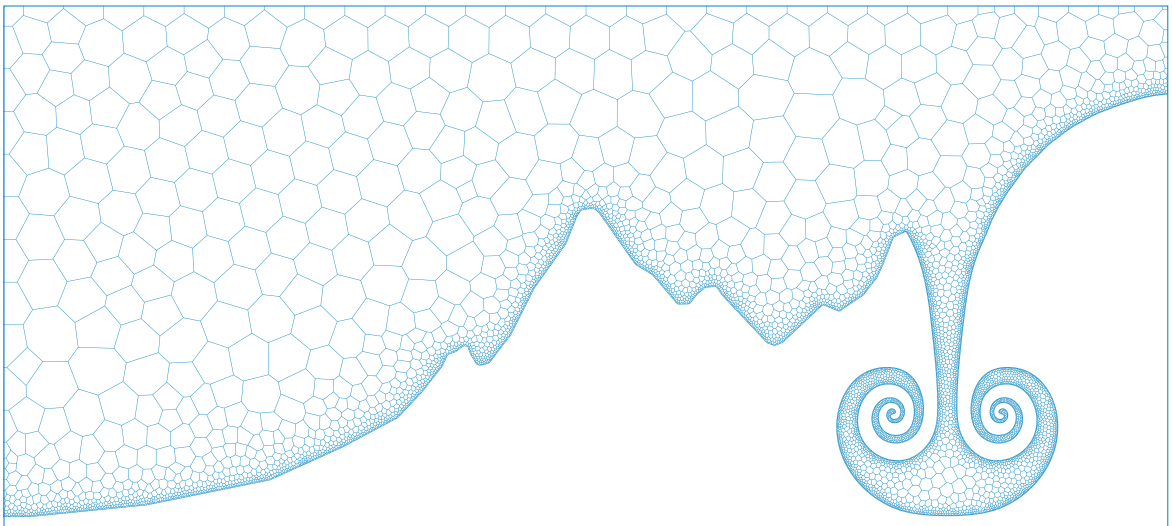


MultiMat 2019

9TH INTERNATIONAL CONFERENCE ON

Numerical methods for multi-material fluid flow

Book of abstracts

9 – 13 September 2019

Hotel Villa Madruzzo, Trento, Italy

Organized by the University of Trento

The instrument that mediates between theory and practice, between thought and observation, is mathematics; it builds the connecting bridge and makes it stronger and stronger. Thus it happens that our entire present-day culture, insofar as it rests on intellectual insight into and harnessing of nature, is founded on mathematics. Already, Galileo said: Only he can understand nature who has learned the language and signs by which it speaks to us; but this language is mathematics and its signs are mathematical figures. Kant declared, "I maintain that in each particular natural science there is only as much true science as there is mathematics." In fact, we do not master a theory in natural science until we have extracted its mathematical kernel and laid it completely bare. Without mathematics today's astronomy and physics would be impossible; in their theoretical parts, these sciences unfold directly into mathematics. These, like numerous other applications, give mathematics whatever authority it enjoys with the general public.

David Hilbert

Radio address given in Königsberg on 8 September 1930, on the occasion of the yearly meeting of the Society of German Natural Scientists and Physicians (english translation by James T. Smith)

Scientific committee:

Remi Abgrall *(Univerity of Zurich, Switzerland)*
Andrew Barlow *(AWE, UK)*
Pavel Bochev *(SNL, USA)*
Jerry Brock *(LANL, USA)*
Alan Dawes *(AWE, UK)*
Stephane Del Pino *(CEA, France)*
Marianne Francois *(LANL, USA)*
Sergey Gavrilyuk *(Aix-Marseille University, France)*
Dmitri Kuzmin *(TU Dortmund, Germany)*
Raphaël Loubère *(CNRS, France)*
Pierre-Henri Maire *(CEA, France)*
Douglas Miller *(LLNL, USA)*
Jim Morel *(Texas A&M)*
Renaud Motte *(CEA, France)*
J. Michael Owen *(LLNL, USA)*
Igor Menshov *(VNIIA and KIAM, Russia)*
William Rider *(SNL, USA)*
Evgeniy Romenskiy *(Sobolev Institute, RAS, Russia)*
Richard Saurel *(Aix-Marseille University, France)*
Mikhail Shashkov *(LANL, USA)*
H.S. Udaykumar *(University of Iowa, USA)*

Organizing committee:

Michael Dumbser *(University of Trento, Italy)*
Walter Boscheri *(University of Ferrara, Italy)*
Elena Gaburro *(University of Trento, Italy)*
Simone Chiocchetti *(University of Trento, Italy)*

Conference secretary:

Lorena Galante (University of Trento, Italy)

This conference has been supported by:

ExaHyPE
European Research Council
University of Trento *(Italy)*
Los Alamos National Laboratory *(USA)*
Commisariat à l'Énergie Atomique et aux Énergie Alternatives *(France)*
Atomic Weapons Enstablishment *(United Kingdom)*
Lawrence Livermore National Laboratory *(USA)*
Kitware SAS *(France)*
Agenzia per il Turismo di Trento *(Italy)*

Welcome to MultiMat 2019!

We are very pleased to welcome you to MultiMat 2019, *the 9^{th} International Conference on Numerical Methods for Multi-Material Fluid Flows, held in Trento, Italy.*

Trento lies in the heart of the majestic Dolomiti Mountains and close to the charming Garda Lake, in a dream scenery rich of arts, history, natural beauties where excellent cuisine and good wine cannot be missed.

MultiMat 2019 builds on the success of previous MultiMat conferences: *Santa Fe in 2017, Würzburg in 2015, San Francisco in 2013, Arcachon in 2011, Pavia in 2009, Prague in 2007, Oxford in 2005, and Paris in 2002.* This year we have received 114 abstracts, which have been carefully reviewed by the members of the scientific committee. There will be 60 talks, 12 additional talks in thematic minisymposia, and 24 posters, given by international researchers coming from *China, Czech Republic, France, Germany, Israel, Italy, Japan, Russia, Switzerland, the United Kingdom, and the United States of America.*

During the conference, we will push forward the state of the art in the field of multiphase and multimaterial flow problems. Researchers from academic and/or laboratory institutions will focus their discussions on relevant numerical methods, including the analysis of such methods as well as the modeling of complex multi-material flows, which is essential for the investigation and development of new sources of energy.

Maintaining the tradition of its previous editions, the conference will focus on the mathematical and physical aspects of:

- Lagrangian hydrodynamics;
- Arbitrary Lagrangian Eulerian (ALE) methods;
- Eulerian methods;
- Radiation hydrodynamics;
- Multi-material diffusion;
- Mesh generation methods and mesh adaptation;
- Interface reconstruction methods;
- Multiphase flows;
- Data transfer between meshes and remapping;
- Advanced discretization methods and High order methods;
- Numerical methods for complex constitutive models.

We would like to thank the scientific committee, our sponsors and all the participants for their enrichening contributions and we wish you a very pleasant stay in Trento and productive scientific and personal interactions during the conference!

Michael Dumbser

Chairman of the MultiMat 2019 organization committee

Elena Gaburro, Simone Chiocchetti, Walter Boscheri

MultiMat 2019 local organizing committee

Table of contents 1/5

Program at-a-glance **10**

Daily program **12**

Abstracts of oral presentations **17**

Remi Abgrall (University of Zürich, Switzerland) 18
Some preliminary results on a kinetic scheme that has an Lattice Boltzmann method flavour

Jason Albright (Los Alamos National Lab, USA) 19
Machine learning-based optimization strategies for artificial viscosity

Paola Bacigaluppi (University of Zürich, Switzerland) 20
Non-conservative explicit residual distribution formulation with a posteriori limiting for multiphase flow systems with source terms

Dinshaw Balsara (University of Notre Dame, USA) 21
The Multidimensional Approximate Generalized Riemann Problem

Brody Bassett (Lawrence Livermore National Lab, USA) 22
Efficient solution of the SPH radiation hydrodynamics equations

Pavel Bochev (Sandia National Lab, Albuquerque, USA) 23
A consistent, conservative and scalable meshfree mimetic method

Walter Boscheri (University of Ferrara, Italy) 24
High order direct Arbitrary-Lagrangian-Eulerian (ALE) PNPM schemes on unstructured meshes

Yibing Chen (IAPCM, Beijing, China) 25
Recent Developments of HGKS: High Order Approach Based On Gas Kinetic Scheme

Florian Chevassu (Kitware SAS, Lyon, France) 26
SHAPO - Recent Advances on the Voronoi Mesh Generation Toolkit

Vincent Chiravalle (Los Alamos National Lab, USA) 27
Subscale Closure Model for Cell-Centered Hydrodynamics using a Multidirectional Approximate Riemann Solution

Sidafa Conde (Sandia National Lab, Albuquerque, USA) 28
On algebraic flux correction in continuous finite element schemes for problems in plasma physics

Andrew Corrigan (US Naval Research Lab, Washington DC) 29
A Moving Discontinuous Galerkin Method with Interface Condition Enforcement Applied to Multi-Material Flows

Marta D'Elia (Sandia National Lab, Albuquerque, USA) 30
Mathematical foundations for nonlocal interface problems: multiscale simulations of heterogeneous materials

Alan Dawes (AWE, Aldermaston, UK) 31
Solving the diffusion equation on a flattened AMR mesh

Stéphane Del Pino (CEA, Arpajon, France) 32
Triangular metric-based mesh adaptation for compressible multi-material flows in semi-Lagrangian coordinates

Michael Dumbser (University of Trento, Italy) 33
High order ADER schemes for a unified first order hyperbolic formulation of Newtonian continuum mechanics coupled with electro-dynamics

Nicolas Favrie (Aix-Marseille University, France) 34
Dynamic compaction of granular material

Elena Gaburro (University of Trento, Italy) 35
Arbitrary high order direct ALE schemes on moving Voronoi meshes with topology changes

Sergey Gavrilyuk (Aix-Marseille University, France) 36
Uncertainty principle in two fluid-mechanics

Table of contents 2/5

Fernando F. Grinstein (Los Alamos National Lab, USA) 37
Eulerian Hydrodynamics Effects in Turbulent Mixing Simulations

Jean-Luc Guermond (Texas A&M, College Station, USA) 38
High-order invariant domain preserving ALE approximation of hyperbolic systems

Hennes Hajduk (TU Dortmund University, Germany) 39
Bound-Preserving High-Order Finite Element Schemes for Advection Problems: II. Matrix-Free Approaches

Philippe Hoch (CEA, Arpajon, France) 40
Well-balanced schemes on two dimensionnal conical meshes

Milan Holec (Lawrence Livermore National Lab, USA) 41
An efficient coupling of thermal radiation transport to ALE hydrodynamics on high-order curvilinear meshes

Kseniya Ivanova (University of Zürich, Switzerland) 42
Multi-dimensional shear shallow water flows

Yuliya Kanarska (Lawrence Livermore National Lab, USA) 43
Semi-implicit compressible DEM multiphase model without acoustic time step restrictions

Matej Klima (Czech Technical University in Prague) 44
A Closure Model for Impacts of All Speeds in Multi-Material Arbitrary Lagrangian-Eulerian Hydrodynamics

Christian Klingenberg (Wuerzburg University, Germany) 45
Kinetic modeling and numerical simulation of multi-species plasma

Dmitri Kuzmin (TU Dortmund University, Germany) 46
Bound-Preserving High-Order Finite Element Schemes for Advection Problems: I. Matrix-Based Approaches

Thomas Leroy (CEA, Arpajon, France) 47
Curved interface reconstruction for 2D compressible multi-material flows

Richard Liska (Czech Technical University in Prague) 49
Cell-centered Lagrangian Lax-Wendroff HLL Hybrid Scheme in Cylindrical Geometry

Na Liu (IAPCM, Beijing, China) 50
High-order spectral volume scheme for multi-component flows using non-oscillatory kinetic flux

Christoph Lohmann (TU Dortmund University, Germany) 51
Algebraic flux correction schemes for symmetric tensors with applications to fiber suspension flows

Raphaël Loubère (University of Bordeaux & CNRS, France) 52
Solution Property Preserving Reconstruction for Finite Volume schemes

Elizabeth Lovegrove (Los Alamos National Lab, USA) 54
Radiation Diffusion in FLAG SGH and CCH

Hong Luo (North Carolina State University, USA) 55
A Moving Discontinuous Galerkin Finite Element Method for Conservation Laws

Pierre-Henri Maire (CEA, Le Barp, France) 56
Thermodynamic consistency of cell-centered Lagrangian hydrodynamics method

Robert Managan (Lawrence Livermore National Lab, USA) 57
Modeling the Free Expansion of an Ideal Gas with and without Shocks

Tomislav Maric (TU Darmstadt, Germany) 58
Distance-gradient normal reconstruction

Igor Menshov (VNIIA, Moscow, Russia) 59
A Diffuse Interface Method for Calculating Multifluid Compressible Flows on Eulerian Grids

Douglas Miller (Lawrence Livermore National Lab, USA) 60
Splitting shock heating between ions and electrons in an ionized gas

Table of contents 3/5

Jim E. Morel (Texas A&M, College Station, USA) 61
Second-Order Coupling of Radiation and Hydrodynamics with Different Spatial and Temporal Discretizations

Nathaniel Morgan (Los Alamos National Lab, USA) 62
A fourth-order accurate Lagrangian discontinuous Galerkin method for cubic cells

Britton Olson (Lawrence Livermore National Lab, USA) 63
An explicit material contact model for simple gaps on structured meshes

Michael Owen (Lawrence Livermore National Lab, USA) 64
Meshfree modeling of the DART mission impactor on the asteroid Didymos-B

Marica Pelanti (ENSTA ParisTech, Palaiseau, France) 66
Numerical modeling of liquid-vapor flows with arbitrary heat and mass transfer relaxation times and general equation of state

Ilya Peshkov (University of Toulouse III, France) 67
Monolithic multiscale modeling of solidification and melting processes

Michael Powell (Sandia National Lab, Albuquerque, USA) 68
Multi-material dynamic domain topology changes in the Lagrangian Grid Reconnection (LGR) code

Barbara Re (University of Zürich, Switzerland) 69
A diffuse interface method for weakly compressible multiphase flows based on the Baer and Nunziato model

William Rider (Sandia National Lab, Albuquerque, USA) 70
The Power and Secrets of the Sigmoid Function: A Numerical Swiss Army Knife

Robert Rieben (Lawrence Livermore National Lab, USA) 71
A matrix-free hyper-viscosity method for high-order finite element ALE hydrodynamics

Evgeniy Romenskiy (University of Trento, Italy) 72
A two-phase model for fluid saturated elastoplastic porous medium based on the theory of thermodynamically compatible systems

Christopher Rousculp (Los Alamos National Lab, USA) 73
Simulation of Magnetically Driven HEDP/ICF Experiments with a Lagrangian/ALE Code

Richard Saurel (Aix-Marseille University, France) 74
Riemann solver with internal reconstruction (RSIR) for compressible single-phase and non-equilibrium two-phase flows

John N Shadid (Sandia National Lab, Albuquerque, USA) 75
An IMEX Continuum Multifluid Electromagnetic Plasma Formulation for Challenging Fusion Related Applications

Mikhail Shashkov (Los Alamos National Lab, USA) 76
Intersection-distribution-based remapping for multi-material staggered arbitrary Lagrangian-Eulerian hydrodynamics

David Sidilkover (Soreq NRC, Yavne, Israel) 77
Vorticity Confinement and Shock Capturing - two sides of the same coin?

Daniil Svyatskiy (Los Alamos National Lab, USA) 78
A higher order approximate static condensation method for multi-material diffusion problems

Petr Sváček (Czech Technical University in Prague) 79
Mathematical Modelling of Multiphase Flows with Surface Tension and the Finite Element Approximation

Joanna Szmelter (Loughborough University, UK) 80
A Multidimensional Positive Definite Remapping Algorithm for Unstructured Meshes

Nicolas Therme (CEA, Le Barp, France) 81
A new segregated-explicit staggered scheme for Lagrangian hydrodynamics

Baolin Tian (IAPCM, Beijing, China) 82
Numerical Simulation of Compressible Multi-Material Multiphase Flows with High Order Eulerian Methods

Vladimir Titarev (Moscow Institute of Physics and Technology, Russia) 83
Near-wall Domain Decomposition for Essentially Unsteady Turbulent Flows

Table of contents 4/5

Svetlana Tokareva (Los Alamos National Lab, USA) 84
Residual Distribution Scheme for Multi-Material Lagrangian Hydrodynamics

Ignacio Tomas (Sandia National Lab, Albuquerque, USA) 85
Invariant domain preserving methods and convex limiting: towards an extension to MhD

Vladimir Tomov (Lawrence Livermore National Lab, USA) 86
Adaptation of High-Order Curved Meshes in ALE Hydrodynamics

Eleuterio Francisco Toro (University of Trento, Italy) 87
On flux splitting schemes for a class of hyperbolic systems

Sergey Utyuzhnikov (University of Manchester, UK) 88
Efficient Full Non-overlapping Domain Decomposition for near-wall Turbulent Flows

Douglas Woods (Los Alamos National Lab, USA) 89
Modeling Shock Wave Speed in MARBLE Foam

Feng Xiao (Tokyo Institute of Technology, Japan) 90
A robust and interface preserving formulation for compressible multiphase flows

Qinghong Zeng (IAPCM, Beijing, China) 91
Sliding interfaces with radiation in multi-material fluid flows

Duan Zhang (Los Alamos National Lab, USA) 92
Dual Domain Material Point Method and Multivelocity Formulation Applied to Sweeping Wave Impact and Plastic Spallation

Qiang Zhao (IAPCM, Beijing, China) 93
A Positivity-Preserving FV Scheme for Diffusion Equations on Polyhedral Meshes and its Application in Electrostatic Particle-In-Cell Simulation

Abstracts of poster presentations **94**

Jayesh Badwaik (Wuerzburg University, Germany) 95
An Arbitrary Lagrangian-Eulerian DG Method on Triangular Grids

Keith Bennet (University of Warwick, Coventry, UK) 96
Investigating the effects of hot electron generation from laser-plasma interactions

Jerome Breil (CEA, Le Barp, France) 97
3D cell-centered Lagrangian second order scheme for the numerical modeling of hyperelasticity system

Rémi Chauvin (CEA, Saclay, France) 98
Recovering discrete Rankine-Hugoniot conditions on uneven meshes with anti-diffusive schemes

Rao Garimella (Los Alamos National Lab, USA) 99
Portage+Tangram: Update on Scalable Multi-Material Remapping

Tom Goffrey (University of Warwick, Coventry, UK) 100
Non-diffusive radiation transport and non-ideal Magnetohydrodynamics on arbitrary structured meshes

Brian Michael Haines (Los Alamos National Lab, USA) 101
Coupling Laser Physics to Radiation-Hydrodynamics

Zhiwei He (IAPCM, Beijing, China) 102
On High-order Finite Difference Algorithm for Compressible Multi-material Flows

Andrew Kercher (US Naval Research Lab, Washington DC) 104
A Moving Discontinuous Galerkin Method with Interface Condition Enforcement for Incompressible Flows with Surface Tension

Tzanio Kolev (Lawrence Livermore National Lab, USA) 105
Recent Developments in the High Order Finite Element Hydrodynamics Code BLAST

Table of contents 5/5

Milan Kucharik (Czech Technical University in Prague) 106
Reducing Diffusion of Remapping by Non-Polynomial Function Reconstructions

Ronit Kumar (Tokyo Institute of Technology, Japan) 107
High-order interface representation in THINC method

E.J. Lieberman (Los Alamos National Lab, USA) 108
A Lagrangian Discontinuous Galerkin Hydrodynamic Method for Elastic-Plastic Solid Dynamics

E.J. Lieberman (Los Alamos National Lab, USA) 109
A Lagrangian Discontinuous Galerkin Hydrodynamic Method for Reactive Materials

Xiaodong Liu (Los Alamos National Lab, USA) 110
A hermite WENO-based limiter for a Lagrangian discontinuous Galerkin method

Gabi Luttwak (Dynamic 123D, Haifa, Israel) 111
Using the SMG scheme to study Rayleigh-Taylor instability growth in solids

Jacob Moore (Los Alamos National Lab, USA) 112
A 2D/3D High-Order Finite Element Library in C++

Renaud Motte (CEA, Bruyères-le-Châtel, France) 113
Anti-diffusive methods for multiphase flows with exchange phenomena at the interfaces

Christina Paulin (CEA, Arpajon, France) 114
Towards Isotropic Transport with Co-Meshes

Alexey Serezhkin (VNIIA, Moscow, Russia) 115
An approximate Riemann solver for non-conservative hyperbolic systems

GS Sidharth (Los Alamos National Lab, USA) 116
Low-dissipation high-order finite volume fluxes for compressible mixing with heat release

Davide Torlo (University of Zürich, Switzerland) 117
High order IMEX deferred correction scheme for multiphase flows

Pavel Vachal (Czech Technical University in Prague) 118
Comparison of Various Equations of State for Laser Plasma Simulations Using the HerEOS Framework

Jan Velechovsky (Los Alamos National Lab, USA) 119
Effects of interface treatment methods on hydrodynamic instabilities between immiscible fluids

Multimat 2019, 9 – 13 September 2019, Trento, Italy

Program of the Ninth International Conference on Numerical Methods for Multi-Material Fluid Flow (1/2)

	Monday, 9.9.2019	Tuesday, 10.9.2019	Wednesday, 11.9.2019	Thursday, 12.9.2019	Friday, 13.9.2019
08:40 – 09:00	*Opening and Welcome*				
09:00 – 09:25	Shashkov	Abgrall	Maire	Bochev	Loubère
09:25 – 09:50	Rieben — ***Kuzmin*** *chairman*	Pelanti — ***Shashkov*** *chairman*	Del Pino — ***Abgrall*** *chairman*	Owen — ***Guermond*** *chairman*	Tomov — ***Balsara*** *chairman*
09:50 – 10:25	Toro	Romenski	Liska	Liu	Szmelter
10:25 – 11:00	*Coffee Break*	*Coffee Break*	*Coffee Break*	Chen	*Coffee Break*
11:00 – 11:25	Rider	Saurel	Guermond	*Coffee Break*	Holec
11:25 – 11:50	Morgan — ***Maire*** *chairman*	Menshov — ***Klingenberg*** *chairman*	Tomas — ***Bochev*** *chairman*	Kuzmin — ***Francois*** *chairman*	Zeng — ***Xiao*** *chairman*
11:50 – 12:15	Powell	Peshkov	Luo	Hajduk	Therme
12:15 – 12:40	Gaburro	Sváček	Boscheri	Zhao	Leroy
12:40 – 13:05	*Discussion*	*Discussion*	*Discussion*	D'Elia	*Discussion*
13:05 – 14:00	*Lunch*	*Lunch*	*Lunch*	*Lunch*	*Lunch*
14:00 – 14:45					
14:45 – 15:10	Hoch	Klingenberg	Lohmann		Managan
15:10 – 15:35	Corrigan — ***Owen*** *chairman*	Balsara — ***Menshov*** *chairman*	Conde — ***Del Pino*** *chairman*	*Social event.*	Woods — ***Miller*** *chairman*
15:35 – 16:00	Rousculp	Xiao	Dawes	*Guided city tour including the Buonconsiglio Castle, the ancient Tridentum and the Cathedral of Trento.*	Maric
16:00 – 16:35	*Coffee Break*	*Coffee Break*	*Coffee Break*		*Coffee Break*
16:35 – 17:00	Klima	Favrie	Shadid		Svyatskiy
17:00 – 17:25	Chevassu — ***Rider*** *chairman*	Re — ***Saurel*** *chairman*	Zhang — ***Tokareva*** *chairman*		Albright — ***Boscheri*** *chairman*
17:25 – 17:50	Morel	Dumbser	Miller		Lovegrove
17:50 – 18:15	*Discussion*	*Discussion*	*Discussion*		*Closing discussion*
18:15 – 19:00					
19:00 – 20:00	*Welcome reception*	*Poster session and wine tasting*			
20:00 – ...			*Conference dinner*		

Saturday 14.9.2019. *Bus tour through the Dolomiti mountains.*

Program of the Ninth International Conference on Numerical Methods for Multi-Material Fluid Flow (2/2)

Monday, 9.9.2019

13:05 – 14:00	*Lunch*
14:00 – 14:45	

Minisymposium I.
Residual distribution

14:45 – 15:10	Tokareva	***Vachal***
15:10 – 15:35	Bacigaluppi	*chairman*

Minisymposium II.
CFD and turbulence

15:35 – 16:00	Ivanova	***Dumbser***
16:00 – 16:35	*Coffe Break*	*chairman*
16:35 – 17:00	Utyuzhnikov	
17:00 – 17:25	Titarev	
17:25 – 17:50	Grinstein	
17:50 – 18:15	*Discussion*	

Wednesday, 11.9.2019

13:05 – 14:00	*Lunch*
14:00 – 14:45	

Minisymposium III.
Methods and algorithms

14:45 – 15:10	Kanarska	***Titarev***
15:10 – 15:35	Olson	*chairman*
15:35 – 16:00	Chiravalle	
16:00 – 16:35	*Coffee Break*	

Minisymposium IV.
Methods and algorithms

16:35 – 17:00	Bassett	***Loubère***
17:00 – 17:25	Tian	*chairman*
17:25 – 17:50	Sidilkover	
17:50 – 18:15	*Discussion*	

Thematic Minisymposia

Daily program: Monday, 9 September 2019

08:40 – 09:00 Opening and Welcome

09:00 – 09:25 **Mikhail Shashkov** (Los Alamos National Lab, USA)
Intersection-distribution-based remapping for multi-material staggered arbitrary Lagrangian-Eulerian hydrodynamics

09:25 – 09:50 **Robert Rieben** (Lawrence Livermore National Lab, USA)
A matrix-free hyper-viscosity method for high-order finite element ALE hydrodynamics

09:50 – 10:25 **Eleuterio Francisco Toro** (University of Trento, Italy)
On flux splitting schemes for a class of hyperbolic systems

10:25 – 11:00 Coffe Break

11:00 – 11:25 **William Rider** (Sandia National Lab, Albuquerque, USA)
The Power and Secrets of the Sigmoid Function: A Numerical Swiss Army Knife

11:25 – 11:50 **Nathaniel Morgan** (Los Alamos National Lab, USA)
A fourth-order accurate Lagrangian discontinuous Galerkin method for cubic cells

11:50 – 12:15 **Michael Powell** (Sandia National Lab, Albuquerque, USA)
Multi-material dynamic domain topology changes in the Lagrangian Grid Reconnection (LGR) code

12:15 – 12:40 **Elena Gaburro** (University of Trento, Italy)
Arbitrary high order direct ALE schemes on moving Voronoi meshes with topology changes

12:40 – 13:05 Discussion

13:05 – 14:45 Lunch

14:45 – 15:35 Thematic Minisymposium: *Residual distribution*

14:45 – 15:10 **Philippe Hoch** (CEA, Arpajon, France)
Well-balanced schemes on two dimensionnal conical meshes

Svetlana Tokareva (Los Alamos National Lab, USA)
Residual Distribution Scheme for Multi-Material Lagrangian Hydrodynamics

15:10 – 15:35 **Andrew Corrigan** (US Naval Research Lab, Washington DC)
A Moving Discontinuous Galerkin Method with Interface Condition Enforcement Applied to Multi-Material Flows

Paola Bacigaluppi (University of Zürich, Switzerland)
Non-conservative explicit residual distribution formulation with a posteriori limiting for multiphase flow systems with source terms

15:35 – 17:50 Thematic Minisymposium: *CFD and turbulence*

15:35 – 16:00 **Christopher Rousculp** (Los Alamos National Lab, USA)
Simulation of Magnetically Driven HEDP/ICF Experiments with a Lagrangian/ALE Code

Kseniya Ivanova (University of Zürich, Switzerland)
Multi-dimensional shear shallow water flows

16:00 – 16:35 Coffe Break

16:35 – 17:00 **Matej Klima** (Czech Technical University in Prague)
A Closure Model for Impacts of All Speeds in Multi-Material Arbitrary Lagrangian-Eulerian Hydrodynamics

Sergey Utyuzhnikov (University of Manchester, UK)
Efficient Full Non-overlapping Domain Decomposition for near-wall Turbulent Flows

17:00 – 17:25 **Florian Chevassu** (Kitware SAS, Lyon, France)
SHAPO - Recent Advances on the Voronoi Mesh Generation Toolkit

Vladimir Titarev (MIPT, Russia)
Near-wall Domain Decomposition for Essentially Unsteady Turbulent Flows

17:25 – 17:50 **Jim E. Morel** (Texas A&M, College Station, USA)
Second-Order Coupling of Radiation and Hydrodynamics with Different Spatial and Temporal Discretizations

Fernando F. Grinstein (Los Alamos National Lab, USA)
Eulerian Hydrodynamics Effects in Turbulent Mixing Simulations

17:50 – 18:15 Discussion

19:00 – ... Welcome reception

Daily program: Tuesday, 10 September 2019

09:00 **Opening**

09:00 – 09:25 **Remi Abgrall** (University of Zürich, Switzerland)
Some preliminary results on a kinetic scheme that has an Lattice Boltzmann method flavour

09:25 – 09:50 **Marica Pelanti** (ENSTA ParisTech, Palaiseau, France)
Numerical modeling of liquid-vapor flows with arbitrary heat and mass transfer relaxation times and general equation of state

09:50 – 10:25 **Evgeniy Romenskiy** (University of Trento, Italy)
A two-phase model for fluid saturated elastoplastic porous medium based on the theory of thermodynamically compatible systems

10:25 – 11:00 **Coffe Break**

11:00 – 11:25 **Richard Saurel** (Aix-Marseille University, France)
Riemann solver with internal reconstruction (RSIR) for compressible single-phase and non-equilibrium two-phase flows

11:25 – 11:50 **Igor Menshov** (VNIIA, Moscow, Russia)
A Diffuse Interface Method for Calculating Multifluid Compressible Flows on Eulerian Grids

11:50 – 12:15 **Ilya Peshkov** (University of Toulouse III, France)
Monolithic multiscale modeling of solidification and melting processes

12:15 – 12:40 **Petr Sváček** (Czech Technical University in Prague)
Mathematical Modelling of Multiphase Flows with Surface Tension and the Finite Element Approximation

12:40 – 13:05 **Discussion**

13:05 – 14:45 **Lunch**

14:45 – 15:10 **Christian Klingenberg** (Wuerzburg University, Germany)
Kinetic modeling and numerical simulation of multi-species plasma

15:10 – 15:35 **Dinshaw Balsara** (University of Notre Dame, USA)
The Multidimensional Approximate Generalized Riemann Problem

15:35 – 16:00 **Feng Xiao** (Tokyo Institute of Technology, Japan)
A robust and interface preserving formulation for compressible multiphase flows

16:00 – 16:35 **Coffe Break**

16:35 – 17:00 **Nicolas Favrie** (Aix-Marseille University, France)
Dynamic compaction of granular material

17:00 – 17:25 **Barbara Re** (University of Zürich, Switzerland)
A diffuse interface method for weakly compressible multiphase flows based on the Baer and Nunziato model

17:25 – 17:50 **Michael Dumbser** (University of Trento, Italy)
High order ADER schemes for a unified first order hyperbolic formulation of Newtonian continuum mechanics coupled with electro-dynamics

17:50 – 18:15 **Discussion**

19:00 – ... **Poster session and Wine tasting**

Daily program: Wednesday, 11 September 2019

09:00 **Opening**

09:00 – 09:25 **Pierre-Henri Maire** (CEA, Le Barp, France)
Thermodynamic consistency of cell-centered Lagrangian hydrodynamics method

09:25 – 09:50 **Stéphane Del Pino** (CEA, Arpajon, France)
Triangular metric-based mesh adaptation for compressible multi-material flows in semi-Lagrangian coordinates

09:50 – 10:25 **Richard Liska** (Czech Technical University in Prague)
Cell-centered Lagrangian Lax-Wendroff HLL Hybrid Scheme in Cylindrical Geometry

10:25 – 11:00 **Coffe Break**

11:00 – 11:25 **Jean-Luc Guermond** (Texas A&M, College Station, USA)
High-order invariant domain preserving ALE approximation of hyperbolic systems

11:25 – 11:50 **Ignacio Tomas** (Sandia National Lab, Albuquerque, USA)
Invariant domain preserving methods and convex limiting: towards an extension to MhD

11:50 – 12:15 **Hong Luo** (North Carolina State University, USA)
A Moving Discontinuous Galerkin Finite Element Method for Conservation Laws

12:15 – 12:40 **Walter Boscheri** (University of Ferrara, Italy)
High order direct Arbitrary-Lagrangian-Eulerian (ALE) PNPM schemes on unstructured meshes

12:40 – 13:05 **Discussion**

13:05 – 14:45 **Lunch**

14:45 – 15:35 **Thematic Minisymposium:** *Methods and algorithms*

14:45 – 15:10 **Christoph Lohmann** (TU Dortmund University, Germany)
Algebraic flux correction schemes for symmetric tensors with applications to fiber suspension flows

15:10 – 15:35 **Sidafa Conde** (Sandia National Lab, Albuquerque, USA)
On algebraic flux correction in continuous finite element schemes for problems in plasma physics

15:35 – 16:00 **Alan Dawes** (AWE, Aldermaston, UK)
Solving the diffusion equation on a flattened AMR mesh

Yuliya Kanarska (Lawrence Livermore National Lab, USA)
Semi-implicit compressible DEM multiphase model without acoustic time step restrictions

Britton Olson (Lawrence Livermore National Lab, USA)
An explicit material contact model for simple gaps on structured meshes

Vincent Chiravalle (Los Alamos National Lab, USA)
Subscale Closure Model for Cell-Centered Hydrodynamics using a Multidirectional Approximate Riemann Solution

16:00 – 16:35 **Coffe Break**

16:35 – 17:50 **Thematic Minisymposium:** *Methods and algorithms*

16:35 – 17:00 **John N Shadid** (Sandia National Lab, Albuquerque, USA)
An IMEX Continuum Multifluid Electromagnetic Plasma Formulation for Challenging Fusion Related Applications

17:00 – 17:25 **Duan Zhang** (Los Alamos National Lab, USA)
Dual Domain Material Point Method and Multivelocity Formulation Applied to Sweeping Wave Impact and Plastic Spallation

17:25 – 17:50 **Douglas Miller** (Lawrence Livermore National Lab, USA)
Splitting shock heating between ions and electrons in an ionized gas

Brody Bassett (Lawrence Livermore National Lab, USA)
Efficient solution of the SPH radiation hydrodynamics equations

Baolin Tian (IAPCM, Beijing, China)
Numerical Simulation of Compressible Multi-Material Multiphase Flows with High Order Eulerian Methods

David Sidilkover (Soreq NRC, Yavne, Israel)
Vorticity Confinement and Shock Capturing - two sides of the same coin?

17:50 – 18:15 **Discussion**

20:00 – ... **Conference dinner**

Daily program: Thursday, 12 September 2019

09:00 **Opening**

09:00 – 09:25 **Pavel Bochev** (Sandia National Lab, Albuquerque, USA)
A consistent, conservative and scalable meshfree mimetic method

09:25 – 09:50 **Michael Owen** (Lawrence Livermore National Lab, USA)
Meshfree modeling of the DART mission impactor on the asteroid Didymos-B

09:50 – 10:25 **Na Liu** (IAPCM, Beijing, China)
High-order spectral volume scheme for multi-component flows using non-oscillatory kinetic flux

10:25 – 11:00 **Yibing Chen** (IAPCM, Beijing, China)
Recent Developments of HGKS: High Order Approach Based On Gas Kinetic Scheme

11:00 – 11:25 **Coffe Break**

11:25 – 11:50 **Dmitri Kuzmin** (TU Dortmund University, Germany)
Bound-Preserving High-Order Finite Element Schemes for Advection Problems: I. Matrix-Based Approaches

11:50 – 12:15 **Hennes Hajduk** (TU Dortmund University, Germany)
Bound-Preserving High-Order Finite Element Schemes for Advection Problems: II. Matrix-Free Approaches

12:15 – 12:40 **Qiang Zhao** (IAPCM, Beijing, China)
A Positivity-Preserving FV Scheme for Diffusion Equations on Polyhedral Meshes and its Application in Electrostatic Particle-In-Cell Simulation

12:40 – 13:05 **Marta D'Elia** (Sandia National Lab, Albuquerque, USA)
Mathematical foundations for nonlocal interface problems: multiscale simulations of heterogeneous materials

13:05 – 14:45 **Lunch**

15:10 – 18:15 **Guided city tour**

Visit to the Buonconsiglio Castle, the ancient Tridentum and the Cathedral of Trento

Daily program: Friday, 13 September 2019

09:00 Opening

09:00 – 09:25 **Raphaël Loubère** (University of Bordeaux & CNRS, France)
Solution Property Preserving Reconstruction for Finite Volume schemes

09:25 – 09:50 **Vladimir Tomov** (Lawrence Livermore National Lab, USA)
Adaptation of High-Order Curved Meshes in ALE Hydrodynamics

09:50 – 10:25 **Joanna Szmelter** (Loughborough University, UK)
A Multidimensional Positive Definite Remapping Algorithm for Unstructured Meshes

10:25 – 11:00 Coffe Break

11:00 – 11:25 **Milan Holec** (Lawrence Livermore National Lab, USA)
An efficient coupling of thermal radiation transport to ALE hydrodynamics on high-order curvilinear meshes

11:25 – 11:50 **Qinghong Zeng** (IAPCM, Beijing, China)
Sliding interfaces with radiation in multi-material fluid flows

11:50 – 12:15 **Nicolas Therme** (CEA, Le Barp, France)
A new segregated-explicit staggered scheme for Lagrangian hydrodynamics

12:15 – 12:40 **Thomas Leroy** (CEA, Arpajon, France)
Curved interface reconstruction for 2D compressible multi-material flows

12:40 – 13:05 Discussion

13:05 – 14:45 Lunch

14:45 – 15:10 **Robert Managan** (Lawrence Livermore National Lab, USA)
Modeling the Free Expansion of an Ideal Gas with and without Shocks

15:10 – 15:35 **Douglas Woods** (Los Alamos National Lab, USA)
Modeling Shock Wave Speed in MARBLE Foam

15:35 – 16:00 **Tomislav Maric** (TU Darmstadt, Germany)
Distance-gradient normal reconstruction

16:00 – 16:35 Coffe Break

16:35 – 17:00 **Daniil Svyatskiy** (Los Alamos National Lab, USA)
A higher order approximate static condensation method for multi-material diffusion problems

17:00 – 17:25 **Jason Albright** (Los Alamos National Lab, USA)
Machine learning-based optimization strategies for artificial viscosity

17:25 – 17:50 **Elizabeth Lovegrove** (Los Alamos National Lab, USA)
Radiation Diffusion in FLAG SGH and CCH

17:50 – 18:15 Closing discussion

Abstracts of oral presentations

Some preliminary results on a kinetic scheme that has an Lattice Boltzmann method flavour

R. Abgrall[†*], D.Torlo[‡]

[†] Institute of Mathematics and Institute of Computational Sciences,
Universität Zürich, Winthertherstrasse 190, Zürich, Switzerland
(remi.abgrall@math.uzh.ch, davide.torlo@math.uzh.ch)

Keywords: ALE FV-DG schemes, arbitrary high order in space and time, moving Voronoi tessellations, fully-discrete one-step ADER approach, Euler and MHD hyperbolic equations.

ABSTRACT

In this short paper, we intend to describe one way to construct arbitrarily high order kinetic schemes on regular meshes. The method can be arbitrarily high order in space and time, and run at CFL one. This is a common feature with the Lattice Boltzmann Methods. However, the type of Maxwellian we use here are different. This results in very simple and CPU efficient methods. I will also indicate how this could be used for the simulation of compressible multiphase and multicomponent flows

Back

Machine Learning-based optimization strategies for artificial viscosity (LA-UR-19-20493)

Jason Albright, Mikhail Shashkov, Nathan Urban

ABSTRACT

In this talk, we present a strategy for using machine learning techniques to optimize the amount of artificial viscosity in Lagrangian-based schemes. Lagrangian-based algorithms for hydrodynamics often employ artificial viscosity to control numerical oscillations behind shocks. The simplest functional form of artificial viscosity introduces two terms into the discrete equations, which are proportional to the divergence of the velocity field and to the square of the divergence, respectively. Hence, the amount of artificial viscosity can be tuned by treating the two unspecified proportionality coefficients as additional control param- eters. For appropriate choices of these parameters, post-shock oscillations can be significantly diminished, however, excessive amounts of artificial viscosity result in shock profiles that are overly-smeared across a large number of computational cells. Moreover, the use of more naive parameter values can also lead to other unintended consequences, including highly oscillatory solutions and negative density profiles. Therefore, properly utilizing artificial viscosity requires choosing these parameters to achieve a careful balance between avoiding excessive dissipation while still attenuating the formation of spurious oscillations near discontinuities. Unfortunately, despite longstanding efforts, in general, there is no systematic procedure dictating how to choose the appropriate values of these additional parameters. Consequently, in practice, these coefficients are often selected merely on the basis of prior user experience with a specific subset of applications, which may not be generalizable to new applications.

In this talk, we view the determination of the coeficients of artificial viscosity as an optimization problem. We introduce two objective functions that quantify the accuracy of the solution and the presence of oscillations for a given choice of parameters, which we then seek to minimize in order to determine a better trade-of between attenuation of post-shock oscillations and the introduction of excessive dissipation. As a proof-of-principle, we explore this approach in 1D using a standard, staggered-grid hydrodynamics scheme with artificial viscosity to approximate the solutions to two well-known shock producing verification tests, the Sod Shock Tube and LeBlanc shock tube problems. First, we apply intensive, large-scale sampling of the parameter space to determine the general shape of the response surfaces of each objective function for the two test cases. Using simple uniform, cartesian grids of the two-parameter space, we are able to determine the best approximation to the optimal parameter values for both test cases. Second, we apply multiple-objective function optimization via constructing the Pareto frontier in phase space to determine whether a common optimal parameter choice can be selected for both problems. In particular, we demonstrate that the parameter choices obtained with this methodology yield an improvement in accuracy relative to default choices used in several production codes.

Although intensive, large-scale sampling has the advantages of being conceptually straight-forward to apply and can be highly informative, the cost of running a large number of forward simulations can become prohibitively expensive, especially in higher dimensions. Therefore, the ultimate goal of this work is to apply several machine learning algorithms to drastically reduce the cost of brute force sampling. In particular, we will construct an emulator response surface using Gaussian process (GP) regression techniques. One salient feature of GP regression is that it can estimate the uncertainty in its predictions. We exploit to design efficient adaptive sampling strategies that significantly decrease the cost of parameter selection by further reducing the number of needed forward simulations to achieve comparable accuracy.

Back

Non-conservative explicit residual distribution formulation with "a posteriori" limiting for multiphase flow systems with source terms

P. Bacigaluppi[†*], R. Abgrall[†], J. Carlier[‡], M. Pelanti[‡] and P. Congedo[◇]
[†] Institute of Mathematics, University of Zurich, Switzerland, (paola.bacigaluppi@math.uzh.ch)
[‡] ENSTA ParisTech, Universit Paris-Saclay, France
[◇]DEFI Team, INRIA Saclay Île-de-France and Ecole Polytechnique, France

Keywords: Multiphase flows, phase transition, residual distributions, non-conservative, MOOD

ABSTRACT

Within the framework of the equilibrium two-phase mixtures with phase transition, this work focuses on a four-equation model, which allows to study certain typologies of cavitation problems, where the assumption of a homogeneous temperature, pressure and velocity are allowed. In particular, we tackle the study of time dependent problems with strong discontinuities and phase transition. Driven by the interest of engineering-based applications towards the treatment of non-conserved variables, this work presents a novel approach to solve systems of equations with a non-conservative formulation which guarantees the actual conservation of the mass, momentum and energy quantities, following [3] . This non-conservative formulation allows avoiding the classical oscillations obtained by many approaches, that might appear for the pressure profile across contact discontinuities. Further, the proposed method is formulated with an "a posteriori limiter" following the recent work [1] and is based on a finite volume-type residual distribution (RD) scheme designed for an explicit second-order time stepping (see [2]). This novel approach is cross-validated on several one- and two-dimensional benchmark problems with the approximated solution obtained via a conservative approach, based on an HLLC solver implemented for the CLAWPACK (CP) software.

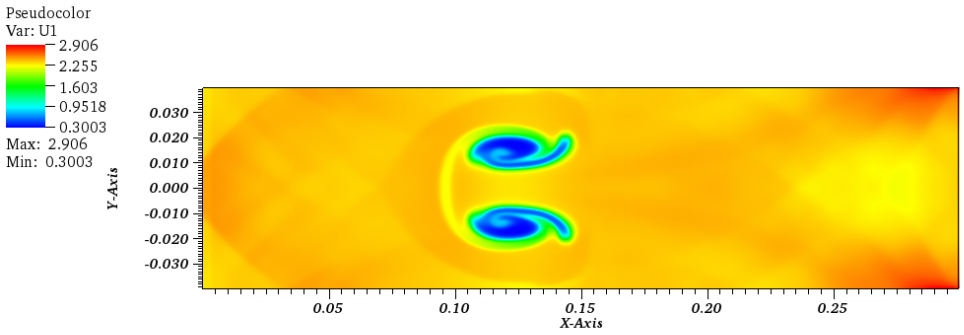


Figure 1: Shocking bubble in a tube at $t = 577\,[\mu s]$.

References

[1] P. Bacigaluppi, R. Abgrall and S. Tokareva, "A Posteriori" Limited High Order and Robust Residual Distribution Schemes for Transient Simulations of Fluid Flows in Gas Dynamics, submitted

[2] R. Abgrall, P. Bacigaluppi and S. Tokareva, A high-order nonconservative approach for hyperbolic equations in fluid dynamics. Computers & Fluids, Vol. 169, pp. 10-22, 2018

[3] R. Abgrall and P. Bacigaluppi. Design of a second-order fully explicit residual distribution scheme for compressible multiphase flows. Sp. Proc. Math. & Stat., FVCA8, Vol. 200, pp. 257-264, 2017

Back

The Multidimensional Approximate Generalized Riemann Problem

Dinshaw S. Balsara
University of Notre Dame (dbalsara@nd.edu)

ABSTRACT

One dimensional Riemann problems have been one of the essential building blocks of higher order Godunov schemes. Exact and approximate Generalized Riemann Problem (GRP) solvers have also been designed. When the GRP is used in a numerical scheme, it has the advantage that higher order in time can be achieved with much fewer stages than in traditional RK timestepping. Multidimensional approximate Riemann solvers have also been designed and have shown themselves to be very valuable for certain systems of hyperbolic PDEs – especially those that have an involution constraint like MHD and CED. Therefore, it becomes reasonable to ask whether there can exist something like a multidimensional GRP solver? In this talk, we answer that question in the affirmative.

We first show that the multidimensional GRP solver is very beneficial for certain types of problems involving CED and MHD. We then develop the viewpoint that the multidimensional GRP solver can also be used as an effective building block for higher order ALE schemes. In such situations the multidimensional GRP solver can provide us with a more accurate nodal solver for the evolution of nodes in an ALE scheme.

Back

Efficient solution of the SPH radiation hydrodynamics equations

Brody Bassett[†] **and J. Michael Owen**[†]

[†] Lawrence Livermore National Laboratory, P.O. Box 808, M/S L-38, Livermore, CA 94550

(bassett4@llnl.gov, owen8@llnl.gov)

Keywords: radiation hydrodynamics; multi-material hydrodynamics; Lagrangian methods; mesh-free methods.

ABSTRACT

The coupling of radiation transport to smoothed particle hydrodynamics (SPH) presents practical difficulties, including the choice of transport discretization and solution methodology. Current discretization methods for the SPH radiation hydrodynamics equations include the method of characteristics, Monte Carlo approaches, and strong-form, flux-limited diffusion (see review in Ref. [1]). In this talk, we compare discretizations of the diffusion equation, including the strong form and a globally conservative weak form derived using nodal integration. Because the discretizations only use data from the particle centers, they retain beneficial SPH properties such as Galilean invariance and full independence from a mesh.

The coupling between the material and radiation energy equations is performed using nonlinear elimination, which reduces the required number of diffusion inverse operations compared to standard Newton iteration [2]. Past approaches to solving the diffusion equation in SPH include using explicit time steps [3], which is simple to implement but severely limits the time step for many problems, and solving the implicit diffusion equations iteratively by calculating particle pair interactions [4], which is too expensive for large-scale problems. Here, the diffusion equations are solved implicitly using scalable linear solver libraries, which significantly speeds up the solution process compared to iterative techniques and allows for larger time steps compared to explicit techniques.

References

[1] V. Springel, "Smoothed particle hydrodynamics in astrophysics", *Annual Review of Astronomy and Astrophysics*, 48, pp. 391-430, 2010.

[2] T. Brunner and P. Nowak, "Nonlinear elimination applied to radiation transport", in review for *Proceedings of M&C 2019*, Portland, Oregon, 2019.

[3] C. Fryer, G. Rockefeller, and M. Warren, "SNSPH: A parallel 3-D smoothed particle radiation hydrodynamics code", *The Astrophysical Journal*, 643(1), pp. 292-305, 2006.

[4] S. Whitehouse, M. Bate, J. Monaghan, "A faster algorithm for smoothed particle hydrodynamics with radiative transfer in the flux-limited diffusion approximation", *Monthly Notices of the Royal Astronomical Society*, 364(4), pp. 1367-1377.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. LLNL-ABS-768166.

Back

A consistent, conservative and scalable meshfree mimetic method

N. Trask[†], P. Bochev[†] and M. Perego[†*]
[†] Center for Computing Research, Sandia National Laboratories, Albuquerque, NM 87185
({ntrask,pbboche,mperego}@sandia.gov)

Keywords: mesh-free method; mimetic discretization; conservation Generalized Moving Least-Squares.

ABSTRACT

Mimetic methods discretize divergence by restricting the Gauss theorem to mesh cells. Because point clouds lack such geometric entities, construction of a compatible meshfree divergence remains a challenge. In this talk, we present an abstract Meshfree Mimetic Divergence (MMD) operator on point clouds defined by contraction of *field* and *virtual face* moments. MMD satisfies a discrete divergence theorem, i.e., it is conservative, and is first-order accurate. We consider two MMD instantiations. The first one assumes a background mesh and uses generalized moving least squares (GMLS) to obtain the necessary field and face moments. This MMD instance is appropriate for settings where mesh is available but its quality is insufficient for a robust and accurate mesh-based discretization. The second MMD operator retains the GMLS field moments but defines *virtual face* moments using computationally efficient weighted graph-Laplacian equations. This MMD instance does not require a background grid and is appropriate for applications where mesh generation creates a computational bottleneck. It allows one to trade an expensive mesh generation problem for a scalable algebraic one, without sacrificing compatibility with the divergence operator. We demonstrate the approach by using the MMD operator to obtain a virtual finite-volume discretization of conservation laws on point clouds. Numerical results for benchmark problems with material discontinuities confirm the mimetic properties of the method and show that it behaves similarly to standard finite volume methods; see Fig.1.

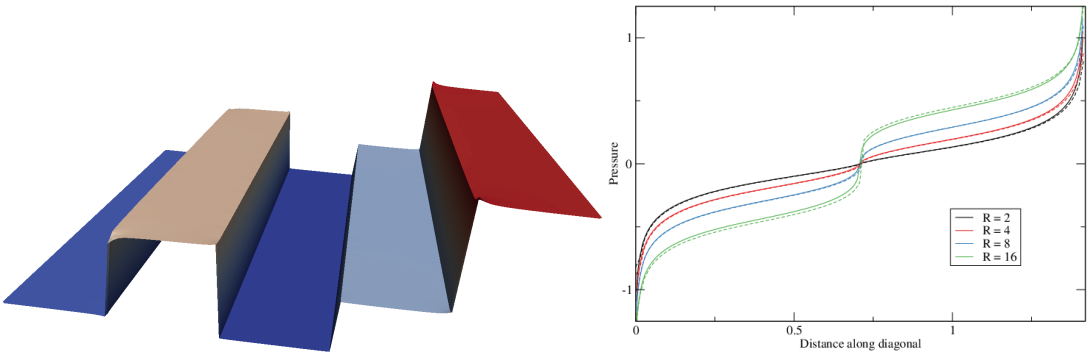


Figure 1: *Left:* Approximation of the horizontal flux component in the five strip benchmark by the virtual finite volume scheme is undistinguishable from that by a mixed method using RT0-P0 elements. *Right:* Comparison of the pressure profiles of the five spot benchmark along $y = x$ by the virtual finite volume scheme (solid lines) and a mixed method using RT0-P0 elements (dashed lines) for increasing diffusivity ratios $R = \varepsilon_1/\varepsilon_2$.

This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Advanced Scientific Computing Research under Award Number DE-SC-0000230927, and the Laboratory Directed Research and Development program at Sandia National Laboratories.

Back

High order direct Arbitrary-Lagrangian-Eulerian (ALE) $P_N P_M$ schemes on unstructured meshes

W. Boscheri[†] and D.S. Balsara[‡*]

[†] Department of Mathematics and Computer Science, University of Ferrara, Via Machiavelli 30, 44121 Ferrara, Italy (walter.boscheri@unife.it)

[‡] Physics Department, University of Notre Dame, 225 Nieuwland Science Hall, Notre Dame, IN 46556, USA (dbalsara@nd.edu)

Keywords: Arbitrary-Lagrangian-Eulerian (ALE); $P_N P_M$ schemes; reconstructed DG schemes; WENO-AO reconstruction; ADER time discretization; high order of accuracy in space and time; moving unstructured meshes; local rezoning; hyperbolic PDE; Euler equations.

ABSTRACT

In this work we present a conservative WENO Adaptive Order (AO) reconstruction operator applied to an explicit one-step Arbitrary-Lagrangian-Eulerian (ALE) discontinuous Galerkin (DG) method. The spatial order of accuracy is improved by reconstructing higher order piecewise polynomials of degree $M > N$, starting from the underlying polynomial solution of degree N provided by the DG scheme. High order of accuracy in time is achieved by the ADER approach, making use of an element-local space-time Galerkin finite element predictor that arises from a one-step time integration procedure. As a result, space-time polynomials of order $M + 1$ are obtained and used to perform the time evolution of the numerical solution adopting a fully explicit DG scheme.

To maintain algorithm simplicity, the mesh motion is restricted to be carried out using straight lines, hence the old mesh configuration at time t^n is connected with the new one at time t^{n+1} via space-time segments, which result in space-time control volumes on which the governing equations have to be integrated in order to obtain the time evolution of the discrete solution. Our algorithm falls into the category of *direct* Arbitrary-Lagrangian-Eulerian (ALE) schemes, where the governing PDE system is directly discretized relying on a space-time conservation formulation and which already takes into account the new grid geometry *directly* during the computation of the numerical fluxes. A local rezoning strategy might be used in order to locally optimize the mesh quality and avoiding the generation of invalid elements with negative determinant. The proposed approach reduces to direct ALE finite volume schemes if $N = 0$, while explicit direct ALE DG schemes are recovered in the case of $N = M$.

In order to stabilize the DG solution, an *a priori* WENO based limiting technique is employed, that makes use of the numerical solution inside the element under consideration and its neighbor cells to find a less oscillatory polynomial approximation. By using a *modal basis* in a reference element, the evaluation of the oscillation indicators is very easily and efficiently carried out, hence allowing higher order modes to be properly limited, while leaving the zero-*th* order mode untouched for ensuring conservation.

Numerical convergence rates for $2 \leq N, M \leq 4$ are presented as well as a wide set of benchmark test problems for hydrodynamics on moving and fixed unstructured meshes.

References

[1] W. Boscheri and D.S. Balsara "High order direct Arbitrary-Lagrangian-Eulerian (ALE) $P_N P_M$ schemes on unstructured meshes", *Journal of Computational Physics*, submitted.

Back

Recent Developments of HGKS: High Order Approach Based On Gas Kinetic Scheme

Yibing Chen, Shiyi Li and Song Jiang

[1]Institute of Applied Physics and Computational Mathematics
(chen_yibing@iapcm.ac.cn,li_shiyi@iapcm.ac.cn,jiang@iapcm.ac.cn)

Keywords: high order in both space and time, gas kinetic scheme, multi-materials flows.

ABSTRACT

In this talk, recent developments of HGKS, a new scheme of arbitrary high order accuracy in both space and time for hyperbolic conservative laws, will be introduced. The basic idea in the construction is that, based on the idea of the kinetic flux vector splitting (KFVS), we split all the spatial and time derivatives in the Taylor expansion of the numerical flux into two parts: one part with positive velocity of particle distribution function of the corresponding equilibrium state, another with negative part. According to a Lax-Wendroff procedure, all the time derivatives are then replaced by spatial derivatives, which are evaluated by using WENO/HWENO reconstruction polynomials. This scheme can be extended to solve the so-called extended Euler equations of compressible multi-materials flows. Numerous numerical tests for linear and nonlinear hyperbolic conservative laws are carried out, and the numerical results demonstrate that the proposed scheme is robust and can be of high order accuracy in both space and time.

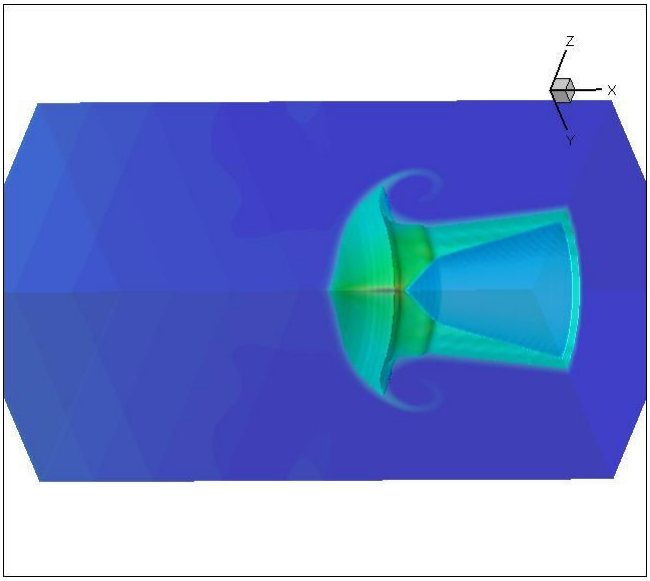


Figure 1: density profile of triple-points problem computed by the fifth order HGKS

References

[1] Q.Li, K.Xu, S.Fu. A high-order gas-kinetic Navier-Stokes solver. J. Comput.Phys., (2010) 229: 6715-6731

[2] Yibing Chen, Song Jiang, Na Liu , HFVS: An arbitrary high order approach based on flux vector splitting, J. Comput.Phys .,322 (2016) 708–722

Back

SHAPO - Recent Advances on the Voronoi Mesh Generation Toolkit

J. Pouderoux[†], F. Chevassu[†], M. Kenamond[‡], M. Shashkov[‡]

[†] Kitware SAS, Lyon - France
(joachim.pouderoux@kitware.com, florian.chevassu@kitware.com)
[‡] Los Alamos National Laboratory, Los Alamos, NM - USA
(kenamond@lanl.gov, shashkov@lanl.gov)

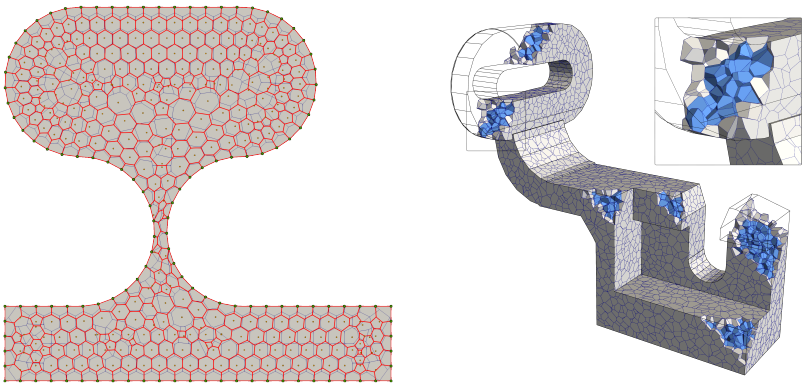


Figure 1: Left: Relaxed 2D Conformal Voronoi Tessellation in a concave domain. Right: Clipped view of a 3D Clipped Voronoi tessellation in a complex domain with sharp features.

Keywords: Meshing; Voronoi; Centroidal; Delaunay; Tessellation.

ABSTRACT

Voronoi meshes are polygonal or polyhedral meshes that have properties which are recognized in many scientific fields like computational mechanics, computer graphics or geophysics.

SHAPO is a cross-platform C++ software library and toolkit we are developing in the particular context of the implementation of Reconnection-Based ALE[1] family of methods at LANL. From the orthogonal dual Delaunay triangulation, SHAPO produces unstructured Voronoi meshes from a set of seeds (user-defined, sampled from Poisson sampling algorithm or regular patterns) defined by a domain made of a set of complex boundaries (convex or non-convex, simply or multi-connected). SHAPO integrates different algorithms to generate, in serial or in data-parallelism context, 2D and 3D Voronoi meshes with different properties. It also provides a simple programming interface to retrieve the full connectivity of the generated meshes from many programming languages like Python or Fortran.

In this talk/poster we present the main algorithms of SHAPO and put the focus on some of its new features. In particular, we present the 2D ConPolM algorithm[2] that allows creating tessellation that guarantee the input boundary edges are preserved untouched in the output mesh. The Weighted Centroidal Voronoi Tessellation framework will also be described. Finally, we present the load balancing capabilities of SHAPO , where generators are distributed across MPI ranks before performing the local tessellations.

References

[1] R. Loubère, P.-H. Maire, M. Shashkov, J. Breil and S. Galera, "ReALE: A reconnection–based arbitrary–Lagrangian-Eulerian method", *Journal of Computational Physics*, 229(12), pp. 4724–4761, 2010.
[2] D. Herring and B. Jean, "Voronoi Meshes with Prescribed Boundaries", *Proceedings of the 24th International Meshing Roundtable*, 2014.

The work was carried out under the auspices of the National Nuclear Security Administration of the U.S. Department of Energy at Los Alamos National Laboratory under Contract No. DE-AC52-06NA25396. The authors gratefully acknowledge the support of the US Department of Energy National Nuclear Security Administration Advanced Simulation and Computing (ASC) Program.

Back

Subscale Closure Model for Cell-Centered Hydrodynamics using a Multidirectional Approximate Riemann Solution

Vincent Chiravalle[1], Andrew Barlow[2] and Nathaniel Morgan[1]

[1]Los Alamos National Laboratory (chiravle@lanl.gov, nmorgan@lanl.gov)
[2]Computational Physics Group, AWE Aldermaston, (Andy.Barlow@awe.co.uk)

Keywords: subscale closure models, cell-centered hydrodynamics, ALE methods

ABSTRACT

We extend the interface-aware subscale dynamics (IA-SSD) closure model [1] to a cell-centered hydrodynamic (CCH) formulation [2] for simulating 3D compressible hydrodynamic problems within an arbitrary Lagrangian-Eulerian (ALE) framework. Our CCH formulation involves a multidirectional approximate Riemann solution with a discrete Mach number as a smoothness indicator to limit dissipation. At the subscale level we determine pair-wise material interactions by solving a distinct approximate Riemann problem at the common interface, using the volume of fluids (VOF) method to find the interface. Material interactions are constrained to ensure material volumes remain in physically justified bounds, the internal energy of each material component is positive, and pressure equilibration among materials occurs smoothly. The accuracy and robustness of our subscale closure model is demonstrated by simulating a suite of 3D Cartesian problems, each involving two or more materials, including the Sedov problem (see Figure 1), as well as a multi-material compression problem with impacting plates.

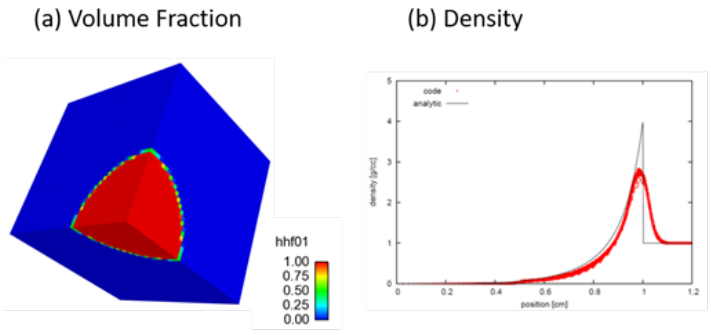


Figure 1: Calculated volume fraction (a) and density (b) for the 2-material Sedov problem on an Eulerian mesh without IA-SSD. The zone at the origin where energy is initially deposited is a separate material.

References

[1] A. Barlow, M. Klima, and M. Shashkov, “Constrained optimization framework for interface-aware sub-scale dynamics models for voids closure in Lagrangian hydrodynamics,” Journal of Computational Physics, 371, pp. 914–944, 2018.

[2] V. Chiravalle and N. Morgan. “A 3D Lagrangian cell-centered hydrodynamic method with higher-order reconstructions for gas and solid dynamics,” Computers and Mathematics with Applications, (in press).

Back

On algebraic flux correction in continuous finite element schemes for problems in plasma physics

S. Mabuza[†*], J.N. Shadid[†], D. Kuzmin[‡], S. Conde[†], E.C. Cyr[†], T.M. Smith[†], R.P. Pawlowski[†]
[†] Center for Computing Research, Sandia National Laboratories (smabuza@sandia.gov)
[‡] TU Dortmund University (kuzmin@math.uni-dortmund.de)

Keywords: algebraic flux correction; iterative limiters; continuous Galerkin methods; magnetohydrodynamics; two-fluid plasma.

ABSTRACT

We present finite element methods for approximating continuum plasma systems with sharp gradients and discontinuities in the solutions. We consider iterative, linearity preserving, nodal variation limiting strategies for the stabilization of hyperbolic systems such as the magnetohydrodynamics (MHD) equations and multifluid plasma equations. These equations, are discretized using piece-wise linear continuous finite elements. The stabilization of the scheme follows the flux corrected transport paradigm by introducing conservative, consistent, diffusion operators into the system for which the magnitude of the dissipative operator is regulated by solution dependent element and nodal limiters. The limiter is designed to be linearity preserving so to ensure that in smooth regions, second order convergence is observed for smooth solutions. The limiters are also designed such that they are continuously dependent on data, guaranteeing solvability of the semi-discrete scheme. The limiting strategy allows for flexible assembly, and utilization of various time integration methods, that include implicit, explicit, and IMEX time integrators. A number of standard inviscid and viscous MHD examples in 1D, 2D and 3D on unstructured quad and simplex meshes are presented. We also consider two-fluid electromagnetic plasma formulations and examples consisting of simulating systems with ion and electron species. Verification results for the numerical methods are presented, along with applications to challenging problems.

References

[1] S. Mabuza, J.N. Shadid, E.C. Cyr, R.P. Pawlowski, D. Kuzmin "A monotone linearity preserving nodal variation limiting algorithm for continuous Galerkin discretization of MHD equations", (submitted).

[2] S. Mabuza, J.N. Shadid, D. Kuzmin, "Local bounds preserving stabilization for continuous Galerkin discretization of hyperbolic systems", *Journal of Computational Physics*, 361, pp. 82–110, 2018.

Back

A Moving Discontinuous Galerkin Method with Interface Condition Enforcement Applied to Multi-Material Flows

A. Corrigan[†*], **A. Kercher**[†] **and D. Kessler**[†]

[†] Laboratories for Computational Physics and Fluid Dynamics, Naval Research Laboratory

(andrew.corrigan@nrl.navy.mil, andrew.kercher@nrl.navy.mil, david.kessler@nrl.navy.mil)

Keywords: shock hydrodynamics; multi-material hydrodynamics; moving discontinuous galerkin method; interface condition enforcement; shock-fitting; interface-tracking.

ABSTRACT

The Moving Discontinuous Galerkin Method with Interface Condition Enforcement (MDG-ICE), introduced by the present authors [1, 2], can accurately and stably compute flows with interfaces, without relying on interface or shock capturing. In order to detect a priori unknown interfaces, MDG-ICE uses a weak formulation that enforces the conservation law and its interface condition separately, while treating the discrete domain geometry as a variable. Thus, in contrast to the standard discontinuous Galerkin (DG) method, MDG-ICE has both the means to detect via interface condition enforcement and satisfy via grid movement the conservation law and its associated interface condition.

The test cases presented by the present authors in earlier work demonstrated that MDG-ICE can be used to compute both steady and unsteady flows with a priori unknown interface topology and point singularities using higher-order elements in arbitrary-dimensional spaces. For example, MDG-ICE was used to compute a Mach-3 bow shock and achieve optimal-order convergence using $p = 1, 2, 3$ elements upon grid refinement. In another example, MDG-ICE was applied to fit intersecting oblique planar shocks in three dimensions. The ability to fit steady shocks extends to unsteady flows using a spacetime formulation with a priori unknown and dynamic interface topology, as demonstrated for the case of a spacetime Burgers shock formation problem, where a continuous temporal initial condition steepens to form a shock. In the case of the Sod shock tube, MDG-ICE successfully fit and tracked the moving shock and contact interfaces, further demonstrating the generality of the method.

In this work we extend MDG-ICE to the case of compressible multi-material flows with complex constitutive models that incorporate material strength. Results for standard multi-material benchmark cases will be presented in order to assess the ability of MDG-ICE to achieve high-order accuracy in the presence of interfaces for the case of multi-material flows, without relying on any form of shock capturing, limiters, or an upwind numerical flux for stability.

References

[1] A. Corrigan, A. Kercher, and D. Kessler. A moving discontinuous Galerkin finite element method for flows with interfaces. Technical Report NRL/MR/6040–17-9765, U.S. Naval Research Laboratory, December 2017.

[2] A. Corrigan, A. Kercher, and D. Kessler. A moving discontinuous Galerkin finite element method for flows with interfaces. *International Journal for Numerical Methods in Fluids*, 89(9):362–406, 2019.

Back

Mathematical foundations for nonlocal interface problems: multiscale simulations of heterogeneous materials

M. D'Elia[1], P. Bochev[1], G. Capodaglio[2] and M. Gunzburger[2]

[1]Center for Computing Research, Sandia National Lab.s (mdelia,pbboche@sandia.gov)
[2]Scientific Computing, Florida State U. (gcapodaglio,mgunzburger@fsu.edu)

Keywords: nonlocal models, interface problems, heterogeneous materials, multiscale

ABSTRACT

By relaxing regularity requirements of PDEs, nonlocal models accurately represent fractures and anomalous behaviors such as prediction of mechanical damage and subsurface transport for, e.g., water storage.
However, wider deployment of nonlocal models remains compromised by the lack of a key mathematical capability: a rigorous theory of nonlocal interfaces, which is required in any simulation of heterogeneous material. In fact, using nonlocal models successfully requires handling of *physical interfaces* arising from material discontinuities, and *virtual interfaces* in domain decomposition methods to improve computational efficiency. Consequently, a mathematically rigorous and physically consistent theory of nonlocal interfaces is essential for physically meaningful and computationally efficient simulations.
The key technical challenge is to discover transmission conditions yielding well-posed interface problems that recover classical formulations in the local limit. We posit that the treatment of local entities (interfaces) in nonlocal terms together with minimization of the (nonlocal) energy of the system provides a mathematically sound foundation to identify transmission conditions leading to well-posed interface problems. By analyzing local limits we will determine which modeling assumptions recover classical formulations, guaranteeing physical consistency.
Today's treatments of interfaces are ad hoc and heuristic, compromising physical consistency of the solutions. Current mathematical approaches [1, 2] fail to establish rigorous theoretical foundations either because they do not ensure uniqueness of solutions or they do not rigorously specify transmission conditions, compromising convergence to local limits. We address these shortcomings by establishing a mathematical theory for nonlocal interfaces mirroring that available for PDEs.
Advantages include: 1) Applicability to existing algorithms and software; 2) Enabling new scalable domain-decomposition solvers; 3) Providing foundation for data-driven discovery of interfaces; 4) Advances in treating heterogeneity in mechanics and subsurface geosciences.
In this talk we present the mathematical formulation of the nonlocal interface problem and show that its local limit recovers the local interface problem with classical transmission conditions. We illustrate our theory in the context of mechanics of heterogeneous materials with two-dimensional numerical tests.

References:

[1] B. Alali, M. Gunzburger, Peridynamics and Material Interfaces, *Journal of Elasticity*, **2**, 2015.
[2] P. Seleson, M. Gunzburger, M.L. Parks, Interface problems in nonlocal diffusion and sharp transitions between local and nonlocal domains, *Computer Methods in Applied Mechanics and Engineering*, **266**, 2013.

Back

"Solving the diffusion equation on a flattened AMR mesh"

A. S. Dawes[#], AWE, UK

MULTIMAT 2019, Trento, Italy

Abstract

Block structured Adaptive Mesh Refinement (AMR) has become a very effective tool at focusing mesh resolution where it is required. Its importance to the community has led to several different libraries being developed, such as SAMRAI [2], AMReX [3] and many others [1]. AMR was originally developed for gas dynamics, and over the years its range has been extended, such as can be found in FLASH [4], Nyx [5] and CASTRO [6] to name but a few.

The AMR algorithm is hierarchal in nature with finer higher-level mesh patches overlapping the coarser lower-level mesh patches. For gas dynamics this route is ideal as the explicit numerical nature allows each patch to be advanced independently of the others (stability must be met) and up to the point where the different levels must be synchronised. This approach was extended to diffusion [7,8] but the philosophy does not lend itself to the same type of patch independence; each patch solve is implicit and sub-cycling must be used with a synchronisation for energy conservation.

An alternative to this is to flatten the AMR mesh, but requires a global implicit solve across a new unstructured mesh decomposition. Energy conservation is maintained but Howell [9] has shown that there are challenges associated with it. Traditionally, simulation codes have been written in FORTRAN, and for them to be integrated into a C++ framework, such as SAMRAI, they must be kernelized. This step is not trivial, but the burden can be reduced if the library has a FORTRAN interface.

In this paper we will describe a method to solve the diffusion equation on a flattened AMR mesh using AMReX's FORTRAN interface. The library does not have a flattening capability and we will describe the steps needed to add one. Results will be shown, and comparisons will be made against different multi-material numerical approaches, as well as analytic solutions where ever possible [10,11,12].

References

[1] A. Dubey et al, "A Survey of High-Level Frameworks in Block Structured Adaptive Mesh Refinement Packages", J. Parallel Distrib. Comput., Pages 3217-3227, 2014
[2] B. Gunney and R. Anderson, "Advances in Patched Based Adaptive Mesh Refinement Scalability", LLNL-JRNL-668337, LLNL, 2015

[3] A. Nonaka, "AMReX – a new framework for block structured adaptive mesh refinement calculations", SciDAC-TEAMS Collaboration Meeting, LBNL, 22 August 2018

[4] http://flash.uchicago.edu/site/flashcode/

[5] https://arxiv.org/abs/1301.4498

[6] http://amrex-astro.github.io/Castro/

[7] L. Howell and J. Greenough, "Radiation Diffusion for Multi-fluid Eulerian Hydrodynamics with Adaptive Mesh Refinement", J. Comp. Phys., 184:53–78 (1981).
[8] W. Zhang et al, "CASTRO: A new compressible astrophysics solver. II. Gray radiation hydrodynamics", The American Astronomical Society, 2011
[9] L. Howell, "Grafting AMR Capability into the Diffusion Package of an Existing ALE Code", LLNL-CONF-609323, 2013
[10] A. Dawes, Computers and Fluids, 156: 485-495 (2017)
[11] E. Kikinzon et al, J. Comp. Phys., 347: 416-436 (2017)
[12] A. Dawes et al, LA-UR-24696, 2016

[#]Alan.Dawes@awe.co.uk

Back

Triangular metric-based mesh adaptation for compressible multi-material flows in semi-Lagrangian coordinates

Stéphane Del Pino and Isabelle Marmajou
CEA, DAM, DIF, F-91297 Arpajon, France.

Lagrangian formulation is a powerful tool to compute compressible multi-material flows. Indeed, contact discontinuities are automatically preserved by construction which avoids the use of mixing models. Lagrangian methods are usually more precise than their Eulerian counterparts but generally fail to calculate vortexes or shears: the mesh following the flow might become too distorted.

To overcome this difficulty, one has to maintain the mesh suitable for the calculation. The more classical remedy is ALE method. It consists in adding two steps to the initial Lagrangian method: smoothing the mesh to improve its quality and then remapping the approximated solution on the new grid. New Lagrangian steps can then be performed.

However, it seems relevant to provide more flexibility to the mesh adaptation step (e.g. connectivity changes). In the Lagrange/Remap context recent works have re-investigated the field of remeshing with modern tools. For instance, [4] deals with polygonal mesh adaptation and smoothing, [6] is based on a Voronoï approach (reconnection and smoothing), [2] uses local triangular remeshing and [5] utilizes patch-based triangular remeshing and mesh smoothing.

The approach we proposed in [2] can be described as an *as lagrangian as possible* AMR (Adaptive Mesh Refinement) method for compressible fluid dynamics. It is very efficient and cheap as well as reproducible in parallel. Conservative remapping is easy to define in the case of Lagrangian cell-centered schemes (such as Glace [3] or Eucclhyd [7] for instance). Also, since it is based on local remeshing techniques [1] and since only few cells are remeshed from one time step to the other, the remapping produces low numerical dissipation.

Dealing with multi-material flows, it is generally not possible to maintain Lagrangian interfaces so that, any remeshing technique (including ALE) usually requires to treat multi-material cells, *i.e.* mixing models. In [2], we avoided mixing treatment by preserving Lagrangian interfaces between materials. This allowed to perform nice calculations but time step could eventually tend to 0 (due to interfaces preservation in vortexes). This is one of the points we address in this presentation.

We shall present multi-material treatment improvements of our method [2] and propose a better remapping strategy (only first-order was used previously). We describe our interface reconstruction procedure in the particular case of local triangular mesh adaptation. We illustrate the efficiency of the method through numerical tests.

[1] H. Bourouchaki, P.-L. George, F. Hecht, P. Laug, and E. Saltel. Delaunay mesh generation governed by metric specifications. *Finite Elem. Anal. Des.*, 1997.

[2] S. Del Pino. Metric-based mesh adaptation for 2D Lagrangian compressible flows. *J. Comput. Phys.*, 2011.

[3] B. Després and C. Mazeran. Lagrangian gas dynamics in two dimensions and Lagrangian systems. *Arch. Rational Mech. Anal.*, 2005.

[4] P. Hoch. Semi-conformal polygonal mesh adaptation seen as discontinuous grid velocity formulation for ALE simulations. MULTI-MAT'09. `http://www.math.univ-toulouse.fr/HYDRO`, September 2009.

[5] Z. Lin, S. Jiang, S. Zu, and L. Kuang. A local rezoning and remapping method for unstructured mesh. *Comput. Phys. Comm.*, 2011.

[6] R. Loubère, P.-H. Maire, M. J. Shashkov, J. Breil, and S. Galera. ReALE: A Reconnection-based Arbitrary-Lagrangian-Eulerian Method. *J. Comput. Phys.*, 2010.

[7] P.-H. Maire, R. Abgrall, J. Breil, and J. Ovadia. A cell-centered Lagrangian scheme for two-dimensional compressible flow problems. *SIAM J. Sci. Comput.*, 2007.

Back

High order ADER schemes for a unified first order hyperbolic formulation of Newtonian continuum mechanics coupled with electro-dynamics

M. Dumbser[1], I. Peshkov[2] and E. Romenski[1,2]

[1]Laboratory of Applied Mathematics, University of Trento, Italy (michael.dumbser@unitn.it)
[2]Sobolev Institute of Mathematics, Russia (peshenator@gmail.com, evrom@math.nsc.ru)

Keywords: symmetric-hyperbolic and thermodynamically compatible systems (SHTC), fluid mechanics, solid mechanics, magnetohydrodynamics (MHD), ADER schemes.

ABSTRACT

In this talk, we present a new unified first order hyperbolic model of Newtonian continuum mechanics coupled with electro-dynamics. The model is derived from the theory of hyper-elasticity and is able to describe the behavior of moving elasto-plastic dielectric solids as well as viscous and inviscid fluids in the presence of electro-magnetic fields. It is a peculiar feature of the proposed PDE system that viscous fluids are treated just as a special case of elasto-plastic solids. This is achieved by introducing a strain relaxation mechanism in the evolution equations of the distortion field **A**, which in the case of purely elastic solids maps the current configuration to the reference configuration. The model also contains a hyperbolic formulation of heat conduction as well as a dissipative source term in the evolution equations for the electric field given by Ohm's law. Via formal asymptotic analysis we show that in the stiff limit, the governing first order hyperbolic PDE system with relaxation source terms tends asymptotically to the viscous and resistive magnetohydrodynamics (MHD) equations. The governing PDE system is symmetric hyperbolic and satisfies the first and second principle of thermodynamics, hence it belongs to the so-called class of symmetric hyperbolic thermodynamically compatible systems (SHTC), which have been studied for the first time by Godunov in 1961 and later in a series of papers by Godunov and Romenski. An important feature of the proposed model is that the propagation speeds of all physical processes, including dissipative processes, are finite. The model is discretized using high order accurate ADER discontinuous Galerkin (DG) finite element schemes with a posteriori subcell finite volume limiters and using high order ADER-WENO finite volume schemes on fixed and moving meshes. We show numerical test problems that explore a rather large parameter space of the model ranging from Euler and Navier-Stokes flows over ideal MHD, viscous and resistive MHD and nonlinear large-strain solid mechanics of elasto-plastic materials to pure electro-dynamics and moving dielectric elastic solids in a magnetic field.

References

[1] S.K. Godunov. An interesting class of quasilinear systems. Dokl. Akad. Nauk SSSR, 139:521–523, 1961.

[2] S.K. Godunov and E.I. Romenski. Nonstationary equations of nonlinear elasticity theory in eulerian coordinates. Journal of Applied Mechanics and Technical Physics, 13:868–884, 1972.

[3] S.K. Godunov and E.I. Romenski. Elements of continuum mechanics and conservation laws. Kluwer Academic/Plenum Publishers, 2003.

[4] I. Peshkov and E. Romenski. A hyperbolic model for viscous newtonian flows. Continuum Mechanics and Thermodynamics, 28:85–104, 2016.

[5] M. Dumbser, O. Zanotti, R. Loubère, and S. Diot. A posteriori subcell limiting of the discontinuous Galerkin finite element method for hyperbolic conservation laws. Journal of Computational Physics, 278:47–75, 2014.

[6] M. Dumbser, I. Peshkov, E. Romenski and O. Zanotti. High order ADER schemes for a unified first order hyperbolic formulation of continuum mechanics: viscous heat-conducting fluids and elastic solids. Journal of Computational Physics 314:824–862, 2016

Back

Dynamic compaction of granular material

N. Favrie[†]*, J. Massoni[†] and S. Gavrilyuk[†]
[†]Aix-Marseille Universite, UMR CNRS 7343, IUSTI, 5 rue E. Fermi, 13453 Marseille Cedex 13, France, (nicolas.favrie@univ-amu.fr, jacques.massoni@univ-amu.fr, sergey.gavrilyuk@univ-amu.fr)

Keywords: Compaction of granular materials, multiphase flows, Godunov type method Eulerian methods;

ABSTRACT

An Eulerian hyperbolic multiphase flow model for dynamic and irreversible compaction of porous materials is constructed. A reversible model for elastic compressible porous material is derived. Classical homogeneisation results are obtained. The irreversible model is then derived in accordance with the following basic principles. First, the entropy inequality is satisfied by the model. Second, the stress coming from the elastic energy decreases in time (the material behave as Maxwell-type materials). The irreversible model admits an equilibrium stat corresponding to a Gurson type limit which varies with the porosity. The sound velocity at the yield limit is smaller than that of the reversible model. Such an embedded model structure assures a thermodynamically corect formulation of the model of porous materials. The usual model used in the detonation community is recovered. The model is than validated on quasi-static loading unloading experiments with HMX. The ability of the model to capture strong shock propagation in porous material as well as his ability to deal with interface between a fluid and a porous material is demonstrated and validated on Hugoniot curve of aluminium with various porosities for a unique set of empirical parameters.

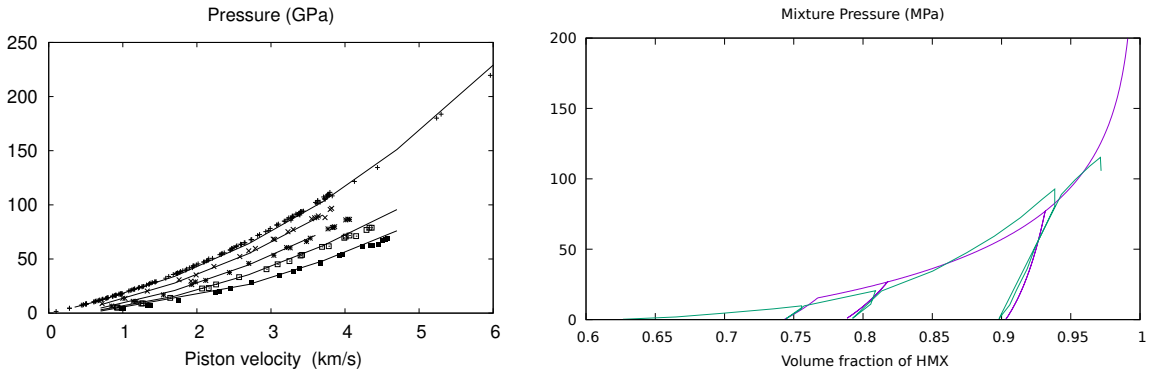


Figure 1: On the left, Hugoniot curve for aluminium 2024 with various porosities. Numerical results are given with continuous lines, experimental results with symbols. On the right, loading-unloading test case for porous HMX. The experimental results are given in green, the numerical results in purple.

This work was partially supported by L'Agence Nationale de la Recherche, France (grant numbers ANR-14-ASTR-0016-01, ANR-11-LABX-0092, and ANR-11-IDEX-0001-02).

Back

Arbitrary high order direct ALE schemes on moving Voronoi meshes with topology changes

E. Gaburro[†*], W. Boscheri[‡], S. Chiocchetti[†], C. Klingenberg[^] and M. Dumbser[†]

[†] University of Trento, Italy (elena.gaburro@unitn.it, simone.chiocchetti@unitn.it, michael.dumbser@unitn.it)

[‡]University of Ferrara, Italy (bscwtr@unife.it)

[^]Würzburg University, Germany (klingen@mathematik.uni-wuerzburg.de)

Keywords: ALE FV-DG, arbitrary high order in space and time, fully-discrete one-step ADER, Voronoi

ABSTRACT

In this talk, we present the first high order accurate direct Arbitrary-Lagrangian-Eulerian (ALE) Finite Volume (FV) and Discontinuous Galerkin (DG) schemes on moving Voronoi meshes that, at each time step, are *regenerated* and are even *free to change their topology*. The Voronoi tessellations are obtained from a set of generator points moving with the fluid flow using an AREPO-type code [1], which rearranges the elements shapes and neighbors in order to maintain a *high quality* mesh even for long computational times and vortical phenomena. Then, the old and new elements associated to the same generator point are connected in space–time to construct the so-called space-time control volumes, whose bottom and top faces may be different polygons; also *degenerating sliver elements* are incorporated in order to *fill the space–time holes* that arise by the topology changes (following the proof of concept [2]). The final ALE FV-DG scheme is obtained by a novel redesign of the high order accurate fully discrete one-step direct ALE $P_N P_M$ scheme [3], which has been adapted to Voronoi and sliver elements: by integrating over arbitrary closed space-time elements, and by using a space-time conservation formulation of the governing hyperbolic PDE system, we directly evolve the solution in time *satisfying the GCL* by construction and being *conservative* thanks to the careful treatment of the space–time holes. Our numerical results show that the new combination of very high order schemes and moving Voronoi meshes with topology changes makes it possible to go further beyond the state of the art in direct ALE methods opening new perspectives.

References

[1] V. Springel, MNRAS, 401:791–851, 2010.
[2] E. Gaburro, M. Dumbser and M.J. Castro, CAF, 159: 254–275, 2017.
[3] M. Dumbser et al., JCP, 227:8209–8253, 2008.

The authors **acknowledge** GNCS-INDAM and the ERC project STiMulUs, grant agreement no 278267.

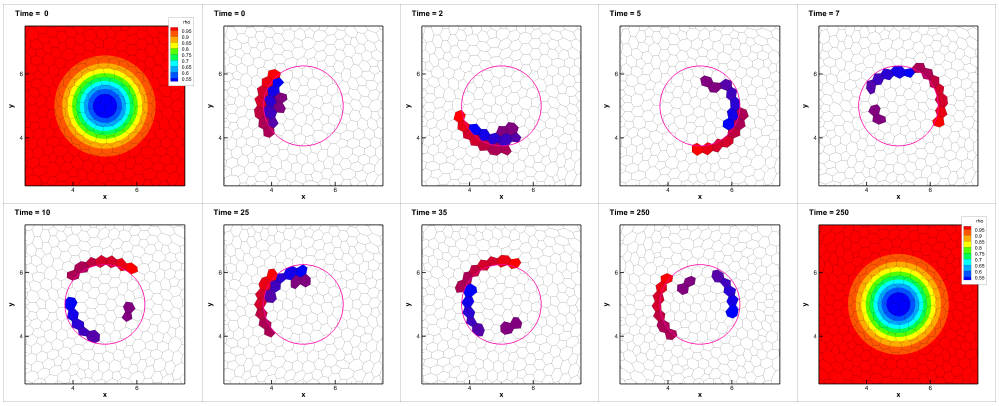


Figure 1: Stationary rotating vortex solved with our 3^{rd} order ALE-DG scheme, on a moving Voronoi mesh with a dynamically *changing grid topology*, for more than 25 loops of the elements located at $r = 1.25$.

Back

Uncertainty principle in two fluid–mechanics

S. Gavrilyuk*

March 7, 2019

Abstract

Hamilton's principle (or the principle of stationary action) is one of the basic modelling tools in classical mechanics. It states that the reversible motion of a mechanical system is completely determined by the corresponding Lagrangian which is the difference between the kinetic and potential energy of the system.

The extension of Hamilton's principle to the continuum mechanics involving fluid-fluid and solid-fluid interaction can be performed (cf. [1, 2]). The motion of a multi–fluid continuum is described by a coupled system of "Newton's laws" for each component that are completely determined by the Lagrangian. The introduction of dissipative terms compatible with the second law of thermodynamics and natural mathematical restrictions on the potential energy allow us to derive the governing equations having nice mathematical properties.

I will consider a simplest example of two-velocity flows where one of the phases is incompressible (for example, flows of dusty air, or flows of compressible bubbles in an incompressible fluid). A very surprising fact is that one can obtain different governing equations from the same Lagrangian. Different types of the governing equations are due to the choice of independent variables and the corresponding virtual motions. The equations differ from each other in the presence (or not) of gyroscopic forces (also called "lift" forces). The total energy does not depend on these forces, but the velocity distribution depends on them. The gyroscopic forces are not usually taken into account in two-fluid models. Even if these forces have no influence on the hyperbolicity of the governing equations, their presence drastically changes the distribution of the energy of each component.

To the best of my knowledge, such an uncertainty in the governing equations of multi-phase flows was never a subject of discussion in a "multi-fluid" community.

Keywords: Hamilton's principle, gyroscopic forces, hyperbolicity

References

[1] S. Gavrilyuk, Multiphase flow modelling via Hamilton's principle, In the book : F. dell'Isola, S. L. Gavrilyuk (Editors), Variational Models And Methods In Solid And Fluid Mechanics, Springer, 2011.

[2] S. Ndanou, N. Favrie, S. Gavrilyuk, Multi-solid and multi-fluid diffuse interface model: applications to dynamic fracture and fragmentation, J. Comput. Phys. **295**(2015) 523–555.

*Aix–Marseille Université, CNRS, IUSTI, UMR 7343, 5 rue E. Fermi, 13453 Marseille Cedex 13, France

Back

Eulerian Hydrodynamics Effects in Turbulent Mixing Simulations

F.F. Grinstein and F.M. Pereira Soares
Los Alamos National Laboratory, Los Alamos, NM 87545, USA

Keywords: shock-driven turbulence, material mixing, eulerian methods

ABSTRACT

Understanding material mixing driven by turbulent motions is a critical element in many programmatic applications of interest -- e.g., ICF capsule implosions. The complexity of the high Reynolds number (Re) turbulent flow typically requires accurate and dependable predictions of highly nonlinear processes with under-resolved computer simulation models. Hydrodynamics of interest is 3D, and involves transition to turbulence and non-equilibrium turbulence development. Such flow physics can be captured with Coarse-Grained Simulation [1] presuming small scale flow-dynamics enslaved to dynamics of the largest scales, and using mixing transition criteria and effective turbulence Reynolds numbers (*Re*) for macroscopic convergence metrics [2]. CGS includes classical Large-Eddy Simulation using explicit subgrid scale (SGS) models and Implicit LES relying on SGS modeling implicitly provided by *physics capturing* numerics. Comparable contributions from explicit and implicit models are involved in the classical LES practice [3]. By combining shock and turbulence emulation capabilities based on single (physics capturing) numerics, ILES is preferred to simulate the high-*Re*-dominating stirring-driven driven turbulent mixing [1]. Depending on the model equations solved -- and actual values of *Re* and other characteristic (Schmidt, Damköhler) numbers, mixed explicit / implicit SGS models are used to address non-convective physics (e.g., diffusive mixing, backscatter, and combustion).

A crucial predictability issue of deterministic CGS is that of identifying effective combination of modeling choices and convergence metrics to achieve a developed-flow target, such as *Re* characterizing the late-time simulated turbulence. Suitable well-resolved 3D initial conditions, appropriate numerics, and fine enough resolution are required. Our 3D high-resolution eulerian simulations are revisited in the light of new directional-unsplit higher-order hydro algorithms in xRAGE [4] including corrections for well-known excessive numerical diffusion of Godunov-type schemes for low Mach numbers. The unsplit algorithms in xRAGE have been recently evaluated for relevant canonical test cases including the Taylor-Green Vortex and the AWE inverse chevron shock tube [5]. New xRAGE simulations and assessments will be reported. At a fundamental level, we reevaluate the TGV case, and systematically examine the evolution of xRAGE ILES initialized with well-characterized isotropic turbulence data from direct numerical simulation. On a more practical note, our previous assessments [6] of simulations of the LANL P-23 shocked gas-curtain experiments are revisited. xRAGE is now capable of simulating transition to turbulence with much higher turbulence *Re* -- and significantly more so with the low Mach number correction, improving agreement with late-time laboratory observations and offering high impact on our 3D hydrodynamics simulation capabilities.

1. Grinstein, F.F., *Coarse Grained Simulation and Turbulent Mixing*, Cambridge, 2016.
2. Zhou, Y., Grinstein, F.F., Wachtor, A.J., Haines, B.M., Estimating the effective Reynolds number in implicit large eddy simulation, *Phys. Rev. E*, **89**, 013303, 2014.
3. Hirt, C.W., Computer studies of time-dependent turbulent flows, *Phys. Fluids Supplement II*, pp. 219–227, 1969; Ghosal, S., An analysis of numerical errors in large-eddy simulations of turbulence, *J. Comput. Phys.*, **125**, 187–206, 1996.
4. J.C. Dolence, T.O. Masser, New Directionally Unsplit Option for Hydrodynamics in the Eulerian AMR Code xRage, 2017 MultiMat, Santa Fe, NM, Sept., 18-22, 2017.
5. F.F. Grinstein, J.A. Saenz, J.C. Dolence, T.O. Masser, R.M. Rauenzahn, M.M. Francois, Effects of operator splitting and low Mach-number correction in turbulent mixing transition simulations, MultiMat 2017 Special Issue of *Computers and Mathematics with Applications* https://doi.org/10.1016/j.camwa.2018.05.008.
6. A.A. Gowardhan and F.F. Grinstein, Numerical simulation of Richtmyer–Meshkov instabilities in shocked gas curtains, *Journal of Turbulence*, 12, No. 43, 2011, 1–24.

Back

High-order invariant domain preserving ALE approximation of hyperbolic systems

Jean-Luc Guermond, Bojan Popov, Laura Saavedra

January 31, 2019

Abstract

The objective of the present paper to propose a second-order continuous finite element technique for solving hyperbolic systems in the Arbitrary Lagrangian Eulerian framework. This is done by revisiting the some recent results from [1] and adapting the recently proposed convex limiting technique from [2], [3] to the ALE setting. The main properties of the method presented in the paper is that, provided the user-defined ALE velocity is reasonable, the approximate solution produced by the algorithm is formally second-order accurate in space, is conservative, satisfies the so-called discrete geometric conservation law, preserves convex invariant domains of the system. The second-order accuracy is shown to hold in the maximum norm on numerical examples with smooth solutions.

[1] J.-L. Guermond, B. Popov, L. Saavedra, and Y. Yang. Invariant domains pre- serving arbitrary Lagrangian Eulerian approximation of hyperbolic systems with continuous finite elements. SIAM J. Sci. Comput., 39(2):A385A414, 2017.

[2] J.-L. Guermond, M. Nazarov, B. Popov, and I. Tomas. Second-order invariant domain preserving approximation of the euler equations using convex limiting. SIAM, J. Sci. Comput., 40:5 (2018) A3211–A3239

[3] J.-L. Guermond, B. Popov, and I. Tomas, Invariant domain preserving discretization-independent schemes and convex limiting for hyperbolic systems, Comput. Methods Applied Mech. Engin., 347 (2019) 143175.

Bound-Preserving High-Order Finite Element Schemes for Advection Problems: II. Matrix-Free Approaches

H. Hajduk[†*], D. Kuzmin[†] and Tz. Kolev[‡]
[†] Institute of Applied Mathematics, TU Dortmund University
(kuzmin@math.uni-dortmund.de, hennes.hajduk@math.tu-dortmund.de)
[‡]Lawrence Livermore National Laboratory (kolev1@llnl.gov)

Keywords: advection equation; local maximum principles; high-order finite element methods; Bernstein polynomials; matrix-free methods; residual distribution schemes; limiting techniques.

ABSTRACT

In this talk, we present a new residual distribution (RD) approach for the design of matrix-free bound-preserving finite element schemes. As a starting point, we consider a continuous or discontinuous Galerkin (DG) discretization of the linear advection equation. To construct the corresponding local extremum diminishing (LED) approximation, we perform mass lumping and redistribute the element residuals in a manner which guarantees the LED property. The proposed residual distribution procedure involves localization to subcells and definition of bound-preserving weights for subcell contributions. Using strong stability preserving (SSP) Runge-Kutta methods for time integration, we prove the validity of discrete maximum principles under CFL-like time step restrictions. The low-order version of our RD scheme has roughly the same accuracy as the one derived from a piecewise (bi)-linear approximation on a submesh with the same nodal points. After presenting the low-order RD scheme, we focus on the limiting techniques that we use to constrain the mass exchange between the nodes of Bernstein finite elements in high-order extensions. Our limiting strategy for time-dependent problems belongs to the family of flux-corrected transport (FCT) algorithms. For stationary problems, we propose residual-based procedures to constrain and redistribute troublesome element contributions. The numerical results for 2D test problems are as good as those obtained with the best matrix-based (algebraic) approaches to discrete upwinding and limiting for high-order Bernstein finite elements (to be presented in Part I). We present 1D illustrations as well as two and three dimensional results on quadrilateral/hexahedral meshes. The extension of our methodology to unstructured/simplicial meshes is straightforward.

References

[1] R. Anderson, V. Dobrev, Tz. Kolev, D. Kuzmin, M. Quezada de Luna, R. Rieben and V. Tomov, "High-Order Local Maximum Principle Preserving (MPP) Discontinuous Galerkin Finite Element Method for the Transport Equation", *Journal of Computational Physics*, 334, pp. 102–124, 2017.

[2] C. Lohmann, D. Kuzmin, J.N. Shadid, S. Mabuza, Flux-Corrected Transport Algorithms for Continuous Galerkin Methods Based on High Order Bernstein Finite Elements, *Journal of Computational Physics*, 344, pp. 151–186, 2017.

[3] R. Abgrall, A Review of Residual Distribution Schemes for Hyperbolic and Parabolic Problems: The July 2010 State of the Art, *Communications in Computational Physics*, 11(4), pp. 1043–1080, 2012.

The Authors acknowledge contributions of Prof. Remi Abgrall (Universität Zürich) and all coauthors of [1-2] to this work.

Back

Well-balanced schemes on two dimensionnal conical meshes

P. Hoch[†]
[†] CEA, DAM-DIF, F-91297 Arpajon, France (philippe.hoch@cea.fr)

Keywords: conservation laws, multi-dimensionnal discretisation, well-balanced scheme, curved mesh.

ABSTRACT

We are interested in the discretization of two-dimensionnal hyperbolic conservation laws with source terms,

$$\partial_t U + div_x F(U) = S(t, x, U).$$

In finite volume context, it was shown that uncoupling flux and source discretization may lead to poor approximation, typically when the physics associated to both terms have too much different scale. The natural centered discretization of S do not take into account his variation. Well-balanced strategy has shown improvement see for instance [1][6][2] [5] which mainly focusses on the case of linear flux and source. For non linear flux and source, we use a multi-dimensionnal antiderivatives concept [3], a nodal numerical flux (localised at some points) and apply the enhanced consistency condition [4] to upwind the source term (see also [8]).
The approach is compatible with curved conical cells (including polygonal cells) for which we can compute nodal normals [7], finally a high order reconstruction can be also used.

References

[1] S. Jin and D. Levermore, Numerical schemes for hyperbolic conservation laws with stiff relaxation terms, Jour. of Comp. Physics, Vol. 126, p. 449-467, 1996.

[2] L. Gosse and G. Toscani, An asymptotic-preserving well-balanced scheme for the hyperbolic heat equations, CRAS, Ser. I 334, p. 337-342, 2002.

[3] P. Hoch, O. Pironneau, A vector HamiltonJacobi formulation for the numerical simulation of Euler flows, C. R. Acad. Sci. Paris, Ser. I 342 (2006).

[4] F. Alouges, J.-M. Ghidaglia, M. Tajchman, On the interaction of upwinding and forcing for non-linear hyperbolic systems of conservation laws, Preprint CMLA.

[5] E. Franck, Design and numerical analysis of asymptotic preserving schemes on unstructured meshes. Application to the linear transport and the Friedrichs systems Ph.D. in Applied Mathematics, CEA DAM and UPMC, 2009-2012.

[6] Greenberg J, Leroux A. Y., A well balanced scheme for the numerical processing of source terms in hyperbolic equations, SIAM J. Numer. Anal - Vol 33 No 1, 1996.

[7] A. Bernard-Champmartin, E. Deriaz, P. Hoch, G. Samba, and M. Schaefer, Extension of centered hydrodynamical schemes to unstructured deforming conical meshes : the case of circles, ESAIM: PRCOCEEDINGS, 2012, Vol. 38, p. 135-162.

[8] F. Bouchut, Nonlinear Stability of Finite Volume Methods for Hyperbolic Conservation Laws and Well-Balanced Schemes for Sources, Birkhäuser Verlag 2004.

Back

An efficient coupling of thermal radiation transport to ALE hydrodynamics on high-order curvilinear meshes

M. Holec[1], T. S. Haut[1] , V. Z. Tomov[1] , B. S. Southworth[2] and B. Yee[1]

[1] Lawrence Livermore National Laboratory, U.S. (holec1@llnl.gov)
[2] University of Colorado Boulder, U.S.

Keywords: radiation transport, curvilinear meshes, high-order methods, DSA.

ABSTRACT

Thermal radiation transport (TRT) belongs to the very important physical phenomena of energy transport in plasmas, i.e. astrophysics and inertial confinement fusion. Since the effect of TRT coupled to plasmas we are interested in exhibits much likely a particle-like (streaming) rather than a fluid-like (low anisotropy) nature, we use a high-dimensional (6D) discrete ordinates (SN) transport model leveraging an arbitrarily high-order discontinuous Galerkin upwind finite elements discretization solved by either an efficient graph-based sweep [1] or nonsymmetric algebraic multigrid [2] on curvilinear meshes. The fixed-point iteration method is adopted for coupling between TRT and the energy equation of hydrodynamics. Although it performs really well for conditions of weak coupling, the number of iteration required to converge under strong coupling is unbearable and one needs to introduce an acceleration strategy.

It is well known that transport can be described as diffusion under conditions of strong coupling. In terms of physics this corresponds to a perturbation theory in small number Kn, which scales as a mean free path of photon, and that the terms ~ Kn^2 are simply neglected. We seek exactly the same property in the discrete sense, while using a diffusion synthetic acceleration (DSA) preconditioner providing that the fixed-point iteration residual also scales as ~ Kn^2 and number of iteration is kept small. This property, however, is not satisfied for any discrete diffusion operator in particular not on curvilinear meshes [3] and we also require that our fixed-point iteration scheme recovers its simple form if Kn >> 1. In our presentation we show an optimal strategy of efficient iteration count for general Kn based on what we learned from math, physics and simulations.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

References

[1] T. S. Haut, P. G. Maginot, V. Z. Tomov, B. S. Southworth, T. A. Brunner and T. S. Bailey, “An Efficient Sweep-based Solver for the SN Equations on High-Order Meshes”, Nuclear Science and Engineering, (accepted / arXiv:1810.11080).

[2] T. A. Manteuffel, J. Ruge and B. S. Southworth, “Nonsymmetric Algebraic Multigrid Based on Local Approximate Ideal Restriction (lAIR)”, SIAM Journal on Scientific Computing, 40(6):A4105–A4130, 2018.

[3] T. S. Haut, B. S. Southworth, P. G. Maginot and V. Z. Tomov, “DSA Preconditioning for DG discretizations of SN transport and High-Order curved meshes”, Journal of Computational Physics, (submitted / arXiv:1810.11082).

Back

Multi-dimensional shear shallow water flows

K. Ivanova, S. Gavrilyuk, B. Nkonga, N.Favrie
Aix-Marseille University, France

Abstract

The mathematical model of shear shallow water flows of constant density is studied. This is a 2D hyperbolic non-conservative system of equations that is mathematically equivalent to the Reynolds-averaged model of barotropic turbulent flows. The model has three families of characteristics corresponding to the propagation of surface waves, shear waves and average flow (contact characteristics). The system is non-conservative: for six unknowns (the fluid depth, two components of the depth averaged horizontal velocity, and three independent components of the symmetric Reynolds stress tensor) one has only five conservation laws (conservation of mass, momentum, energy and mathematical 'entropy'). A splitting procedure for solving such a system is proposed allowing us to define a weak solution. Each split subsystem contains only one family of waves (either surface or shear waves) and contact characteristics. The accuracy of such an approach is tested on 2D analytical solutions describing the flow with linear with respect to the space variables velocity, and on the solutions describing 1D roll waves. The capacity of the model to describe the full transition scenario as commonly seen in the formation of roll waves: from uniform flow to 1D roll waves, and, finally, to 2D transverse 'fingering' of the wave profiles, is shown.

Finally, we model a circular hydraulic jump formed in a convergent radial flow of water. Obtained numerical results are qualitatively similar to those observed experimentally: oscillation of the hydraulic jump and its rotation with formation of a singular point.

Keywords— shear shallow water flows, non-conservative system of equations, Reynolds stress tensor

References

[1] K.A. Ivanova, S.L. Gavrilyuk, "Structure of the hydraulic jump in convergent radial flows", *Journal of Fluid Mechanics*, Volume 860, 10 February 2019 , pp. 441-464

[2] S.L. Gavrilyuk, K.A. Ivanova, N. Favrie, "Multi-dimensional shear shallow water flows : problems and solutions", *Journal of Computational Physics*, Volume 366, 1 August 2018, Pages 252-280

[3] K.A. Ivanova, S.L. Gavrilyuk, B. Nkonga, G.L. Richard, "Formation and coarsening of roll-waves in shear shallow water flows down an inclined rectangular channel", *Computers& Fluids*, 159, pp 189–203, 2017

[4] A. Bhole, B. Nkonga, S. Gavrilyuk, K. Ivanova, "Fluctuation splitting Riemann solver for a non-conservative modeling of shear shallow water flow ", *Journal of Computational Physics*, Volume 392, 1 September 2019, Pages 205-226

Back

Semi-implicit compressible DEM multiphase model without acoustic time step restrictions

Yuliya Kanarska[†], Timothy Dunn, Charles Noble, Katherine Lundquist, Lee Glascoe

[†]Lawrence Livermore National Laboratory, 7000 East ave. Livermore, CA
(kanarska1@llnl.gov)

ABSTRACT

ALE3D is a multi-physics numerical simulation software tool utilizing arbitrary-Lagrangian- Eulerian (ALE) techniques (Noble et al., 2017). The ALE3D multiphase model is based on the finite volume method of discrete equation model (DEM) solution (Chinnaya et al., 2003). Rather than solving all phase equations simultaneously, the DEM reduces the equations to a system of single-phase Riemann solves, where each phase has its own velocity and thermodynamic state. Exchanges between the phases are modeled through source terms accounting for the phase interactions. Since the current multiphase scheme uses an explicit time advancement scheme, it has time step restrictions dictated by the speed of sound and limits its applicability to weakly compressible flows. We propose to extend the current multiphase formulation by implementing a pressure-correcting step to enable implicit calculations and remove acoustic time step limitations. This method is compatible with previously developed multi-domain method for multiphase flow interaction with Lagrangian structural meshes (Kanarska et al., 2019). Therefore, newly developed feature makes it suitable for two-way coupling between compressible and weakly compressible multiphase flows and solid structures. We illustrate applicability of the method on several examples of the air blast wave interaction with the complex terrain and subsequent cloud formation as well as simulations of underwater explosions.

Back

A Closure Model for Impacts of All Speeds in Multi-Material Arbitrary Lagrangian-Eulerian Hydrodynamics

A. Barlow[†], M. Klima[‡*], M. Kucharik[‡], M. Shashkov[◇]
[†] Computational Physics Group, AWE Aldermaston, Reading, Berkshire, RG7 4PR, UK
(Andy.Barlow@awe.co.uk)
[‡] Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague, Brehova 7, Praha 1, 115 19, Czech Republic
(klimamat@fjfi.cvut.cz, kucharik@newton.fjfi.cvut.cz)
[◇] XCP-4 Group, Los Alamos National Laboratory, Los Alamos, NM 87545, USA
(shashkov@lanl.gov)

Keywords: multi-material hydrodynamics; ALE methods; closure models; voids;

ABSTRACT

The multi-material Arbitrary Lagrangian-Eulerian (ALE) framework combines the advantages of a purely Lagrangian computation with an ability to smooth the computational mesh if it gets too distorted. This makes it an efficient strategy for simulations of high-speed impact problems. In such cases, there are often difficulties transitioning from a free movement in vacuum to a contact state. As an alternative to multi-mesh slide-line interactions or artificial gas environments, the notion of *voids* was developed – a material with zero density and internal energy. Voids can represent closing gaps in shocked cavities or between impacting bodies. At the same time, they can serve as an ambient environment surrounding the impact zone, eliminating the need for a moving boundary condition to encompass the expanding material. And at last, there is a possibility for two materials that are in contact to become separated due to tension forces, opening new voids.

The modeling of interaction of multiple materials follows the interface-aware sub-scale dynamics (IA-SSD) concept , which consists of two stages:

- The equal compressibility stage, dealing with the movement of the mixed cell as a whole.
- The sub-scale stage where only interactions of the materials inside the multi-material cell are taken into account.

Each material interacts in a pair-wise fashion with other materials that share a common boundary and the volume and energy exchanges are limited using physically justified constraints. The IA-SSD model was recently extended to include void closure in fluids.We present an improvment of this model adapted to describe both high-speed high-deformation impacts and low-speed elastic-dominated collision and rebound phenomena. This is based on a new formulation of the interface velocity in sub-scale interactions which adapts to the level of elastic loading. Usage of independent material strain tensors at the first stage of the closure model is also discussed. It can increase accuracy if the interacting materials have different strength parameters (and in void-solid interactions).

Back

Kinetic modeling and numerical simulation of multi-species plasma

C. Klingenberg,
Dept. of Mathematics, Würzburg University, Germany
(klingen@mathematik.uni-wuerzburg.de)

Keywords: multi-fluid mixture; kinetic model; BGK approximation; plasma flow.

ABSTRACT

This project is inspired by an attempt to compute plasma in a regime found in inertial confinement fusion. To this end we developed a multi-species kinetic model. For two species, this is modelled by a system of kinetic BGK equations featuring two interaction terms for each species to account for momentum and energy transfer between the species. Our model is an extension of the model [1]. In addition the collison frequency depends on the difference of micro- and macroscopic velocity. Consistency of this model is shown via a maximum entropy procedure. Next we peresent a a robust numerical appraoch, which mimics this theoretical procedure. We expect this to be able to deal with the very stiff case where we model ions and electrons.

This is joint work among others with Jeff Haack, Cory Hauck, Marlies Pirner and Sandra Warnecke.

References

[1] Klingenberg, C., Pirner, M., Puppo, G.: A consistent kinetic model for a two component mixture with an application to plasma, *Kinetic and Related Models* Vol. 10, No. 2, pp. 445465 (2017)

Back

Bound-Preserving High-Order Finite Element Schemes for Advection Problems: I. Matrix-Based Approaches

D. Kuzmin[†*], H. Hajduk[†] and Tz. Kolev[‡]
[†] Institute of Applied Mathematics, TU Dortmund University
(kuzmin@math.uni-dortmund.de, hennes.hajduk@math.tu-dortmund.de)
[‡]Lawrence Livermore National Laboratory (kolev1@llnl.gov)

Keywords: advection equation; local maximum principles; high-order finite element methods; Bernstein polynomials; limiting techniques; hp-adaptivity.

ABSTRACT

In this talk, we introduce some new matrix-based (algebraic) approaches to enforcing discrete maximum principles for high-order Bernstein finite element discretizations of time-dependent and stationary advection problems. We begin with the derivation of optimal bound-preserving low-order schemes from element matrices of a standard continuous or discontinuous Galerkin (DG) approximation. Using a local mass lumping preconditioner for element residuals, we reduce the levels of numerical dissipation that must be applied to achieve the M-matrix property. The accuracy of the resulting low-order solutions depends on the number of nodes but not on the degree of the Bernstein finite elements. To recover the high-order target discretization, we either limit the perturbations of the Galerkin element matrices in an iterative manner, or perform antidiffusive corrections of the low-order solutions using the flux-corrected transport (FCT) algorithms developed in [1,2]. The new features to be discussed include the definition of nodal correction factors, the design of built-in limiters for discrete diffusion operators, and adaptive mass lumping for boundary terms in DG schemes. The use of Hessian-based smoothness indicators makes it possible to circumvent the second-order accuracy barrier for problems with local extrema. We also discuss the possibility of using such smoothness indicators to construct hp-adaptive schemes in which bound-preserving algebraic corrections are restricted to subdomains discretized using low-order finite elements [3]. Our methods are applicable to simplicial as well as tensor product meshes. Numerical results will be presented for steady and unsteady test problems in 1D, 2D, and 3D.

References

[1] R. Anderson, V. Dobrev, Tz. Kolev, D. Kuzmin, M. Quezada de Luna, R. Rieben and V. Tomov, "High-Order Local Maximum Principle Preserving (MPP) Discontinuous Galerkin Finite Element Method for the Transport Equation", *Journal of Computational Physics*, 334, pp. 102–124, 2017.

[2] C. Lohmann, D. Kuzmin, J.N. Shadid, S. Mabuza, Flux-Corrected Transport Algorithms for Continuous Galerkin Methods Based on High Order Bernstein Finite Elements, *Journal of Computational Physics*, 344, pp. 151–186, 2017.

[3] D. Kuzmin, M. Quezada de Luna and C. Kees, A Partition of Unity Approach to Adaptivity and Limiting in Continuous Finite Element Methods, *Computers and Mathematics with Applications*, (submitted). Preprint version: *Ergebnisberichte des Instituts für Angewandte Mathematik* 590, TU Dortmund University, 2018.

The Authors acknowledge contributions of all coauthors of [1-3] to this work.

Back

Curved interface reconstruction for 2D compressible multi-material flows

I. Chollet [*], G. Lissoni [†], T. Corot, P. Hoch, T. Leroy [‡], L. Dumas [§]

Abstract

A curved interface reconstruction procedure is presented here in the case of a 2D compressible flow made of two or more materials. Built with a dynamic programming procedure already introduced in [1], the curve interface is continuous and volume preserving in each cell. It is applied here to general test cases with non cartesian grids as well as triple point configurations.

Interface reconstruction (IR) methods are encountered in numerical simulation of multi-material or multi-fluid flows. The objective of IR methods is to define a geometric interface separating material 1 and material 2 with the following properties:

- P1: volume fractions conservation,
- P2: continuity of the interface,
- P3: robustness,
- P4: low or moderate computational cost.

There exists various IR methods based on a VOF approach. The first one that has been introduced in 1982 is due to D.L. Youngs [3]. Even though this method is still largely used up to now because of its simplicity and robustness, it suffers from the non continuity of the interface.

Another family of IR methods is the level-set method. Introduced by S. Osher [2], thie method consists in defining the interface between the two materials as an isoline contour of a function $\Phi : \mathbb{R}^3 \to \mathbb{R}$ advected by the flow field. Compared to a VOF scheme, Φ is a solution of a similar equation to the one satisfied by C but, contrarily to the VOF approach, the isoline $\Phi = 0$ exactly defines the interface. This method, very popular in free surface simulations, has here the major drawback of not fulfilling the mandatory conservation property P1. Some variants of this method have been proposed that remedy to this drawback. One of the idea is to define a new control point inside each mixed cell but it is done at the expense of an increased cost and a reduced robustness.

[*]Sorbonne Université , institut des sciences du calcul et des données, ISCD, F-75005 Paris, France

[†]Université Côte d'Azur, Inria, CNRS, LJAD, Parc Valrose, 06108 Nice, France

[‡]CEA DAM DIF, BP 12, 91297 Arpajon Cedex, France

[§]Laboratoire de Mathématiques de Versailles, UVSQ, CNRS, Université Paris-Saclay, 78035 Versailles, France

Back

Recently, in [1], a new reconstruction method which ensures continuity of the interface and preserves volume fractions have been introduced. This new interface reconstruction method, called DPIR (*Dynamic Programming Interface Reconstruction*), consists of two main steps. First, minimize a suitable energy functional gives a continuous linear interface. Secondly, add a control point in each cell to find the correct volume fractions. This last step in usually made by searching the point in the normal direction of the interface, in the line passing through the center of this one.

In this work there is three main goals. First, the DPIR method is extended for curved interfaces. It is of interest in particular in the case of curved meshes, where an exact reconstruction of the interface is expected. In order to be a real candidate for being used in multi-material hydrodynamic simulation using ALE remap methods, the DPIR method must be able to deal with distored meshes. Although the principle of the method remains unchanged (one minimization step, one correction step), several improvment are proposed, in particular to deal with strongly distorded cells and small volumic fraction issues. Finally, this work ends with a generalization of the method for three materials. The proposed method applies the DPIR method for all the materials *without choosing any material ordering* and a suitable average is applied to obtain the final interfaces. The method is tested on several test cases, including triple point and advection configurations.

References

[1] L. Dumas *A new volume-preserving and continuous interface reconstruction method for 2D multimaterial flow*, Int. Journ. for Num. Met. in Fluids (1) 1, 2017.

[2] S. Osher, R. P. Fedkiw *Level set methods: an overview and some recent results*, Numerical Methods for Fluid dynamics 169, 463-502, 2011.

[3] D. L. Youngs *Time dependent multi-material flow with large fluid distorsion*, Numerical Methods for Fluid dynamics, 273-285, 1982.

Cell-centered Lagrangian Lax-Wendroff HLL Hybrid Scheme in Cylindrical Geometry

D. Fridrich[†], R. Liska[†*] and B. Wendroff[‡]
[†] Czech Technical University in Prague, Faculty of Nuclear Sciences and Physical Engineering
(d.fridrich@volny.cz, liska@siduri.fjfi.cvut.cz)
[‡] Retired Fellow, Los Alamos National Laboratory,

Keywords: shock hydrodynamics; Lagrangian methods; cell-centered methods; Lax-Wendroff scheme.

ABSTRACT

We have recently developed a new Lagrangian cell-centered hydrodynamical scheme based on the Richtmyer two-step version of the Lax-Wendroff (LW) scheme and using Hartern-Lax-van Leer (HLL) type dissipative fluxes [1]. The dissipative fluxes are included as an artificial viscosity in the momentum equation and also as an artificial energy flux in the energy equation, which was proposed originally by Noh [2] and which considerably reduces the wall heating effect. The LW-HLL scheme preserves very nicely symmetry for the Noh problem on initially rectangular mesh. The LW-HLL hybrid method has been generalized from compressible gas dynamics to hypoelastic model for elasto-plastic flows [3].

Our first approach to generalize the LW-HLL hydrodynamical method from Cartesian to cylindrical geometry [4] has employed only the first order approximation to the momentum equation. Here we present a second order method. The proposed LW method in cylindrical geometry keeps symmetry of a polar symmetric problem on a polar mesh. The standard HLL dissipation in the momentum equation however breaks this symmetry and we propose a symmetry correction, so that the whole LW-HLL method keeps the symmetry. We have tested the newly developed method on a series of standard hydrodynamical tests in cylindrical geometry.

References

[1] D. Fridrich, R. Liska, and B. Wendroff. Some cell-centered Lagrangian Lax-Wendroff HLL hybrid schemes. *J. Comput. Phys.*, 326:878–892, 2016.

[2] W. F. Noh. Errors for calculations of strong shocks using an artificial viscosity and artificial heat flux. *J. Comp. Phys.*, 72:78–120, 1987.

[3] D. Fridrich, R. Liska, and B. Wendroff. Cell-centered Lagrangian Lax-Wendroff HLL hybrid method for elasto-plastic flows. *Computers & Fluids*, 157:164–174, 2017.

[4] D. Fridrich, R. Liska, and B. Wendroff. Cell-centered Lagrangian Lax-Wendroff HLL hybrid scheme in cylindrical geometry. In C. Klingenberg and M. Westdickenberg, editors, *Theory, Numerics and Applications of Hyperbolic Problems I. HYP 2016*, volume 236 of *Springer Proceedings in Mathematics and Statistics*, pages 565–576, 2018.

Back

High-order spectral volume scheme for multi-component flows using non-oscillatory kinetic flux

Na Liu[†‡], Xihua Xu[†] and Yibing Chen[†*]
[†] Institute of Applied Physics and Computational Mathematics, P.R. China
(liu_na@iapcm.ac.cn, xu_xihua@iapcm.ac.cn, chen_yibing@iapcm.ac.cn)
[‡] Software Center for High Performance Numerical Simulation, P.R. China

Keywords: multi-component flows; spectral volume method; simple weighted essentially non-oscillatory limiter; NOK flux.

ABSTRACT

In this talk, a kinetic-theory-based arbitrary high-order compact method is introduced for compressible multi-component flows with a stiffened gas equations of state(EOS). The main contribution is combining the high-order, conservative, compact spectral volume scheme(SV) with the non-oscillatory kinetic scheme(NOK) to solve the quasi-conservative extended Euler equations of compressible multi-component flows. The new scheme consists of two parts: the conservative part and the non-conservative part. The original high order compact SV scheme is used to discretize the conservative part directly. To keep high accuracy and efficiency, a new simple weighted essentially non-oscillatory limiter is proposed. And in order to treat the equation of state of the stiffened gas, the NOK scheme is utilized to compute the numerical flux. Then, careful analysis is made to satisfy the necessary condition to avoid unphysical oscillation near the material interfaces. After that, a high-order compact scheme for the non-conservative part is obtained. This new scheme has the following advantages for numerical simulations of compressible multi-component stiffened gas: high order accuracy with compact stencil and oscillation-free near the material interfaces. Numerical tests demonstrate the good performance and the efficiency of the new scheme for multi-component flow simulations.

References

[1] N.Liu and X.H.Xu and Y.B.Chen, "High order spectral volume scheme for multi-component flows using non-oscillatory kinetic flux", *Computers and Fluids*, 152, pp. 120–133, 2017.

[2] N.Liu and H.Z. Tang, "A high-order accurate gas-kinetic scheme for one- and two- dimensional flow simulation", *Communications in Computational Physics*, 15(4), pp. 911–943, 2014.

[3] Y.B.Chen and S.jiang and N.Liu, "HFVS:Arbitrary High Order Flux Vector Splitting Method", *Journal of Computational Physics*, 322, pp. 708–722, 2016.

[4] N.Liu and X.H.Xu and Y.B.Chen, "A new hybrid simple WENO-SV scheme for hyperbolic conservation laws", (In preparing).

Na Liu, doctorate from Peking university, associate research fellow at Institute of Applied Physics and Computational Mathematics, Beijing 100088, PR China, mainly work on hyperbolic conservation law, high order scheme, kinetic scheme and multi-component flow.

Back

Algebraic flux correction schemes for symmetric tensors with applications to fiber suspension flows

C. Lohmann[†]
[†] Institute of Applied Mathematics, TU Dortmund University
(christoph.lohmann@math.tu-dortmund.de)

Keywords: Fiber suspensions; finite elements; algebraic flux correction; eigenvalue range limiting.

ABSTRACT

A new physics-compatible numerical method for the simulation of fiber suspension flows is developed using an extension of the algebraic flux correction (AFC) methodology to symmetric tensor fields [2]. In the model under consideration, the incompressible Navier-Stokes equations are coupled with an inhomogeneous advection equation which governs the evolution of a so called second order orientation tensor. This quantity is needed to calculate fiber-induced stresses. It approximates the orientation states of rigid slender particles suspended in a Newtonian carrier fluid. By definition, an orientation tensor must stay positive semidefinite and preserve its unit trace property to be physically admissible.

In our numerical treatment, as proposed in [3], an operator splitting approach is used to separate the evolution equation for the symmetric tensor quantity into a nonlinear ordinary differential equation and a homogeneous advection equation. The former is known as the space-independent Folgar-Tucker equation. It describes the local orientation dynamics and preserves the physical properties of orientation tensors if suitable numerical approximations are employed and certain time step restrictions are satisfied. The presented algorithm for the advection equation constrains the eigenvalue range of the tensor quantity by imposing discrete maximum principles on the maximal and minimal eigenvalues. That is, the maximal eigenvalue is bounded above in a suitable manner, while a lower bound is enforced on the minimal eigenvalue. This design criterion was originally proposed in [1] and is satisfied by the proposed extensions of the AFC methodology to symmetric tensor quantities [2]. Generalized discrete maximum principles are formulated and enforced by adding nonlinear artificial diffusion to the semi-discrete residual of the Galerkin discretization. A priori CFL-like time step restrictions guarantee that bound-preserving solutions can be obtained even for the forward Euler time discretization.

The analysis and design of numerical algorithms for the two subproblems lead to a provably physics-compatible solution method for the coupled problem. The potential of the developed 3D simulation tool is illustrated by numerical results for the fiber suspension flow through an axisymmetric contraction.

References

[1] C. Lohmann, “Flux-corrected transport algorithms preserving the eigenvalue range of symmetric tensor quantities”, *Journal of Computational Physics* 350, pp. 907–926, 2017.

[2] C. Lohmann, “Algebraic flux correction schemes preserving the eigenvalue range of symmetric tensor fields”, *ESAIM: M2AN*, (forthcoming).

[3] C. Lohmann, “Physics-compatible finite element methods for scalar and tensorial advection problems”, *PhD thesis*, TU Dortmund University, 2019.

The research was sponsored by the German Research Association (DFG) under grant KU 1530/13-1.

Back

Solution Property Preserving Reconstruction for Finite Volume schemes

R. Loubère[1], S. Tann[2] and F. Xiao[2]

[1]Institut de Mathématiques de Bordeaux, Université de Bordeaux, France
(raphael.loubere@u-bordeaux.fr)
[2]Department of Mechanical Engineering, Tokyo Institute of Technology, Japan
(xiao.f.aa@m.titech.ac.jp, tann.s.aa@m.titech.ac.jp)

Keywords: THINC, BVD, MOOD, non-linear scheme, Euler equations

ABSTRACT

The purpose of this work is to build a general framework to reconstruct the underlying fields within a Finite Volume (FV) scheme solving an hyperbolic system of PDEs (Partial Differential Equations). In a FV context, the data are piece-wise constants per computational cell and the physical fields are reconstructed taking into account neighbor cell values. These reconstructions are further used to evaluate the physical fields which are usually used to feed a Riemann solver.
The physical field reconstructions must obey some physical properties associated to the system of PDEs (such as the positivity, entropy property, admissibility...) but also some numerically based properties like an essentially non-oscillatory behavior, computer admissibility representation (such as NaN, Inf). Moreover the reconstructions should be high accurate for smooth flows and, at minima, robust/stable on discontinuous solutions and possibly “accurate”, ie fews cells of numerical diffusion. Such reconstruction is called “Solution Property Preserving Reconstruction”.
In this work we introduce a methodology to blend high or low order polynomials and non-linear hyperbolic tangent reconstructions (THINC functions). A Boundary Variation Diminishing (BVD) algorithm is employed to select the least dissipative reconstruction in each cell. An *a posteriori* MOOD detection procedure is further employed to ensure the physical admissibility and computer representation in the rare problematic cells (where admissibility is not ensured) by a local re-computation of the solution with a robust first-order FV scheme.
We illustrate the performance of the proposed scheme via the numerical simulations for some benchmark tests which involve vacuum or near vacuum states, strong discontinuities, high Mach flows, etc. The proposed scheme maintains high accuracy on smooth profile, preserves the positivity and can eliminate the oscillation in the vicinity of discontinuities while maintaining sharp discontinuity. (see Figure 1).

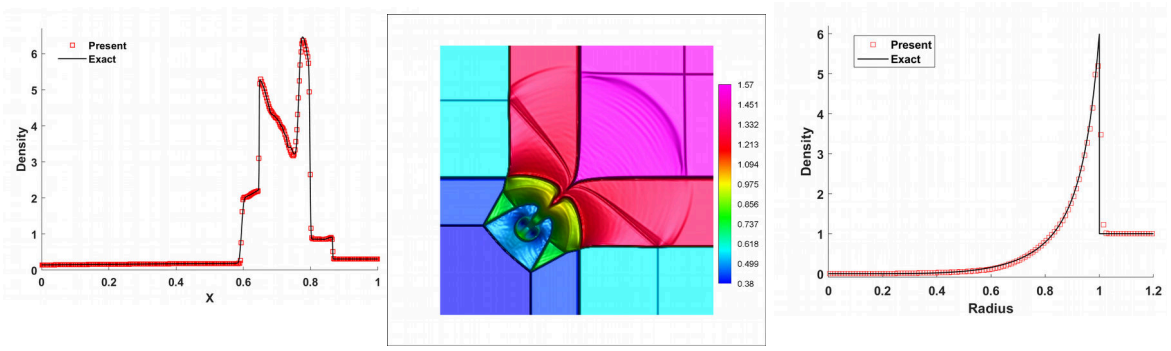


Figure 1: 1D Blastwave problem (density, 400 cells), 2D Riemann problem (density 400x400), 2D Sedov problem (density as function of radius 120x120 cells)

Back

References

[1] Solution Property Preserving Reconstruction for Finite Volume scheme, Siengdy Tann, Xi Deng, Yuya Shimizu, Raphaël Loubère, Feng Xiao, to be submitted 2019.

[2] Limiter-free discontinuity-capturing scheme for compressible gas dynamics with reactive fronts. X. Deng, B. Xie, R. Loubère, Y. Shimizu, F. Xiao, Computer & Fluids, 171, p. 1-14, 2018

[3] A New Family of High Order Unstructured MOOD and ADER Finite Volume Schemes for Multidimensional Systems of Hyperbolic Conservation Laws Raphaël Loubère and Michael Dumbser and Steven Diot , Communication in Computational Physics, 16, pp. 718-763 (2014)

[4] A fifth-order shock capturing scheme with cascade boundary variation diminishing algorithm, Xi Deng, Yuya Shimizu, Feng Xiao, in revision 2019.

Radiation Diffusion in FLAG SGH and CCH

E. Lovegrove[†*], D. Burton[‡], J. Fung[†], M. Kenamond[†], C. Malone[†], and M. Charest[§]
[†] XCP-1, Los Alamos National Laboratory (lovegrove@lanl.gov, fung@lanl.gov, kenamond@lanl.gov, malone@lanl.gov)
[‡] XCP-4, Los Alamos National Laboratory (burton@lanl.gov)
[§] CCS-7, Los Alamos National Laboratory (charest@lanl.gov)

LA-UR-19-21846

Keywords: radiation hydrodynamics; Lagrangian methods; verification and validation.

ABSTRACT

The diffusion approximation for radiation provides a simple way to incorporate basic radiation behavior into hydrodynamic codes. Slightly more complex behavior can be modeled using the flux-limited diffusion (FLD) approximation, which allows for propagation between optically-thick and optically-thin regions. We have implemented flux-limited diffusion in FLAG's staggered-grid hydro module and present results in test problems. We have also implemented grey radiation diffusion in FLAG's cell-centered hydro module and tested it against the grey nonequilibrium shocks in Lowrie & Edwards 2008 [1]. We discuss the challenges of adding radiation diffusion to the existing CCH module and differences from SGH.

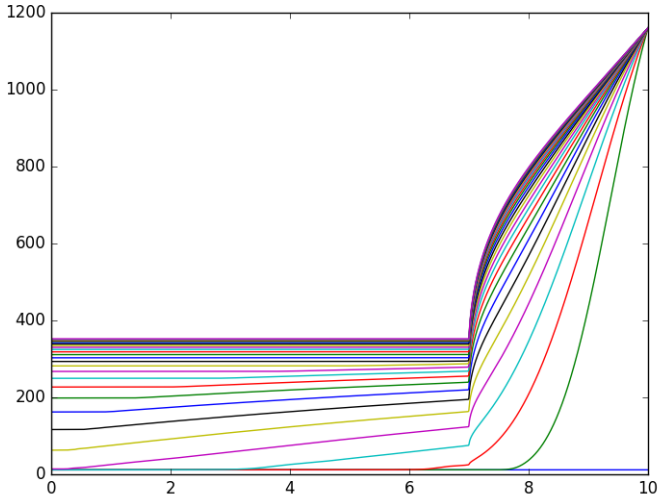


Figure 1: Behavior of light in a volume containing optically-thick and -thin media, simulated using FLAG SGH. In this simulation, the region from 0-7 cm is optically thin, while the region from 7 - 10 cm is optically-thick. The right wall (10 cm) is heated to a high radiation temperature. When the simulation is run with flux-limited diffusion, radiation energy diffuses outwards from the wall until it reaches the transition to optically-thin material and transitions stably to freestreaming behavior.

References

[1] R. Lowrie and J. Edwards, "Radiative shock solutions with grey nonequilibrium diffusion", *Shock Waves*, 18(2), pp. 129–143, 2008.

Back

A Moving Discontinuous Galerkin Finite Element Method for Conservation Laws

H. Luo[1], Y. Jiang[1], and R. Nourgaliev[2]

[1]Department of Mechanical and Aerospace Engineering, North Carolina State University
(hong_luo@ncsu.edu, yjiang28@ncsu.edu)
[2] Lawrence Livermore National Laboratory
(nourgaliev1@llnl.gov)

Keywords: moving discontinuous Galerkin methods, interface condition enforcement, conservation laws

ABSTRACT

Recently, a moving discontinuous Galerkin (MDG) finite element method was developed for compressible flows with interfaces[1]. Unlike the traditional DG methods, this MDG method treats both conservative quantities and discrete grid geometry as independent variables. A space-time DG formulation is used to solve the governing equations in the standard discontinuous solution space, and the geometry variables are determined by enforcing the interface condition in its discontinuous solution trace space. Two attractive features of the MDG method, among others, are 1) no strategies in the form of a limiter or an artificial viscosity are required to eliminate spurious oscillations in the vicinity of discontinuities and thus maintain the nonlinear stability of the DG methods, as interfaces are detected by the interface condition enforcement, and tracked by the grid movement and the interface condition; and 2) no numerical fluxes in the form of a Riemann solver are needed to maintain linear stability of the DG methods. However, this MDG formulation leads to an over-determined system of nonlinear equations. Although this over-determined nonlinear system can be solved as a stationary problem in practice, the residuals for both governing equations and interface condition are, in theory, not zero.

A new MDG formulation, designed to address this issue, is presented in this study to solve the conservation laws. In this new formulation, the conservation laws are solved using a space-time formulation, although space and time are not treated in the same way. The major difference between this formulation and the one presented in Reference 1 is that the discrete grid geometry is solved using a variational formulation in a continuous space. As a result, this new formulation leads to a determined system of nonlinear equations, where the number of unknowns is equal to the number of the nonlinear equations. Consequently, both conservation laws and interface condition are satisfied when the system of nonlinear equations is solved. Furthermore, since the space and the time are not treated exactly the same way, the method of line can be adopted to advance the solution in time. A classical arbitrary-Lagrangian-Eulerian formulation can also be recovered using this new MDG formulation, where the grid movement is determined by enforcing the interface condition, thus providing a new elegant ALE method, which can track not only material interfaces but also detect and fit shock waves. Numerical experiments for a number of benchmark test cases indicate that our new MDG method is able to deliver the designed order of accuracy for smooth solutions, and detect interfaces, via interface condition enforcement and satisfy, via grid movement, the conservation law and its associated interface condition.

References

[1] A. Corrigan, A.D. Kercher, and D.A. Kessler, “A Moving Discontinuous Galerkin Finite Element Method for Flows with Interfaces”, International Journal for Numerical Methods in Fluids, DOI: 10.1002/fld.4697, 2019.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344, and funded by the Laboratory Directed Research and Development Program at LLNL under project tracking code 19-ERD-015.

Back

Thermodynamic consistency of cell-centered Lagrangian hydrodynamics method

I. Bertron[†], R. Chauvin[‡], B. Rebourcet[‡] and P.-H. Maire[†*]
[†] CEA/CESTA, Le Barp France (isabelle.bertron@cea.fr, pierre-henri.maire@cea.fr)
[‡] CEA/DAM Ile de France, Arpajon, France (remi.chauvin@cea.fr, bernard.rebourcet@laposte.net retired fellow)

Keywords: shock hydrodynamics; Lagrangian methods; thermodynamic consistency.

ABSTRACT

It is well known that gas dynamics equations may develop singularities,*i.e.*, shock waves, at a finite time. The related discontinuous solutions are thus sought under a weak form which corresponds to the integral form of the underlying conservation laws of mass, momentum and total energy. Weak solutions being not uniquely defined, the physically relevant solution is singled out by means of an extra admissibility criterion termed entropy condition [1]. In other words, this means that the solutions of gas dynamics equations have to be consistent with the second law of thermodynamics: for smooth flows entropy has to be conserved, whereas for non smooth flows, such as shock waves, it has to be dissipated ensuring the conversion of kinetic energy into internal energy.

Bearing this in mind, the purpose of the present work is to address the thermodynamic consistency of cell-centered Finite Volume discretizations dedicated to the numerical simulation of Lagrangian hydrodynamics[2]. Firstly, we describe explicitly a general procedure to construct affordable entropy conservative numerical fluxes, extending Tadmor's work [3, 4] to the Lagrangian framework. Secondly, the entropy stability of these fluxes enhanced by proper dissipation operators is investigated. Then, a multi-dimensional extension of this work is explored. Finally, these theoretical studies are assessed by various numerical experiments.

References

[1] E. Godlewski and P.-A. Raviart "Numerical Approximation of Hyperbolic Systems of Conservation Laws" *Springer*, 1996.

[2] R. Loubère, P.-H. Maire and B. Rebourcet "Staggered and Colocated Finite Volumes Schemes for Lagrangian Hydrodynamics" *Chapter 13 in Handbook of Numerical Methods for Hyperbolic Problems, edited by R. Abgrall and C.-W. Shu, Elsevier*, 2016.

[3] E. Tadmor "The numerical viscosity of entropy stable schemes for systems of conservation laws" *Mathematics of Computation*, 49, pp. 91–103, 1987.

[4] E. Tadmor "Entropy stability theory for difference approximations of nonlinear conservation laws and related time-dependent problems" *Acta. Numer.*, 12, pp. 451–512, 2003.

Back

LLNL-ABS-768598

Modeling the Free Expansion of an Ideal Gas with and without Shocks

R. A. Managan[†]
[†] WCI/DP Div., Lawrence Livermore National Laboratory (managan1@llnl.gov)

Keywords: shock hydrodynamics; multi-material hydrodynamics; Lagrangian methods; Eulerian methods; ALE methods; mesh-free methods.

ABSTRACT

Many hydro-codes do not do a good job of modeling a gas expanding into vacuum. In addition, many test problems for this involve discontinuous initial conditions that hydro-codes have trouble modeling. An analytic solution that has no discontinuities is used to compare a second-order hydro-code to one that is higher-order. The goal is is see if the high-order hydro-code can exactly match of the analytic solution. In addition the transition from solutions without shocks to those with shocks is compared.

Copson [1] and Pack [2] presented solutions for the adiabatic expansion of an ideal gas into vacuum. The solutions were given in terms of the characteristics. Copson's solutions have a non-homogeneous layer at the surface of the gas to remove the initial discontinuities present in other solutions and are suitable for use in hydrocodes. Copson gives the constraints on the initial conditions that avoid having the characteristics cross and thus to avoid shocks. Therefore the initial conditions at which a shock will occur are known. It also allows testing of how well adiabatic flow is maintained.

Copson's solution is evaluated for initial conditions based on a monotonic cubic function[3]. The conditions for no shocks to be present, i.e. the characteristics don't cross, result in constraints on the slopes of the cubic function. Methods to evaluate the density, internal energy, pressure, and sounds speed for the gas at any (x, t) point are reviewed. Comparisons of the analytic solutions and hydro-code calculations are given.

For the initial conditions where there are no shocks the code's artificial viscosity should not be activated. However, this solution allows us to smoothly change the initial conditions from those without shocks to those that will generate shocks. This allows us to compare how the shocks turn on in the two codes. This also will allow us to compare the different artificial viscosities in the two codes.

References

[1] E. T. Copson. The Expansion of a Gas Cloud into a Vacuum. *MNRAS*, 110:238–246, 1950.

[2] D. C. Pack. The Motion of a Gas Cloud Expanding into a Vacuum. *MNRAS*, 113:43–51, 1950.

[3] Frederick N. Fritsch and Ralph E. Carlson. Monotone piecewise cubic interpolation. *SIAM Journal on Numerical Analysis*, 17(2):238–246, April 1980.

Back

Distance-gradient normal reconstruction

T. Marić[†*], **D. Bothe**[†]
[†] Mathematical modeling and analysis, TU Darmstadt
(maric@mma.tu-darmstadt.edu, bothe@mma.tu-darmstadt.de)

Keywords: Volume-of-fluid; Interface reconstruction; Lagrangian methods; Eulerian methods;

ABSTRACT

Many interface reconstruction algorithms have been developed so far in the context of the unsplit geometrical Volume-of-Fluid method for multiphase flow simulation on unstructured meshes. Some of the first algorithms [1, 2, 3] are still used, either unchanged, or in a modified form [8, 10]. Most algorithms [4, 5, 9] have used the information from the surrounding interface cells to increase the accuracy of the interface normal estimation.

(E)LVIRA [5] is still prevalently used on unstructured meshes, however it is reported to be computationally expensive. The Moment-of-Fluid (MoF) [6] is most accurate, however it introduces volume centroids that need to be advected with the flow.

The Distance-Gradient Normal Reconstruction (DGNR) algorithm improves the accuracy of the interface reconstruction without introducing additional information that needs to be advected. The idea behind the DGNR relies on using signed distances from the PLIC interface to improve the interface orientation. This idea was already used for the RDF algorithm [7], or any of the hybrid Level Set / VoF methods that rely on the geometrical distance calculation. The key difference introduced by DGNR is the way the compact signed distances associated with cell-corner points are used to improve the normal orientation. DGNR avoids the construction of larger stencils on unstructured meshes, and greatly simplifies the parallel algorithm implementation.

References

[1] D. Youngs, "Time-Dependent Multi- material Flow with Large Fluid Distortion.", *Numerical Methods for Fluid Dynamics*, pp. 273-–285., 1982

[2] B. Swartz, "The second-order sharpening of blurred smooth borders." *Mathematics of Computation*, 52(186), pp. 675–714, 1989

[3] S. J. Mosso, B. K. Swartz, D. B. Kothe, R. C. Ferrell, "A Parallel, Volume-Tracking Algorithm for Unstructured Meshes." In Proc., Parallel Computational Dynamics: Algorithms and Results Using Advanced Computers, pp. 368-–375. Capri, Italy, 1996

[4] R. Scardovelli and S. Zaleski, "Interface reconstruction with least-square fit and split Eulerian-Lagrangian advection.", *Int J Numer Methods Fluids*, 41(3), pp. 251—74., 2003

[5] J. E. Pilliod and E.G. Puckett, "Second-order accurate volume-of-fluid algorithms for tracking material interfaces." *Journal of Computational Physics*, 199(2), pp. 465-–502. (2004).

[6] Dyadechko, V. and Shashkov, M., "Reconstruction of multi-material interfaces from moment data." *Journal of Computational Physics*, 227(11), pp. 5361—5384., 2008

[7] S. J. Cummins, M. M. Francois, D. B. Kothe, "Estimating curvature from volume fractions." *Computers and Structures*, 83(6–7), pp. 425-–434., 2005

[8] P. Liovic, M. Rudman, J. L. Liow, D. Lakehal, D. B. Kothe, "'A 3D unsplit-advection volume tracking algorithm with planarity-preserving interface reconstruction."' *Computers and Fluids*, 35(10), pp. 1011-–1032., 2005

[9] J. López, C. Zanzi, P. Gomez, F. Faura, J. Hernández, "A new volume of fluid method in three dimensions—Part II: Piecewise-planar interface reconstruction with cubic-Bezier fit." *International Journal For Numerical Methods in Fluids*, 14(14), pp. 4427–4436., 2008

[10] T. Marić, T., H. Marschall and D. Bothe, "An enhanced un-split face-vertex flux-based VoF method." *Journal of Computational Physics*, 371, pp. 967-–993., 2018

Back

A Diffuse Interface Method for Calculating Multifluid Compressible Flows on Eulerian Grids

I. Menshov[1,2], Ch. Zhang[3]

[1]VNIIA, ROSATOM Company, ul. Sushchevskaya, 22,127055 Moscow, Russia
[2]Keldysh Institute for Applied Mathematics, Russian Academy of Sciences (KIAM RAS)
Miusskaya sq., 4, 125047 Moscow, Russia (menshov@kiam.ru)
[3]Lomonosov Moscow State University (MSU) Moscow 119991, Russia (zhang-c@mail.ru)

Keywords: multifluid flow, diffuse interface, Eulerian grids.

ABSTRACT

A numerical approach for modeling compressible heterogeneous multiphase flows with interfaces separating materials with different physical properties is considered. We use Eulerian grids that are not consistent with interfaces and the diffuse interface model based on the single velocity reduced equations for multiphase flows [1]. The phase distribution is defined by characteristic order functions so that the interface is represented by a narrow transition (mixed) zone [3]. We give thermodynamically consistent derivation of the interface model that takes into account dissipative factors – viscosity and heat conduction, and also surface tension effects. The surface tension in the considered diffuse interface model is modeled with the approach of continuum surface force (CSF) originally proposed for incompressible two-phase flows in [2]. We extend the CSF method to the case of compressible fluids and arbitrary number of components. To do this, by means of splitting coefficients of surface tension, effective coefficients are introduced that denote an effective phase-related surface tension. With these effective coefficients, the thermodynamically consistent phase energy of surface tension is introduced. Finally, the closed system of governing equations is derived that models the flow of heterogeneous compressible multiphase medium in terms of diffuse interfaces defined by the order functions, with accounting for heat conduction and viscosity in phases and the surface tension at the interfaces. The proposed mathematical model is tested on several benchmark problems concerned multiphase flows as, e.g., a liquid lens between two stratified fluids and rising a bubble due to buoyancy in a stratified fluid. The results obtained clear display advantages of the proposed model in accuracy and robustness.

References

[1] A.K. Kapila., R. Menikoff, J.B. Bdzil, S.F. Son, D.S. Stewart, "Two-phase modeling of deflagration-to-detonation transition in granular materials: Reduced equations", Physics of Fluids, 13, pp. 3002–3024, 2001.

[2] J.U. Brackbill, D.B. Kothe, C. Zemach, "A Continuum Method for Modeling Surface Tension", J.Comp.Phys.,100, pp. 335-354, 1992.

[3] Ch. Zhang, I.S. Menshov, "Continuous Method for Calculating the Transport Equations for a Multicomponent Heterogeneous System on Fixed Euler Grids", Mathematical Models and Computer Simulations, 4, pp. 111–130, 2019.

Acknowledgements. The reported study was partially supported by RFBR, research project No. 18-01-00921. The second author thanks the China Scholarship Council for their financial support.

Back

Splitting shock heating between ions and electrons in an ionized gas

Douglas S. Miller[†*]
[†] Lawrence Livermore National Laboratory
(dougmiller@llnl.gov)

Keywords: shock hydrodynamics; radiation hydrodynamics; plasma physics.

ABSTRACT

When the temperature of a material becomes large enough to strip some or all of the electrons off of the atoms, then there are two fluids to consider; the ions and the electrons. When a shock passes through the fluids, a question is raised about how much of the shock energy should go to the ions and how much should go to the electrons. Until recently, we have used the simplest possible model (based on Zel'dovich and Razier [1], dumping all of the shock energy into the ions and ignoring the electronic fluid completely. However, we have become aware of work from the early 2000's by Velikovich *et al*[2] that has convinced us that a more sophisticated approach can be worthwhile in problems that involve ionization of elements with atomic number (Z) as low as five or six.

We describe an approach for splitting the shock energy according to the values of ion and electron viscosity. We examine several calculations to explore the difference between our previous approach and our new one. Finally, we conclude with a brief discussion of when ion/electron shock heat splitting will matter and when it will not.

References

[1] Ya. B. Zel'dovich, Yu. P. Raizer, *Physics of Shock Waves And High-Temperature Hydrodynamic Phenomena*, Ch VII, Sec. 12, Academic, New York, 1966, Dover edition 2002.

[2] A. L. Velikovich, K. G. Whitney, and J. W. Thornhill, "A role for electron viscosity in plasma shock heating", *Physics of Plasmas* 8, 4524 (2001)

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344, LLNL-ABS-768156.

Second-Order Coupling of Radiation and Hydrodynamics with Different Spatial and Temporal Discretizations

Jijie Lou[†], **Jim E. Morel**[†]
[†] Department of Nuclear Engineering, Texas A&M University
(loujijie1991@tamu.edu, morel@tamu.edu)

Keywords: radiation-hydrodynamics, mixed finite-element, discontinuous Galerkin finite-element

ABSTRACT

Lawrence Livermore National Laboratory has an ALE radiation-hydrodynamics (RH) code project based upon an arbitrary-order Mixed Finite-Element (MFEM) discretization for the hydrodynamics equations [1]. Unfortunately, MFEM discretizations are seriously flawed for radiative transfer (RT). As an initial step towards achieving the same arbitrary order of accuracy for both the radiation and MFEM hydrodynamics solutions in radiation-hydrodynamics calculations, we have developed a 1-D High-Order/Low-Order (HOLO) Implicit-Explicit (IMEX) method for coupling radiation and hydrodynamics that uses a lumped linear-discontinuous-Galerkin spatial discretization for a HO grey S_n transport equation in conjunction with a constant-linear MFEM spatial discretization for the LO radiation energy equation, the LO radiation momentum equation, and the material internal energy equation. A standard second-order predictor-corrector scheme is used in time for the explicit solution steps of the algorithm, while a trapezoidal/BDF2 scheme is used for the implicit steps. The material densities and velocities are always treated explicitly, and the radiation variables are always treated implicitly, but the material internal energies are treated both explicitly and implicitly. The LO equations provide the Thompson scattering sources, the emission sources, and the material temperatures in the transport equation, while the HO transport equation provides an Eddington factor in the LO radiation momentum equation that closes the LO system as a whole. The scheme is second-order accurate in space and time, is asymptotic preserving in the equilibrium-diffusion limit, behaves well with unresolved radiation boundary layers, and gives excellent Marshak wave speeds with reasonably coarse meshes, even though the opacities and emission sources have a constant spatial dependence within each cell.

References

[1] V. Dobrev, Tz. Kolev, R. Rieben", "High-Order Curvilinear Finite Element Methods for Lagrangian Hydrodynamics," *SIAM Journal on Scientific Computing*, 34, pp. B606–B641, 2012.

This work was supported by Lawrence Livermore National Laboratory under Task Order B623251 and Task Agreement B575363.

Back

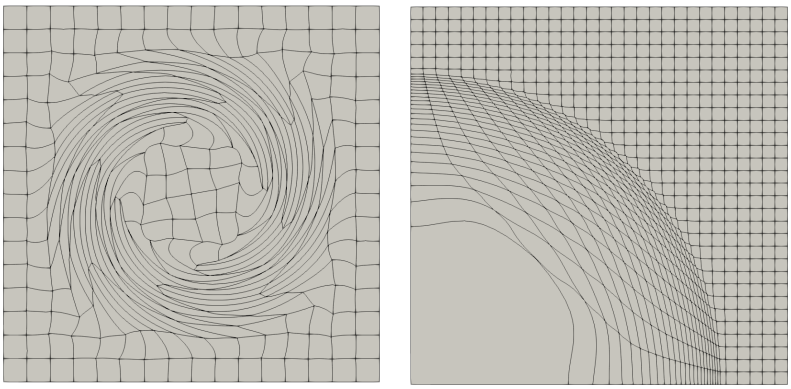
A fourth-order accurate Lagrangian discontinuous Galerkin method for cubic cells

N. Morgan†, X. Liu† and D. Burton†
† X: Computational Physics Division, Los Alamos National Laboratory
(nmorgan@lanl.gov, xliu@lanl.gov, burton@lanl.gov)

Keywords: Lagrangian hydrodynamic methods; Discontinuous Galerkin; High-order; Curvilinear meshes.

ABSTRACT

We present a new fourth-order accurate discontinuous Galerkin (DG) Lagrangian hydrodynamic method for cubic cells, which have edges that can bend and deform with the flow. The specific volume, velocity, and specific total energy fields within a cell are represented with a cubic Taylor-series polynomial. The discontinuity in the polynomials at the cell boundary is addressed by solving a multi-directional Riemann problem at the surface vertices of the cell and at additional locations along the edges so that the surface integration is exact for the polynomial order. To ensure robust mesh motion, the reconstructed density at the cell boundary includes a correction term that is a function of the difference between the density variation over the cell and a density field calculated using a subcell mesh [1] that is suitable for a cubic cell. The accuracy and robustness of the new high-order DG Lagrangian hydrodynamic method is demonstrated by simulating a diverse suite of challenging test problems covering smooth flows and strong shocks. The results from two calculations with cubic cells are shown in Figure 1.



(a) (b)

Figure 1: The deformed mesh for the Gresho vortex problem using cubic cells at t=0.6 is shown in (a), and the deformed mesh for the Sedov blast wave using cubic cells at t=1.0 is shown in (b).

References

[1] X. Liu, N. Morgan and D. Burton, "A high-order Lagrangian discontinuous Galerkin hydrodynamic method for quadratic cells using a subcell mesh stabilization scheme", *Journal of Computational Physics*, (accepted for publication)

We gratefully acknowledge the support of the Laboratory Directed Research and Development (LDRD) program at Los Alamos National Laboratory. The document release number is LA-UR-19-21224.

Back

An explicit material contact model for simple gaps on structured meshes

B. Olson[1] and B. Pudliner[1]

[1]Lawrence Livermore National Laboratory, California, USA (olson45@llnl.gov)

Keywords: contact, slidelines, ALE

ABSTRACT

A methodology for computing the dynamics of contact between two materials on a structured mesh is presented. The method explicitly solves for the contact of the materials after the Arbitrary Lagrangian Eulerian (ALE) hydrodynamic equations are integrated in time, and is therefore operator-split. Numerical experiments have shown that numerical stiffness associated with multi-material "void model" is greatly reduced, enabling larger time steps and improved calculation throughput. We present the formulation in one-dimension and show results from several test cases that demonstrate improved conservation and accuracy. The model is extended to two- and three-dimensions and additional test cases are shown which exhibit similar improved behavior. Performance estimates for large three-dimensional problems are presented to give a notion of the actual realized speedup in the Ares rad-hydro code [1,2] over the traditional multi-material "void model".

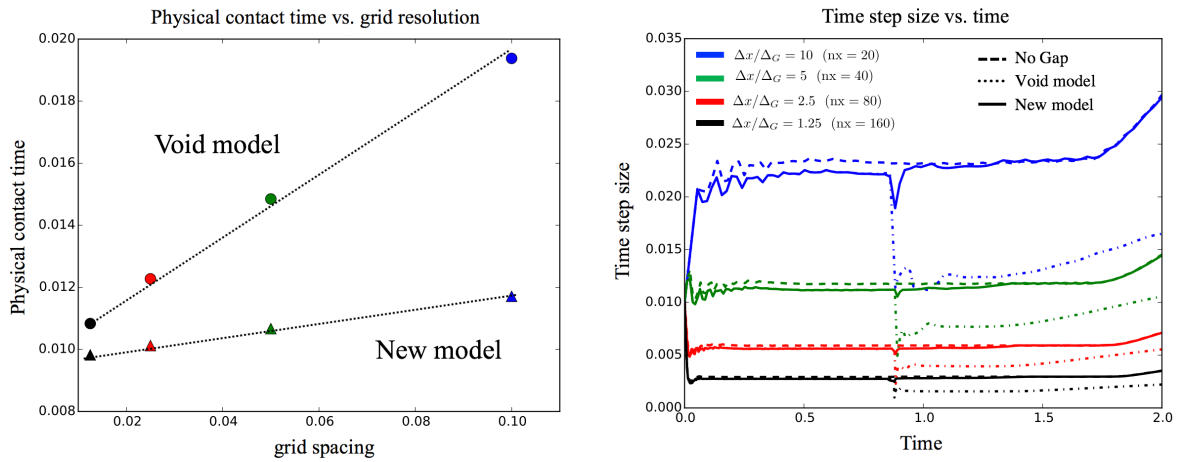


Figure 1: Results from a simple 1D contact problem where (Left) the new model captures the physical contact time more accurately and (Right) can do so with larger time steps sizes as compared to the multi-material void model.

References

[1] M. Wilkins, "Calculation of elastic-plastic flow", Report UCRL-7322, 1963.

[2] R. Sharp and R. Barton, "Hemp advection model", Report UCID 17809, 1981.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Back

Multiple material treatments for Conservative Reproducing Kernel Smoothed Particle Hydrodynamics

J. Michael Owen[†]
[†] Lawrence Livermore National Laboratory, P.O. Box 808, M/S L-38, Livermore, CA 94550
(mikeowen@llnl.gov)

Keywords: shock hydrodynamics; multi-material hydrodynamics; Lagrangian methods; mesh-free methods.

ABSTRACT

Meshfree methods such as Smoothed Particle Hydrodynamics (SPH, Monaghan (2005)) are often applied to problems with multiple materials, which on the face of it seems a trivial extension of the single material form of such techniques. The individual materials can be broken up into pure component "particles" in the meshfree discretization, each following their own Lagrangian evolution in response to interactions with their neighbors, never necessitating explicit mixed material models as the mass in each particle remains pure for all time. However, upon closer inspection there are a few vexing issues with multiple materials that plague simple meshfree methods like SPH:

- Each SPH point needs to sample many neighbors, typically ~ 50 in 2D or ~ 268 in 3D. This means particles near a material boundary interact with many particles of a different material, blending potentially quite different material properties over such interfaces.
- SPH is sensitive to mixing particles with different masses and different spacings – discrepancies of more than a factor of two can lead to pronounced artifacts. However, requiring points of different materials to have similar point masses and spacings near material boundaries with very different material densities is overconstrained, forcing compromises in fidelity and how a calculation can be initialized.

Conservative Reproducing Kernel Smoothed Particle Hydrodynamics (CRKSPH, Frontiere et al. (2017)) offers some interesting possibilities to improve multiple material treatments. The improved interpolation theory of Reproducing Kernels (RK) allows accurate interpolation of properties in point distributions up to surfaces, allowing the neighbor sets for points in a given material to only include neighbors of that material and not sample over different species. We can extract the surface elements between points of different materials as a by-product of the Voronoi-like point volume construction for solid CRKSPH (Owen, 2017), allowing the points of different materials to communicate indirectly via this reconstructed interface. Combined these properties remedy both of the weaknesses outlined above: points in a given material never directly sum over points of different materials, but rather only interact with neighbors from their own material type, negating both the blending effect and the need to mix very different particle masses. Material–material interactions can be modeled as interactions of points with the material interfaces, also affording the opportunity to introduce new surface physics at such interfaces, such as friction. This talk will present work investigating novel multiple material extensions to CRKSPH such as these.

Back

References

Frontiere, N., Raskin, C. D., and Owen, J. M. (2017). CRKSPH - A Conservative Reproducing Kernel Smoothed Particle Hydrodynamics Scheme. *Journal of Computational Physics*, 332:160 – 209.

Monaghan, J. J. (2005). Smoothed particle hydrodynamics. *Reports on progress in physics*, 68(8):1703–1759.

Owen, J. M. (2017). Advances in CRKSPH: volumes, surfaces, solids, and fracture. 2017 Mutlimaterial Hydrodynamics Conference.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. LLNL-ABS-768143.

Numerical modeling of liquid-vapor flows with arbitrary heat and mass transfer relaxation times and general equation of state

M. Pelanti[†*], M. De Lorenzo[‡] and P. Lafon[†]
[†] IMSIA, UMR 9219 ENSTA ParisTech - EDF - CNRS - CEA, Palaiseau, France
(marica.pelanti@ensta-paristech.fr, philippe.lafon@edf.fr)
[‡]Compressor Controls Corporation, Italy (marco.de.lorenzo@hotmail.com)

Keywords: two-phase compressible flows; liquid-vapor transition; thermodynamic relaxation; finite volume schemes; approximate Riemann solvers.

ABSTRACT

We describe liquid-vapor flows by a single-velocity six-equation two-phase compressible flow model, which is composed of the phasic mass and total energy equations for the two phases, one volume fraction equation, and the mixture momentum equation [1]. The model contains relaxation source terms accounting for volume, heat and mass transfer. The system of equations is numerically solved by a classical fractional step algorithm, where we alternate between the solution of the homogeneous hyperbolic portion of the model system via a second-order accurate HLLC-type finite volume scheme, and the solution of a sequence of three systems of ordinary differential equations for the relaxation source terms driving the flow toward mechanical, thermal and chemical equilibrium. In the literature often numerical relaxation procedures are based on simplifying assumptions, namely simple equations of state, such as the stiffened gas one, and instantaneous relaxation processes. These simplifications of the flow physics, which were also assumed in our previous work [1], are convenient for designing more easily efficient and robust numerical methods. Nonetheless, they might be inadequate for a precise description of the thermodynamical processes involved in various flow problems. For instance, in some transient phenomena such as fast depressurizations, the delay of vaporization and the appearance of metastable states are key features in the flow evolution [2]. In the present work we introduce new numerical relaxation procedures to integrate interphase transfer terms with two significant properties: the capability to describe heat and mass transfer processes of arbitrary relaxation time, and the applicability to a general equation of state. Some methods with these features were developed in our recent work [3]. Here we propose novel efficient techniques suited for both non-stiff and stiff relaxation processes. We present several simulations of evaporation and condensation problems, including blowdown experiments, which show the effectiveness of the proposed numerical liquid-vapor flow model.

References

[1] M. Pelanti and K.-M. Shyue, "A mixture-energy-consistent six-equation two-phase numerical model for fluids with interfaces, cavitation and evaporation waves", *Journal of Computational Physics*, 259, pp. 331–357, 2014.

[2] M. De Lorenzo, P. Lafon, M. Di Matteo, M. Pelanti, J.-M. Seynhaeve and Y. Bartosiewicz, "Homogeneous Two-Phase Flow Models and Accurate Steam-Water Table Look-up Method for Fast Transient Simulations", *International Journal of Multiphase Flow*, 95, pp. 199–219, 2017.

[3] M. De Lorenzo, P. Lafon and M. Pelanti, "A hyperbolic phase-transition model with non-instantaneous EoS-independent relaxation procedures", *Journal of Computational Physics*, 379, pp. 279–308, 2019.

Back

Monolithic multiscale modeling of solidification and melting processes

I. Peshkov[1], **E. Romenski**[2,3] **and M. Dumbser**[2]

[1] Institut de Mathématiques de Toulouse, Université Toulouse III, France (peshenator@gmail.com)

[2] University of Trento, Italy (michael.dumbser@unitn.it)

[3] Sobolev Institute of Mathematics SB RAS, Novosibirsk, Russia (evrom@math.nsc.ru)

Keywords: Solid-fluid phase transition; diffuse interface; hyperbolic equations.

ABSTRACT

We discuss some aspects of the modeling of solid-fluid phase transformations within the unified continuum mechanics formulation of solids and fluids [3, 2]. In our approach, fluids and solids are described by a single system of partial differential equations and therefore, it is very suitable for the modeling of physical phenomena with the coexistence of the fluid and solid states. For example, dynamical solid-fluid transformations can be encountered in many industrial and natural processes such as additive manufacturing of metals (3D laser printing, see Fig.1), debris flows and avalanches, general granular flows and flows of viscoplastic fluids, development of new alloys, etc. The state of the art modeling of solid-fluid phase transformations relies on either over simplified approaches when the solid state is approximated by the fluid dynamics equations with a very high viscosity or over complicated models when two different sets of equations (or even two different computational codes) for the solid and liquid phase are coupled in a sophisticated manner. On the other hand, our unified approach allows for the transition between the fluid and solid states be literally described in a continuous and thermodynamically consistent manner. This then provides intriguing opportunities for reducing the complexity of the mathematical and computational modeling but simultaneously for increasing the precision of the physical modeling by naturally incorporating new physical features such as residual stresses, dislocation nucleation, proper heat and mass transfer across the solidification fronts, etc.

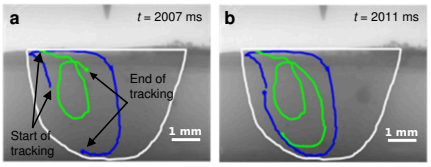


Figure 1: *An example of **fluid flow** observed in a steel melt pool, from [1]. The green and blue lines depict the trajectories of two tracer particles at two time instants $t = 2007$ ms (left) and $t = 2011$ ms (right). The white line shows the borders of the melted pool. Flow velocities are ranging in 0.1 – 0.5 m/s.*

In this talk, we briefly discuss our unified formulation for fluid and solid dynamics and present a few preliminary computational examples of modeling solid-fluid phase transformations.

I.P. greatly acknowledges the support by ANR-11-LABX-0040-CIMI within the program ANR-11-IDEX-0002-02.

References

[1] L. Aucott, H. Dong, W. Mirihanage, R. Atwood, A. Kidess, S. Gao, S. Wen, J. Marsden, S. Feng, M. Tong, T. Connolley, M. Drakopoulos, C. R. Kleijn, I. M. Richardson, D. J. Browne, R. H. Mathiesen, and H. V. Atkinson. "Revealing internal flow behaviour in arc welding and additive manufacturing of metals". *Nature Communications* (2018), pp. 1–7. DOI: 10.1038/s41467-018-07900-9.

[2] M. Dumbser, I. Peshkov, and E. Romenski. "A Unified Hyperbolic Formulation for Viscous Fluids and Elastoplastic Solids". In: *Theory, Numerics and Applications of Hyperbolic Problems II. HYP 2016*. Ed. by C. Klingenberg and M. Westdickenberg. Vol. 237. Springer Proceedings in Mathematics and Statistics. Cham: Springer International Publishing, 2018, pp. 451–463. DOI: 10.1007/978-3-319-91548-7_34.

[3] M. Dumbser, I. Peshkov, E. Romenski, and O. Zanotti. "High order ADER schemes for a unified first order hyperbolic formulation of continuum mechanics: Viscous heat-conducting fluids and elastic solids". *Journal of Computational Physics* 314 (2016), pp. 824–862. DOI: 10.1016/j.jcp.2016.02.015. arXiv: 1511.08995.

Back

Multi-material dynamic domain topology changes in the Lagrangian Grid Reconnection (LGR) code

D. Ibanez[†], **M. Powell**[*] **T. Fuller, B. Granzow, and G. Hansen**[†]
[†] Sandia National Laboratories, Albuquerque, NM (daibane@sandia.gov, micpowe@sandia.gov, gahanse@sandia.gov)

Keywords: shock hydrodynamics; multi-material hydrodynamics; Lagrangian methods;

ABSTRACT

LGR is a continuation of the Alexa research code presented at previous MULTIMAT conferences. We have previously presented the use of tetrahedral mesh adaptation as a viable mechanism for implementing the remesh and remap steps in a Lagrange-remesh-remap implementation of shock hydrodynamics. We now present further progress by extending this method with a mechanism for domain topology change, which allows objects to break up and inter-penetrate. Domain topology change is still based on a cavity approach similar to that used in mesh adaptation, except this cavity operation "floods", or replaces, the entire cavity with background material state, as inspired by the work of Del Pino [1]. We first apply mesh adaptation, which is allowed to change element connectivity but not domain topology, and will ensure high-quality elements as much as possible within the domain topology constraint. After adaptation, any elements which are still low-quality are indicators that domain topology is the limiting factor. Examples of such scenarios include two objects colliding resulting in a thin gas material between them, and a material being folded which creates a pinch region where element angles are forced to zero. When such low-quality elements are detected, nearby cavities containing those elements are evaluated for potential "flooding". Criteria for preferring one cavity over another include the quality of background material and the magnitude of the resulting mass error. We present simulations to demonstrate that this approach handles complex material flows and multi-material interactions. We have further extended the suite of strength models and equations of state in LGR as well, showing that more complex models can still be efficiently executed on NVIDIA GPUs. This includes the evaluation of tabular equations of state on GPUs, as well as strength and damage models such as Johnson-Cook. All simulations presented were executed on a single NVIDIA Volta GPU, and we show good whole-simulation speedup on these accelerators.

References

[1] S. Del Pino "Metric-based mesh adaptation for 2D Lagrangian compressible flows", *Journal of Computational Physics*, 203(5), pp.1793–1821, 2011.

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc. for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Back

A diffuse interface method for weakly compressible multiphase flows based on the Baer and Nunziato model

R. Abgrall[†] **and B. Re**[†*]
[†] Institut für Mathematik, Universität Zürich (remi.abgrall@math.uzh.ch, barbara.re@math.uzh.ch)

Keywords: multiphase flows; weakly compressible flows; Baer and Nunziato model.

ABSTRACT

In this work, we present a novel diffuse interface method (DIM) for the simulation of weakly compressible, multiphase flows. The proposed approach is based on the non-equilibrium Baer and Nunziato model, according to which each phase is described by its own thermodynamic model and no equilibrium is assumed between phase pressure, velocity, nor internal energy [1]. Indeed, the governing equations consist in a hyperbolic relaxation system, where the interface parameters model phase interaction and source terms control how phase equilibrium is reached. Particular care has taken to discretize the non-conservative terms, in order to avoid the occurrence of spurious oscillations across interfaces.

The target applications involve weakly compressible flows. As it is known from single-phase computational fluid dynamics, at low Mach numbers the performances of standard compressible schemes deteriorate significantly, especially in terms of accuracy and efficiency, and, if using explicit time integration schemes, the acoustic effects result in a severe restriction of the time step. Moreover, in multiphase simulations, the source terms may become stiff when the phases are far from equilibrium. In the present work, we use a special scaling for the pressure and a staggered spatial discretization to retrieve asymptotically the correct incompressible behavior, together with a careful time discretization which treats implicitly the acoustic part of the governing equations [2].

Transient numerical simulations involving CO2-rich mixtures are presented to assess the validity of the proposed method. Flow behavior is first described through the simplified "stiffened gas" model. Then, more accurate, engineering-relevant equation of states are used to investigate pipe-flows closer to real applications.

References

[1] R. Saurel and R. Abgrall. "A Multiphase Godunov Method for Compressible Multifluid and Multiphase Flows", *Journal of Computational Physics*, 150, pp. 425–467, 1999.

[2] H. Bijl and P. Wesseling. "A Unified Method for Computing Incompressible and Compressible Flows in Boundary-Fitted Coordinates", *Journal of Computational Physics*, 141, pp. 153–173, 1998.

Acknowledgments: This publication has been produced with support from the NCCS Centre, performed under the Norwegian research program Centres for Environment-friendly Energy Research (FME). The authors acknowledge the following partners for their contributions: Aker Solutions, Ansaldo Energia, CoorsTek Membrane Sciences, Emgs, Equinor, Gassco, Krohne, Larvik Shipping, Norcem, Norwegian Oil and Gas, Quad Geometrics, Shell, Total, Vår Energi, and the Research Council of Norway (257579/E20).

Back

The Power and Secrets of the Sigmoid Function: A Numerical Swiss Army Knife

William J. Rider[1]

[1]Sandia National Laboratories, Albuquerque, Center for Computing Research(wjrider@sandia.gov)

Keywords: sigmoid, THINC, limiter.

ABSTRACT

Occasionally one runs across techniques that provide utility in a myriad of applications and demand that one sits up, focus and take notice. The sigmoid function is one such technique. What is a sigmoid function? The most well-known and widely used member of the family is the hyperbolic tangent. There are numerous versions of the sigmoid, which is the continuously differentiable version of the sign function. The sigmoid can be adjusted to provide the level of smoothness and width of the transition. Its most powerful and famous utility comes in the implementation of neural nets where sigmoid functions act as switching functions. Closer examination shows that the sigmoid has broader utility to remove numerical discontinuities from computer codes, as an example could replace an "if" test in a code with a continuous switch. One of the little mysteries of the sigmoid is how sharp to make the transition and what sort of deeper principles are connected to this numerical "trick".

More provocatively, the sigmoid can be used for solving differential equations. The first example of this is the THINC method that uses the hyperbolic tangent to numerically propagate material interfaces without dissipation [1]. More recently, this method has moved into the role of an alternative path for monotonicity-preserving methods. Usually monotonicity preservation takes a general function and modifies it with a "limiter" to render it monotone. As we will show, other sigmoid functions may be used for this purpose and these functions have an interesting connection to the traditional class of methods. With the sigmoid we have an intrinsically monotone function that needs to be rendered conservative. In a nutshell, limiters are usually the way a reconstruction method is rendered monotone. With sigmoids, the limiter arises from making the intrinsically monotone function conservative (in subtle opposition to [2]). This connection is powerful and worthy of exploiting. It also unifies this new class of approximations with the traditional form, hopefully making them more attractive for adoption and less mysterious in their utility for approximating hyperbolic equations [3].

References

[1] Xiao, F., Ii, S., & Chen, C. (2011). Revisit to the THINC scheme: a simple algebraic VOF algorithm. *Journal of Computational Physics*, *230*(19), 7086-7092.

[2] Deng, X., Xie, B., Loubère, R., Shimizu, Y. and Xiao, F., 2018. Limiter-free discontinuity-capturing scheme for compressible gas dynamics with reactive fronts. *Computers & Fluids*, *171*, pp.1-14.

[3] Sweby, P.K., 1984. High resolution schemes using flux limiters for hyperbolic conservation laws. *SIAM journal on numerical analysis*, *21*(5), pp.995-1011.

Back

A matrix-free hyper-viscosity method for high-order finite element ALE hydrodynamics

P. D. Bello-Maldonado, V. A. Dobrev, Tz. V. Kolev, R. N. Rieben and V. Z. Tomov

Lawrence Livermore National Laboratory
(belloma2@illinois.edu, dobrev1@llnl.gov, tzanio@llnl.gov, rieben1@llnl.gov, tomov2@llnl.gov)

Keywords: artificial viscosity; ALE hydrodynamics; finite element methods; high-order methods.

ABSTRACT

The numerical approximation of shock hydrodynamics is at the core of multiphysics simulations as shocks are the driving force in experiments like inertial confinement fusion. In this work, we describe our extension of the hyperviscosity technique of [1] for use in arbitrarily high-order finite element methods for Lagrangian hydrodynamics [2]. Hyperviscosity enables shock capturing while preserving the high-order properties of the underlying discretization away from the shock region. Specifically, we compute a high-order term based on a product of the mesh length scale to a high power scaled by a hyper-Laplacian operator applied to a scalar field. We then form the total artificial viscosity by taking a non-linear blend of this term and a traditional artificial viscosity term. We also present a matrix-free formulation for computing the finite element based hyper-Laplacian operator. Such matrix-free methods have superior performance characteristics compared to traditional full matrix assembly approaches and offer advantages for GPU based HPC hardware. We show results in numerical convergence of our method and its application to complex, multi-material ALE simulations on high-order (curved) meshes.

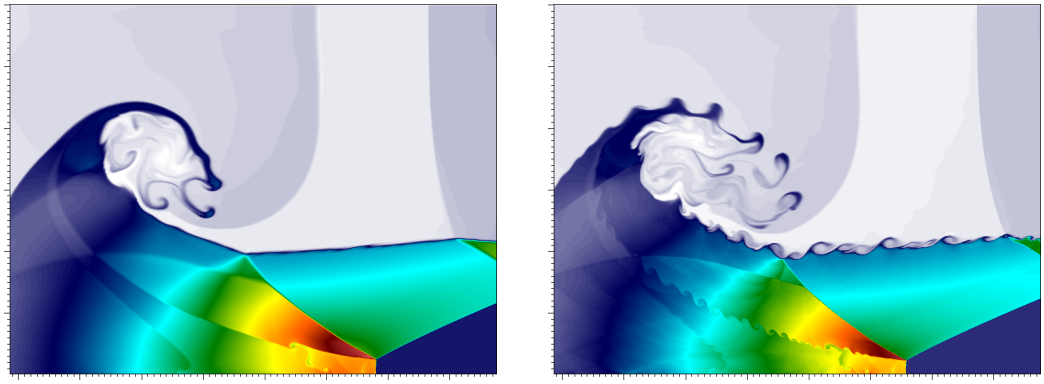


Figure 1: Example of a tradtional (low-order) artifical viscosity method (*left*) compared to a high-order hyper-viscosity method (*right*) in the multi-material shock triple-point test problem using high-order finite elements.

References

[1] A. W. Cook and W. H. Cabot, "Hyperviscosity for shock-turbulence interactions", *Journal of Computational Physics*, (203) 2005, pp. 379-385.

[2] V. A. Dobrev, Tz. V. Kolev and R. N. Rieben, "High-order Curvilinear Finite Element Methods for Lagrangian Hydrodynamics", *SIAM Journal on Scientific Computing*, (34) 2012, pp. B606-B641.

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344, LLNL-ABS-768215

Back

A two-phase model for fluid saturated elastoplastic porous medium based on the theory of thermodynamically compatible systems

E. Romenski[1,2], G. Reshetova[3], I. Peshkov[2,4] and M. Dumbser[1]

[1]University of Trento, Italy (michael.dumbser@unitn.it)
[2]Sobolev Institute of Mathematics SB RAS, Novosibirsk, Russia (evrom@math.nsc.ru)
[3]Institute of Computational Mathematics and Mathematical Geophysics SB RAS, Novosibirsk, Russia (kgv@nmsf.sscc.ru)
[4]Institut de Mathématiques de Toulouse, Université Toulouse III, France (peshenator@gmail.com)

Keywords: hyperbolic thermodynamically compatible system, saturated porous medium.

ABSTRACT

Modeling of fluid flows in porous media is of permanent interest in many geophysical and industrial applications. The starting point of research developments in this field was the pioneering work of Bio, in which a model of elastic wave propagation in the saturated porous media was proposed. Some generalizations of the model have been done in the past and at present Biot's approach is the commonly accepted and widely used in geophysical community. Nevertheless, many technological and scientific problems such as geothermal energy extraction, CO2 storage, hydraulic fracturing, require a development of new advanced models and methods.

For the development of nonlinear processes in deforming porous media we apply the theory of Symmetric Hyperbolic Thermodynamically Compatible (SHTC) systems for multiphase mixture [1] and recently developed unified SHTC model of Newtonian continuum mechanics [2]. The latter describes at the same time the dynamics of elastoplastic solids as well as the viscous compressible fluid flow.

We extend the SHTC unified model of continuum mechanics by consideration of flow of compressible fluid in elastoplastic deforming porous media. The governing equations of the model also belong to the class of SHTC systems. The interphase friction between liquid and solid phases and shear stress relaxation are implemented in the model in accordance with laws of thermodynamics. We also derive PDEs for the small amplitude wave propagation in the stationary fluid saturated porous medium and study the properties of wavefields. Results of the solution of some numerical test problems are presented.

References

[1] E. Romenski, A.A. Belozerov, I.M. Peshkov, “Conservative Formulation for Compressible Multiphase Flow”, Quarterly of Applied Mathematics, 74, pp. 113–136, 2015.

[2] M. Dumbser, I. Peshkov, E. Romenski, O. Zanotti, “High order ADER schemes for a unified first order hyperbolic formulation of continuum mechanics: Viscous heat-conducting fluids and elastic solids”, Journal of Computational Physics, 314, pp. 824-862, 2016.

Back

Simulation of Magnetically Driven HEDP/ICF Experiments with a Lagrangian/ALE Code

C. L. Rousculp[†], T. A. Gianakon[†], K. Lipnikov,[†] T. R. Waters[†], A. Beresnyak[‡]
[†] Los Alamos National Laboratory
[‡] Naval Research Laboratory

Keywords: Magnetohydrodynamics; Lagrangian methods; ALE methods.

ABSTRACT

Magnetic drive has recently received a great deal of attention in the context of high energy density physics (HDEP) as well as inertial confinement fusion (ICF). Here, stored electrical energy in converted into mega-Gauss level magnetic fields that accelerate a conductor that, in turn, drives materials to HEDP regimes or compresses fusion fuel. Most prevalent are cylindrical Z-pinch configurations where a pulsed, axial current generates an azimuthal field via Lorentz forces. The system may or may not be complemented by a static axial field to aid in confinement. Another configuration utilizes a planar geometry for either shocked or quasi-isentropic loading. In order to study the performance of these emerging designs, sophisticated computational tools are required. At the very least, a single-fluid, resistive, magneto-hydrodynamics (MHD) model must be implemented. Shown here are recent developments and applications of the Lagrangian/ALE FLAG code to such problems. Through verification test problems, an explicit, ideal MHD algorithm is shown to be second order on smooth test problems and first-order on problems involving shock discontinuities. The operator-split, implicit, resistive diffusion algorithm is shown to be second-order on arbitrary polyhedral/polygonal meshes. Finally, results of simulation of relevant Z-pinch and planer configurations for HEDP and ICF applications are shown.

This work was supported by the US Department of Energy through the Los Alamos National Laboratory. Los Alamos National Laboratory is operated by Triad National Security, LLC, for the National Nuclear Security Administration of U.S. Department of Energy (Contract No. 89233218CNA000001).

Back

Riemann solver with internal reconstruction (RSIR) for compressible single-phase and non-equilibrium two-phase flows

Quentin Carmouze[1,2], Richard Saurel [1,3] and Emmanuel Lapebie [4]

[1] Aix Marseille Univ, CNRS, Centrale Marseille, LMA, Marseille, France
[2] University of Nice, LJAD UMR CNRS 7351, Parc Valrose, 06108 Nice Cedex, France
[3] RS2N SAS, Saint Zacharie, France
[4] CEA Gramat, France

Abstract

A new Riemann solver is built to address numerical resolution of complex flow models. The research direction is closely linked to a variant of the Baer and Nunziato (1986) model developed in Saurel et al. (2017a). This recent model provides a link between the Marble (1963) model for two-phase dilute suspensions and dense mixtures. As in the Marble model, Saurel et al. system is weakly hyperbolic with the same 4 characteristic waves, while the system involves 7 partial differential equations. It poses serious theoretical and practical issues to build simple and accurate flow solver. To overcome related difficulties the Riemann solver of Linde (2002) is revisited. The method is first examined in the simplified context of compressible Euler equations. Physical considerations are introduced in the solver improving robustness and accuracy of the Linde method. With these modifications the flow solver appears as accurate as the HLLC solver of Toro et al. (1994). Second the two-phase flow model is considered. A locally conservative formulation is built and validated removing issues related to non-conservative terms. However, two extra major issues appear from numerical experiments: The solution appears not self-similar and multiple contact waves appear in the dispersed phase. Building HLLC-type or any other solver appears consequently challenging. The modified Linde (2002) method is thus examined for the considered flow model. Some basic properties of the equations are used, such as shock relations of the dispersed phase and jump conditions across the contact wave. Thanks to these ingredients the new Riemann solver with internal reconstruction (RSIR), modification of the Linde method, handles stationary volume fraction discontinuities, presents low dissipation for transport waves and handles shocks and expansion waves accurately. It is validated on various test problems showing method's accuracy and versatility for complex flow models. Its capabilities are illustrated on a difficult two-phase flow instability problem, unresolved before.

Keywords: two-phase, dense-dilute, weakly hyperbolic, Riemann solver

Email: Richard.Saurel@univ-amu.fr

Back

An IMEX Continuum Multifluid Electromagnetic Plasma Formulation for Challenging Fusion Related Applications*

John N. Shadid[1,2], Michael Crockatt[1], Sibu Mabuza[1], Sidafa Conde[1], Ignacio Tomas[1], Roger P. Pawlowski[1]

[1]Center for Computer Research, Sandia National Laboratories (jnshadi@sandia.gov, mmcrock@sandia.gov, smbuza@sandia.gov, sconde@sandia.gov, itomas@sandia.gov, rppalow@sandia.gov)

[2]Department of Mathematics and Statistics, Univ. of New Mexico

Keywords: multifluid plasmas, Maxwell equations, IMEX, AFC

ABSTRACT

This talk considers the development and evaluation of an implicit / explicit (IMEX) formulation for a continuum multifluid electromagnetic plasma model. The general form of the model is based on the governing partial differential equations (PDEs) describing conservation of mass, momentum, and total energy for each fluid species, collisional transfer and ionization / recombination / charge-exchange effects, and the coupling to electromagnetics with various forms of Maxwell's equations for the electromagnetic fields [1,2]. The resulting systems are characterized by strong nonlinear and nonsymmetric coupling of fluid and electromagnetic phenomena, strong source term coupling, as well as a significant range of time- and length-scales that these interactions produce. This talk presents recent progress in developing robust temporal and spatial discretizations of this system. The spatial discretizations are based on continuous Galerkin methods employing algebraic flux correction (AFC) with an iterative nodal variation limiting techniques that enforces local bounds and positivity preservation constraints [3,4]. To evaluate these methods, we consider both smooth analytic solutions of the multifluid system and challenging multifluid electromagnetic shock problems in both the non-collisional and collisional regimes. Applications of interest for these methods include plasma fusion related problems in magnetic implosions and for tokamak disruption mitigation strategies.

References

[1] E. T. Meier, and U. Shumlak, A general nonlinear fluid model for reacting plasma-neutral mixtures, Phys. of Plasmas, 19, 072508 (2012)

[2] Shadid, Cyr, Phillips, Pawlowski, et. al., Towards Scalable and Efficient Solution of Full Maxwell Electromagnetics - Multifluid Plasma Systems NECDC, 2016

[3] D. Kuzmin and M. Moller and M. Gurris, Algebraic flux correction II, Flux-Corrected Transport: Principles, Algorithms, and Applications, 2012, pp. 193–238

[4] Mabuza, Shadid, Kuzmin, Local bounds preserving stabilization for continuous Galerkin discretization of hyperbolic systems, Journal of Computational Physics 361 (2018), 82 –110.

*This work was partially supported by the DOE Office of Science Advanced Scientific Computing Research (ASCR) - Applied Math Research program and an ASCR/Office of Fusion Energy SciDAC Partnership Project at Sandia National Laboratories. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Back

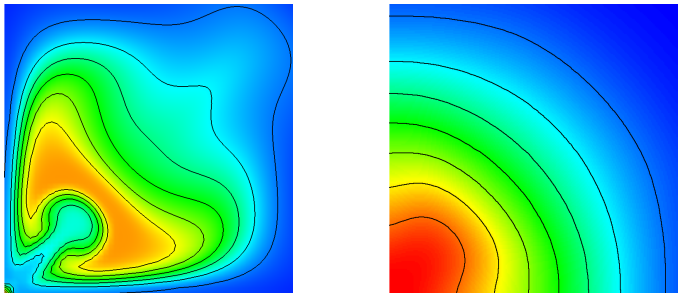
Intersection-distribution-based remapping for multi-material staggered arbitrary Lagrangian-Eulerian hydrodynamics

M. Kenamond[†]**, and M. Shashkov**[‡*]
[†] Lagrange Applications Project (XCP-1), X-Comput. Phys. Div., Los Alamos National Laboratory
(kenamond@lanl.gov)
[‡] Methods and Algorithms (XCP-4), X-Comput. Phys. Div., Los Alamos National Laboratory
(shahkov@lanl.gov)

Keywords: shock hydrodynamics; multi-material hydrodynamics; Lagrangian methods; ALE methods.

ABSTRACT

We present a new distribution-based method for remapping nodal mass and momentum between arbitrary source (Lagrangian) and arbitrary target (rezoned) meshes for indirect staggered arbitrary Lagrangian-Eulerian hydrodynamics, [1]. The method is based on the following ideas: we first define the cell-centered momentum and mass on the source mesh and conservatively remap those cell-centered quantities from source to target meshes using an intersection-based remap. Next, we use a local constrained optimization approach for each cell of the target mesh to conservatively distribute cell mass and momentum between nodes of the cell. The new method is efficient, conservative, accurate and bound preserving and can be used for remapping between two arbitrary meshes which may have completely different connectivity. Using the new method we present results for several test problems: Sod, Sedov, Triple-point and Taylor-Green vortex. and compare our results with the standard flux-based remapping, [2]. In Fig. 1 we present a comparison of the remapping methods for the Sedov problem. One can see that the new method preserves symmetry of the flow much better than the standard flux-based method.In our talk we will demonstrate other advantages of new method with respect to flux based methods.



Swept Remap Intersection-Distribution-Based Remap

Figure 1: Sedov problem, color map for specific internal energy at $t = 1$ (zoom near origin) - comparison of flux-based (left panel) and intersection-based distribution (right panel) remapping methods.

References

[1] M. Kenamond and M. Shashkov, "The distribution-based remapping of the nodal mass and momentum between arbitrary meshes for staggered arbitrary Lagrangian-Eulerian hydrodynamics", *Report of Los Alamos National Laboratory*, LA-UR-18-25326, 2018.

[2] A.J. Barlow, P.-H. Maire, W.J. Rider, R.N. Rieben and M.J. Shashkov, "Arbitrary Lagrangian-Eulerian methods for modeling high-speed compressible multimaterial flows", *J. Comput. Phys.*, 322, pp. 603–665, 2016.

This work was performed under the auspices of the National Nuclear Security Administration of the US Department of Energy at Los Alamos National Laboratory under Contract No. DE-AC52-06NA25396. The authors gratefully acknowledge the support of the US Department of Energy National Nuclear Security Administration Advanced Simulation and Computing (ASC) Program. LA-UR-19-20080.

Back

Vorticity Confinement and Shock Capturing - two sides of the same coin?

D. Sidilkover
Soreq NRC, Yavne 81800, Israel (sidilkov@soreq.gov.il)

Keywords: Eulerian methods; Shock Capturing; Vorticity Confinement.

ABSTRACT

Improving numerical resolution of the vortical structures in fluid flow, both incompressible and compressible, is one of the outstanding difficulties facing both the CFD practitioners and numerical analysts. A remarkable achievement in this direction was the introduction of the Vorticity Confinement (VC) method by John Steinhoff in the early 90's. This method was developed for incompressible flow computations and has been demonstrated to be successful in practice. Several extensions of it to compressible flow were suggested. However, most of them were applicable to problem's concerning the subsonic regime only.

The so-called Shock Capturing (SC) approach originated several decades ago and is under continuous development ever since. It comprises a class of methods designed for resolving compressible flow with shocks and includes schemes of various order of accuracy. This approach is widely accepted and is being used in practice extensively.

We show that these two seemingly unrelated methodologies (VC and SC) are in fact closely related. Exploring their commonality allows to construct a new unified methodology that acquires both VC and SC capabilities by means of a single mechanism. This new approach can be regarded as novel multidimensional extensions of the TVD and finite difference ENO/WENO classes of schemes. Performance of these new methods will be demonstrated on several test-problems involving compressible flow at various flow regimes.

References

[1] J. Steinhoff, N. Lynn and L. Wang, "Computation of High Reynolds Number Flows using Vorticity Confinement: I. Formulation", UTSI preprint, UTSI, 2005.

[2] J. Steinhoff, N. Lynn and L. Wang, "Computation of High Reynolds Number Flows using Vorticity Confinement: II. Results", UTSI preprint, UTSI, 2005.

[3] G. Jiang and C.-W. Shu, "Efficient implementation of weighted ENO schemes", *Journal of Computational Physics* 126 (1996) 202–228.

[4] P.K. Sweby, "High resolution schemes using flux-limiters for hyperbolic conservation laws", *SIAM J. Numer. Anal.* 21(5) (1984) 995–1011.

[5] D. Sidilkover, "Towards unification of the Vorticity Confinement and Shock Capturing (TVD and ENO/WENO) methods", *Journal of Computational Physics*, 358(2018), pp. 235–255.

Back

A higher order approximate static condensation method for multi-material diffusion problems

A. Zhiliakov[†], D. Svyatskiy[‡*], M.Olshanskii[†], E.Kikinzon[‡] and M. Shashkov[‡]
[†] University of Houston, Department of Mathematics (alex@math.uh.edu, molshan@math.uh.edu)
[‡] Los Alamos National Laboratory (dasvyat@lanl.gov, kikinzon@lanl.gov, shashkov@lanl.gov)

Keywords: multi-material hydrodynamics; interface reconstruction; heterogeneous diffusion;

ABSTRACT

Past decades evidenced an explosive growth in developing of efficient computational techniques for problems with evolving interfaces. Depending on how the interface is treated numerically, one can distinguish between methods that smear the interface over a strip of finite thickness which should be further resolved by the mesh, like in the phase field approach, and methods that use a sharp interface representation, as in the level-set method. If one applies a sharp representation to handle complex geometries or interfaces undergoing large deformations, it is convenient to allow the interface to cut through the background mesh in an arbitrary way. In turn, this leads to the problem of building accurate and stable approximations for so-called multi-material cells, i.e. the mesh cells intersected by material interfaces. In particular, we are interested in discretizations which are robust with respect to how interfaces intersect the mesh and with respect to the contrast of material properties, e.g. the ratio of physical parameters. This is the setting and the problem we focus in our research.

We introduce a higher order approximate static condensation method (ASC) for the diffusion problem with discontinuous diffusion coefficients. The present method builds upon the algorithm proposed in [1]. The method allows for a general polygonal mesh which is unfitted to the material interfaces. We assume that interface reconstruction is performed using the extended MOF method [2], which provides local single-material meshes with full topological data. The interfaces can be discontinuous across the mesh edges as typical for numerical reconstructions. We apply a mimetic finite difference method to solve local diffusion problems and use P_1 edge(face) elements to couple local problems into the global system. The properties of the resulting algebraic system are discussed. It is demonstrated that the method is second order accurate on smooth solutions and performs well for problems with high contrast in diffusion coefficients. Experiments also show the robustness with respect to position of the interface against the underlying mesh, [3].

References

[1] A. Kikinzon, Y.Kuznetsov, K. Lipnikov and Mikhail Shashkov., "Approximate static condensation algorithm for solving multi-material diffusion problems on meshes non-aligned with material interfaces.", *Journal of Computational Physics*, 347:416436, 2017.

[2] H.T. Ahn and M. Shashkov, "Adaptive moment-of-fluid method", *Journal of Computational PhysicsComputers and Fluids*, 228(8):27922821, 2009.

[3] A. Zhiliakov, D. Svyatskiy, M. Olshanski, A. Kikinzon, and Mikhail Shashkov. "A higher order approximate static condensation method for multi-material diffusion problems", *Journal of Computational Physics*, (submitted)

Back

Mathematical Modelling of Multiphase Flows with Surface Tension and the Finite Element Approximation

P. Sváček †
†

Department of Technical Mathematics, Faculty of Mechanical Engineering, Czech Technical University in Prague, Technick 4, 166 07 Praha 6, Czech Republic (petr.svacek@fs.cvut.cz)

Keywords: finite element method; discontinuous finite element method; free surface; surface tension

ABSTRACT

This paper is interested in the finite element approximation of mathematical models of flow of molten glass during the production process. Glass is in solid-like state at low temperatures, but at sufficiently high temperatures the (molten) glass behaves like a liquid. This phenomena is used partially during the glass production processes. Here, several aspects of float glass and glass blowing/pressing process shall be considered.

First a mathematical model describing the production of the flat glass by the float process is considered as introduced by Pilkington in the 1950s. In such a process the raw material is given to the furnace and melted at 1500 degrees of Celsia. The material is further homogenized by convection to eliminate bubbles. The viscous liquid then flows out of the melting furnace through the part called lip onto the surface of an enclosed bath made of tin. The formed ribbon of glass on the tin bath is then transported through the so called stretching part of the tin bath. This is a complicated multiphisycal phenomena influenced by the heat transfer which includes the radiation, the glass flow interacts with the tin flow in the tin bath and with the surrounding atmosphere. The difficulties to be overcome are the dimensions of the computational domain (the tin bath is about 60 m long, but the produced flat glass height is in the range 1 - 20 mm), the turbulent flow of the tin depending on the structure of the domain (in order to divide hot and cold zones), the heat transfer with radiation (with the large variations throughout the domain). Here, a simplified mathematical model shall be discussed together with the surface tension forces included. The resulting model will be approximated by the finite element method.

Further, the several aspects of modelling of the pressing/blowing glass production process shall be considered. This forming process involves extreme temperatures and large deformations. The process can be modelled as a coupled thermodynamical/mechanical problem with corresponding interaction between glass, air and equipment. In this case the dimensions of the computational domain are much smaller and thus the surface tension treatment is much more important. Here, a simplified 2D mathematical model shall be considered and the realization of the surface tension shall be discussed. The involved numerical approximation method is based on the finite element method, where for the transport of the two phases either the finite element method or the discontinuous finite element method is used. The extended finite element method is used to treat the pressure discontinuity caused by the surface tension. The numerical results will be presented. The comparison of different strategies will be presented and discussed.

Author acknowledges support from the project no. CZ.02.1.01/0.0/0.0/16_019/0000778 of the EU Operational Programme Research, Development and Education.

Back

A Multidimensional Positive Definite Remapping Algorithm for Unstructured Meshes

J. Szmelter[1], M. Gillard[1]

[1]School of Mechanical, Electrical and Manufacturing Engineering, Loughborough University (j.szmelter@lboro.ac.uk, m.gillard@lboro.ac.uk)

Keywords: unstructured mesh, MPDATA, ALE, remapping, conservative interpolation.

ABSTRACT

We report on developments of a second-order, conservative, sign-preserving remapping scheme for Arbitrary Lagrangian-Eulerian (ALE) methods operating on unstructured meshes. The remapping uses concepts of the Multidimensional Positive Definite Advection Transport Algorithm (MPDATA) [1] and is an extension of the earlier work on using MPDATA remapping for Cartesian grids [2,3]. The non-oscillatory infinite gauge option of MPDATA remapping is derived in volume co-ordinates and is based upon a general and compact edge-based data structure, developed for use within an arbitrary finite volume framework. Monotonicity preservation in the remapping is ensured in the spirit of Flux Corrected Transport. The construction of volume coordinates utilises median dual polygonal finite volume cells and in ALE solutions it employs a collocated mesh arrangement of all prognostic variables. The remapping algorithm benefits from the inherent qualities of MPDATA, such as multidimensionality, positive definiteness, and is formally second order accurate.

Theoretical developments are supported by numerical testing; with examples involving idealised cases with prescribed mesh movement for advection of scalars [4] and a single material ALE benchmark for the explosion problem [5]. The numerical investigations include an asymptotic mesh convergence study and comparisons with both MPDATA and Van Leer MUSCL remapping schemes operating on Cartesian meshes. The results demonstrate that the MPDATA gauge option is suitable for providing accurate ALE remapping for unstructured meshes while preserving the multidimensionality and sign of both scalar and vector fields.

References

[1] P.K. Smolarkiewicz and J. Szmelter “MPDATA: An edge-based unstructured-grid formulation”, Journal of Computational Physics, vol: 206, pp:624-649, 2005.

[2] R.N. Hill, J. Szmelter “A multidimensional positive definite remapping algorithm for arbitrary Lagrangian-Eulerian methods”, International Journal for Numerical Methods in Fluids, 65((11-12)), 1338-1350, 2011.

[3] R.N. Hill, J. Szmelter “A multidimensional positive definite remapping for Lagrangian solutions of the Noh problem”, Computers and Fluids, 46((1)), 257-262, 2011.

[4] L.G. Margolin and M. Shashkov “Second order sign preserving remapping on general grids”, Technical Report LA-UR-02-525, Los Alamos National Laboratory.

[5] A. Barlow “An Adaptive Multi-Material Arbitrary Lagrangian Eulerian Algorithm for Computational Shock Hydrodynamics”, Ph.D. Thesis, University of Wales, Swansea, 2002.

Back

A new segregated-explicit staggered scheme for Lagrangian hydrodynamics

N. Therme[†], **P.-H. Maire**[‡]
[†] CEA/CESTA (nicolas.therme@cea.fr)
[‡] CEA/CESTA (pierre-henri.maire@cea.fr)

Keywords: Lagrangian methods, Finite Volumes, Staggered discretizations, Numerical Analysis.

ABSTRACT

In the field of gas dynamics, the design of positivity-preserving numerical methods is of main importance. Indeed, negative pressure and density can lead to nonlinear instabilities and a crash of the code. From this perspective, we propose a new staggered numerical scheme to solve Lagrangian hydrodynamics. It is part of the staggered grid hydrodynamics (SGH), a class of numerical discretization inspired from the initial work of von Neumann and Richtmyer [1]. In SGH, all the thermodynamic variables of the fluid, such as density, pressure and internal energy are cell-centered, whereas the velocity is defined at the nodes of the mesh. The internal energy equation is discretized instead of the total energy equation.

To ensure the local mass, momentum and total energy conservations a particular structure of the discrete div and grad operators, derived from the framework of mimetic methods [2, 3], is used. The dissipation of kinetic energy into internal energy through shock waves is ensured by means of an artificial viscosity added in the discrete momentum equation. Following the method used in [4, 5], the viscosity residual derived from the discrete kinetic energy equation is compensated with a positive source term in the internal energy balance. This makes the scheme consistent with the conservative system of Euler equations. Furthermore the discretization preserves by construction the convex admissible states under a CFL condition. Finally, we illustrate this theory with some numerical results.

References

[1] J. von Neumann and R.D. Richtmyer, "A method for the numerical calculations of hydrodynamical shocks", *IJ. Appl. Phys.*, 21, pp. 232–238, 1950.

[2] L. G. Margolin, M. Shashkov and P. K. Smolarkiewicz, "A discrete operator calculus for finite difference approximations", *Comput. Methods Appl. Mech. Engrg.*, 187, pp. 365–383, 2000.

[3] K. Lipnikov, G. Manzini, M. Shashkov, "Mimetic finite difference method", *J. Comput. Phys.*, 257, pp. 1163–1227, 2014.

[4] R. Herbin, J. C. Latché and T. T. Nguyen, "Consistent segregated staggered schemes with explicit steps for the isentropic and full Euler equations", *ESAIM, Math. Model. Numer. Anal.*, 52, pp. 893–944, 2018.

[5] L. Gastaldo, R. Herbin, J. C. Latché and N. Therme "A MUSCL-type segregated – explicit staggered scheme for the Euler equations.", *Comput. Fluids*, 175, pp. 91–110, 2018.

Back

Numerical Simulation of Compressible Multi-Material Multiphase Flows with High Order Eulerian Methods

Baolin Tian, Yousheng Zhang, Zhiwei He, Li Li, Haifeng Li, Baoqing Meng

Institute of Applied Physics and Computational Mathematics, Beijing 100094

Keywords: Multimaterial flows; Multiphase flows; High order Eulerian methods; MP-PIC.

ABSTRACT

Compressible multi-material flows, multiphase flows and turbulent mixing can be found in many engineering and nature science fields, such as inertia confined fusion (ICF), astrophysics and so on. In this work, a high order multi- physics code, CFD2 (Code of Finite Difference for Compressible Flow Dynamics), was developed for the simulation of compressible multi-material and multiphase flows under extreme conditions. The code solves the equations of multidimensional hydrodynamics with high order accuracy in space and time, including a series of high order difference schemes, such as WENO, MP, GVC and WCNS schemes based on flux splitting techniques. The CFD2 code is implemented on non-uniform mesh and can simulate flow problems with billion mesh cells on thousands CPU cores with MPI parallelization. Recently, a multiphase particle-in-cell method is presented for compressible dense particle flows and implemented in CFD2 code. Overall, the code can simulate multi-physics flow problems, such as detonation, radiation, particle flows and so on. Some recent progress on high order schemes has been integrated into the code in order to prevent the non-physical oscillations near material interfaces. A series of typical model problems have been simulated to validate the code. Moreover, turbulent mixing induced by RM and RT instability was simulated systematically to study the turbulent mixing mechanism.

Back

Near-wall Domain Decomposition for Essentially Unsteady Turbulent Flows

S. Utyuzhnikov[†] [‡], A. Chikitkin[‡], M. Petrov[‡] and V. Titarev[‡*]
[†] Department of Mechanical, Aerospace and Civil Engineering, University of Manchester
(s.utyuzhnikov@manchester.ac.uk)
[‡] Moscow Institute of Physics and Technology, Dolgoprudny
(chikitkin.av@mipt.ru, petrov.mn@mipt.ru)
[*] Federal Research Center "Computer Science and Control" of RAS, Moscow,
(titarev.va@mipt.ru)

Keywords: non-overlapping domain decomposition; interface boundary conditions; near-wall turbulent flows; unsteady flows; RANS models; LES.

ABSTRACT

The key problem of near-wall turbulence modeling is a correct resolution of a thin area near the wall, which includes a laminar sublayer. Sufficiently enough prediction of the turbulent layer structure usually takes most computational time. The problem even becomes worse in the case of essentially unsteady flows. To avoid time-consuming computations, a new approach based on a non-overlapping domain decomposition was developed in [2]. In this approach the entire computational domain is split into the inner region near the wall and the outer region. At the interface boundary a Robin boundary condition is set for the outer region, which is achieved via transfer of the boundary condition from the wall [1], [3]. In the case of unsteady flows the problem becomes much more complicated. As shown in [4] for a model equation, the interface boundary condition must contain a memory term which is nonlocal in time. The memory term was derived in [5] for the Navier-Stokes equations but not implemented. In the current paper, it is shown that the memory term must depend on the unsteadiness of not only the solution at the interface boundary but also the driving force in the inner region. For the first time, this approach is applied the Reynolds-averaged Navier-Stokes equations for compressible flows.

References

[1] S. Utyuzhnikov, "The method of boundary condition transfer in application to modeling near-wall turbulent flows", *Computers & Fluids*, 35 (10), pp. 1193–1204, 2006.

[2] S. Utyuzhnikov, "Domain decomposition for near-wall turbulent flows", *Computers & Fluids*, 38 (9), pp. 1710–1717, 2009.

[3] S. Utyuzhnikov, "Interface boundary conditions in near-wall turbulence modeling", *Computers & Fluids*, 68, pp. 186–191, 2012.

[4] S. Utyuzhnikov, "Towards development of unsteady near-wall interface boundary conditions for turbulence modelling", *Computer Physics Communications*, 185 (11), pp. 2879–2884, 2014.

[5] S. Utyuzhnikov, M. Petrov, A. Chikitkin, V. Titarev, On Extension of Near-Wall Non-overlapping Domain Decomposition to Essentially Unsteady Turbulent Flows, Smart Modeling for Engineering Systems Proceedings of the Conference 50 Years of the Development of Grid-Characteristic Method, Editors: Petrov, I.B. et al. Springer, 199-209, 2019.

The Authors acknowledge the support by the Russian Science Foundation (Project N 18-19-00098).

Back

Residual Distribution Scheme for Multi-Material Lagrangian Hydrodynamics

S. Tokareva[†], R. Abgrall[‡], K. Lipnikov[†] and N. Morgan[*]

[†] Applied Mathematics and Plasma Physics Group (T-5), Los Alamos National Laboratory
(tokareva@lanl.gov, lipnikov@lanl.gov)

[‡] Institute of Mathematics, University of Zurich (remi.abgrall@math.uzh.ch)

[*] Methods and Algorithms Group (XCP-4), Los Alamos National Laboratory
(nmorgan@lanl.gov)

Keywords: residual distribution; finite elements; matrix-free methods; shock hydrodynamics; multimaterial hydrodynamics; Lagrangian methods

ABSTRACT

We will present the high-order multimaterial Staggered Grid Residual Distribution (SGH RD) scheme for Lagrangian hydrodynamics. The SGH RD scheme is based on the staggered finite element discretization which uses continuous polynomial approximation of the kinematic variables and cell-centered polynomial representation of the thermodynamic variables. Our finite element RD scheme needs the inversion of an auxiliary diagonal matrix instead of the full mass matrix, i.e. it is an essentially a matrix-free method. It can be shown that for the Lagrangian formulation written in non-conservative form, our scheme ensures the exact conservation of the total energy. We shall also discuss stabilization techniques for the SGH RD schemes allowing to improve the robustness of the method at high orders and at the same time minimize the dissipation of the numerical solution. In particular, we will show how the excessive artificial viscosity affects the resolution of vorticity and demonstrate that using MARS artificial viscosity improves the accuracy of the numerical solution. Thanks to the generic formulation of the staggered grid residual distribution scheme, it can be applied to both single- and multimaterial and multiphase models. Finally, we shall demonstrate computational results obtained with the proposed residual distribution scheme for several challenging test problems involving strong shocks and vortical flows.

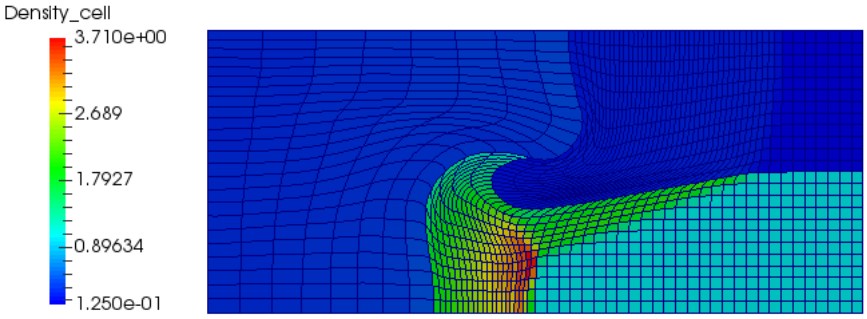


Figure 1: Triple point problem: density computation using MARS viscosity.

Research presented in this talk is supported by the Laboratory Directed Research and Development program of Los Alamos National Laboratory under project number 20170051DR. The unlimited public release number is LA-UR-19-21167.

Back

Invariant domain preserving methods and convex limiting: towards an extension to MhD

Ignacio Tomas

CCR, Sandia National Laboratories

ABSTRACT

The first step in the development of a high-order scheme is the development of a robust first-order method (ideally) endowed with a sound theoretical basis. With that goal in mind, we develop a general framework of first-order fully-discrete numerical schemes that are guaranteed to preserve every convex invariant of the hyperbolic system and satisfy every entropy inequality. This framework is not tied to any particular space discretization technique (e.g. finite volumes, continuous or discontinuous finite elements) and it is of general applicability: it works in any mesh, in any space dimension, and uses neither exact nor approximate Riemann solvers. We also lay out the main steps taken in the direction of MhD, which requires taking into account the involution constraint and/or jump conditions required to have a well defined projected Riemann problem. We then proceed to present a new flux-limiting (hybridization) technique. This technique does not preserve or enforce bounds on conserved variables, but rather bounds on quasiconvex/concave functionals of the conserved variables. This flux-limiting technique, is suitable to enforce/preserve convex constraints of the numerical solution which are natural of hyperbolic systems. Examples of such bounds are positivity of the internal energy and minimum principle of the specific entropy in the context of Euler's equations. We have coined this technique "convex limiting".

Back

Adaptation of High-Order Curved Meshes in ALE Hydrodynamics

Veselin Dobrev[†], **Patrick Knupp**[‡], **Tzanio Kolev**[†], **Robert Rieben**[†] **and Vladimir Tomov**[†*]
[†] Lawrence Livermore National Laboratory (dobrev1@llnl.gov, kolev11@llnl.gov, rieben1@llnl.gov, tomov2@llnl.gov)
[‡] Dihedral LLC (zg37rd@gmail.com)

Keywords: mesh optimization; mesh adaptation; curved meshes; ALE methods; shock hydrodynamics; multi-material hydrodynamics;

ABSTRACT

We present a framework for adaptive optimization of high-order curved meshes in the context of multi-material ALE compressible shock hydrodynamics. The optimization process is driven by information that is provided by the simulation in which the optimized mesh is being used, e.g., shock positions, material regions, amount of Lagrangian motion (see Figure 1), known error estimates, etc. These simulation features are usually given by discrete representations, for instance, as a finite element function on the Lagrangian mesh. This is a critical step for the practical applicability of the algorithms we propose and distinguishes us from approaches that strictly require analytical information. This work extends the methods from [1] by including information about discrete simulation features in the method's target construction step, which is used to specify the desired mesh characteristics. This extension requires more involved derivative calculations, appropriate nonlinear solvers, and reconstruction of discrete quantities on intermediate (produced during the optimization process) meshes. The benefits of the proposed methods are illustrated on various examples from the high-order ALE application BLAST [2].

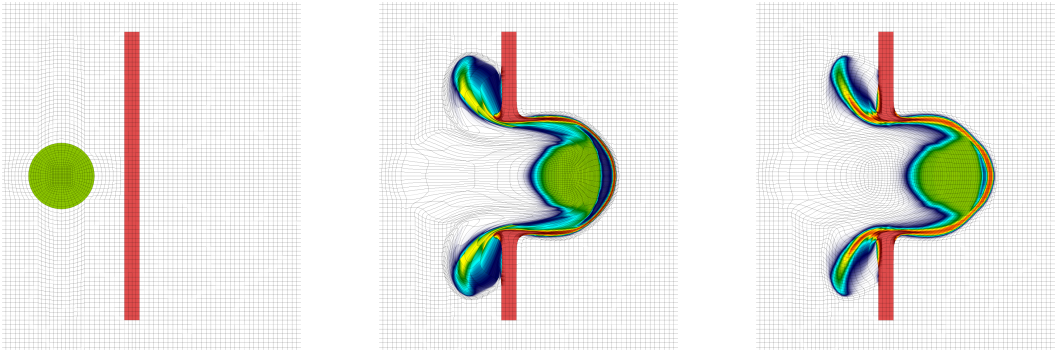


Figure 1: Two strategies for motion-informed mesh optimization in an ALE simulation of an impact.

References

[1] V. Dobrev, P. Knupp, Tz. Kolev, K. Mittal and V. Tomov, *The Target-Matrix Optimization Paradigm for High-Order Meshes*, SIAM J. Sci. Comp., Vol 41(1), pp. B50-B68, (2019).

[2] R. Anderson, V. Dobrev, Tz. Kolev, R. Rieben and V. Tomov, *High-Order Multi-Material ALE Hydrodynamics*, SIAM J. Sci. Comp., Vol. 40(1), pp. B32-B58, (2018).

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344 (LLNL-ABS-768321)

Back

On flux splitting schemes for a class of hyperbolic systems

Eleuterio Toro
Laboratory of Applied Mathematics, DICAM, University of Trento, Italy
(eleuterio.toro@unitn.it)

ABSTRACT

This talk begins with a brief review of flux vector splitting schemes followed by the presentation of a novel splitting scheme for a class of hyperbolic systems [1] which, compared to existing splitting methods, has some distinctive advantages, such as exact recognition of stationary isolated contact waves, simplicity, robustness and efficiency. Two features of the new splitting are: complete separation of pressure from advection terms and identification of a reduced pressure system that furnishes all required information for constructing the full numerical flux in a simple manner. The first order method was originally proposed for the 1D Euler equations for ideal gases in [1], while in [2] the scheme is extended to the 3D Euler equations with general equation of state and high- order of accuracy in both space and time, on unstructured meshes, using the ADER approach. In [3] the scheme is applied to the MHD equations, while in [4] the new splitting is applied to the compressible two-phase flow equations. In this talk I review the main features of the scheme and show computational results for a carefully selected suit of test problems.

References

[1] E F Toro and M E Vázquez-Cendón., "Flux splitting schemes for the Euler equations", *Computers and Fluids*, Vol. 70, Pages 1-12, 2012.

[2] Eleuterio F. Toro, Cristobal Castro and Bok Jick Lee, "A novel numerical flux for the 3D Euler equations with general equation of state", *Journal of Computational Physics*, Vol. 303, pages 80-94, 2015.

[3] Dinshaw S. Balsara, Gino Montecinos, and Eleuterio F. Toro. "Exploring Various Flux Vector Splittings for the Magnetohydrodynamic System", *Journal of Computational Physics*, Vol. 311, pages 1-21, 2016.

[4] Svetlana Tokareva and Eleuterio F. Toro "A flux vector splitting method for the Baer-Nunziato equations of compressible two-phase flow", *Journal of Computational Physics*, Vol. 323, pp 45-74, 2016.

Back

Efficient Full Non-overlapping Domain Decomposition for New-wall Turbulent Flows

S. Utyuzhnikov[†] [‡], M. Petrov[‡], A. Chikitkin[‡] and V. Titarev[‡*]
[†] Department of Mechanical, Aerospace and Civil Engineering, University of Manchester
(s.utyuzhnikov@manchester.ac.uk)
[‡] Moscow Institute of Physics and Technology, Dolgoprudny
(petrov.mn@mipt.ru, chikitkin.av@mipt.ru)
[*] Federal Research Center "Computer Science and Control" of RAS, Moscow,
(titarev.va@mipt.ru)

Keywords: non-overlapping domain decomposition; near-wall turbulent flows; preconditioning; interface boundary conditions; RANS models.

ABSTRACT

The near-wall domain decomposition (NDD) approach proposed in [1] and developed in [2], [3] and other papers proved to be very efficient for modeling turbulent flows. It leads to a non-overlapping domain decomposition with a Robin-to-Dirichlet map. For the outer region interface boundary conditions of Robin type equivalently replace the boundary conditions at the wall and simplified governing equations in the inner region. In contrast, to the widely used approach based on wall functions, it does not contain free parameters, mesh independent and can be applied to low-Reynolds number turbulence models. Since in the near-wall region it exploits the thin-layer model, the approach effectively represents a trade-off between the accuracy and computational time. As shown in [3], it can reduce the computational time by one order of magnitude while retaining a practically high accuracy. Despite its clear advantages, the approach can suffer significant problems if the wall is not smooth enough or in the areas of laminar-turbulent transition where the assumptions of the thin-layer model are not valid. In the current paper, the technique is extended to a full domain decomposition applied to the original Reynolds-averaged Navier-Stokes equations without simplifications near the wall. A Robin-Dirichlet map is realized in such a way that the approximate NDD is effectively used to invert a preconditioning operator. The approach is applied to the Spalart-Almaras turbulence model for compressible flows implemented in code "FlowModellium" [4].

References

[1] S. Utyuzhnikov, "Domain decomposition for near-wall turbulent flows", *Computers & Fluids*, 38 (9), pp. 1710–1717, 2009.

[2] S. Utyuzhnikov, "Interface boundary conditions in near-wall turbulence modeling", *Computers & Fluids*, 68, pp. 186–191, 2012.

[3] A. Jones, S.V. Utyuzhnikov, "Application of a near-wall domain decomposition method to turbulent flows with heat transfer", *Computers & Fluids*, 119, pp. 87–100, 2015.

[4] M.N. Petrov, A.A. Tambova, V.A. Titarev, S.V. Utyuzhnikov, A.V. Chikitkin, "FlowModellium software package for calculating high-speed flows of compressible fluid", *Computational Mathematics and Mathematical Physics*, 58 (11), pp. 1865–1886, 2018.

The Authors acknowledge the support by the Russian Science Foundation (Project N 18-19-00098).

Back

Modeling Shock Wave Speed in MARBLE Foam

D. Woods[†*], B. Haines[†], Y. Kim[†], P. Kozlowski[†], T. Murphy, B. Albright[†], C. Di Stefano[†], T. Day[†], T. Cardenas[†], D. Barnak[†], R. Olson[†], M. Gunderson[†], M. Douglas[†]

[†]Los Alamos National Laboratory

[*]Presenter (dwoods@lanl.gov)

Keywords: shock hydrodynamics; multi-material hydrodynamics; Eulerian methods.

ABSTRACT

Understanding material mixing is of particular importance to achieving inertial confinement fusion (ICF) ignition. The amount of contaminant mixing with fuel reactant impacts the fusion yield as do heterogeneities generated from capsule material plunging into the hot spot. The MARBLE campaign [1] at Los Alamos National Laboratory (LANL) is a series of separated reactant ICF experiments employing plastic foams with engineered macro-pores designed to investigate heterogeneous material mixing during spherical implosions. The initial conditions are varied by controlling the foam pore sizes. Accurately modeling the dynamics of these foams is challenging for radiation-hydrodynamics codes due to the complex geometry that stresses multi-material sub-grid modeling of equation of state (EOS), opacity, thermal conduction, and thermonucler burn.

We discuss the results of companion MARBLE Void Collapse experiments performed on the OMEGA laser at the Laboratory for Laser Energetics (LLE). These experiments were designed to validate the radiation-hydrodynamics modeling of shock propagation through foams with macropores. In particular, we will discuss experiments that stress mixed-material EOS modeling. Foam-filled shock tubes were directly-driven by lasers on one end and x-ray radiographs were generated at various times, enabling the direct measurement of shock speed, shock front shape, and shock/interface dynamics, which is not possible in a spherically convergent geometry. We employed xRAGE [2, 3], a LANL Eulerian radiation-hydrodynamics code, to perform the simulations and study the material effects. The pore sizes were varied to investigate the effects on shock speed. Additionally, the effect of neopentane fill gas on shock speed was investigated. Our simulations are in good agreement with the experimental shock wave speeds. We will present the conditions necessary for accurate simulation of these experiments and discuss modeling implications.

References

[1] T. J. Murphy et al. “Progress in the development of the MARBLE platform for studying thermonuclear burn in the presence of heterogeneous mix on OMEGA and the National Ignition Facility.”, *J. Phys.: Conf. Ser.*, 717, 012072, 2016.

[2] M. Gittings et al. “The rage radiation-hydrodynamic code”, *Computational Science & Discovery*, 1(1), 015005, 2008.

[3] B. M. Haines et al. “High-resolution modeling of indirectly driven high-convergence layered inertial confinement fusion capsule implosions”, *Physics of Plasmas*, 24, 052701, 2017.

This work was supported by the US Department of Energy through the Los Alamos National Laboratory. Los Alamos National Laboratory is operated by Triad National Security, LLC, for the National Nuclear Security Administration of U.S. Department of Energy (Contract No. 89233218CNA000001). Document number LA-UR-19-21734.

Back

A robust and interface preserving formulation for compressible multiphase flows

F.Xiao[1] and X.Deng[1,2]
[1]Department of Mechanical Engineering, Tokyo Institute of Technology, Japan
(xiao.f.aa@m.titech.ac.jp)
[2]M2P2, Aix-Marseille Universite, France

Keywords: Compressible interfacial multiphase flow, THINC, BVD algorithm, high-fidelity interface capturing

ABSTRACT

Compressible interfacial multiphase flows involve strong discontinuous flow structures, like shocks and material interfaces. Numerical simulation of such flows brings a big challenge to computational fluid dynamics. An acceptable numerical method to solve this sort of problems must be able to at least (1) suppress spurious oscillation in the presence of discontinuities, and (2) resolve accurately the moving interfaces that separate different fluids. The currently available high-resolution finite volume schemes, which combine polynomial-based reconstructions and nonlinear limiting projections to compromise between spurious oscillation and numerical dissipation, can hardly provide adequate solution quality for either smooth or discontinuous solution due to excessive numerical dissipation, which tends to smear out the moving interface and is thus fatal in simulating compressible interfacial multiphase flows.
In this talk, we will present a novel numerical formulation, based on the Boundary Variation Diminishing (BVD) principle, to capture discontinuous flow structures with superior solution quality. The BVD principle minimizes the jumps of the reconstructed physical variables at cell boundaries, and thus effectively reduces the dissipation errors. With the THINC function as one of the BVD-admissible reconstruction functions, we have developed a scheme of great practical significance for compressible interfacial multiphase flows. As shown in Figure 1, the moving interface is accurately resolved with compact thickness, and all flow structures are reproduced with greatly improved solution quality compared to other existing methods [1,2].

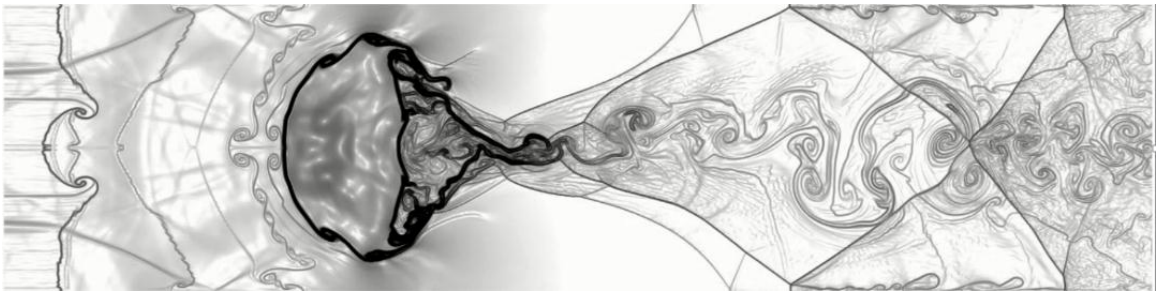


Figure 1: Schlieren image of density field of the shock-droplet interaction benchmark test.

References

[1] R.K. Shukla, C. Pantano, J.B. Freund, An interface capturing method for the simulation of multi-phase compressible flows, J. Comput. Phys. 229, 7411–7439 (2010).

[2] X.Deng, S.Inaba, B.Xie, K.M.Shyue, F.Xiao, High fidelity discontinuity-resolving reconstruction for compressible multiphase flows with moving interfaces, J. Comput. Phys. 371, 945–966 (2018).

Back

An Embedded-Boundary/ALE Framework for Multi-Material Flow Computations

X. Zeng[1*], K. Li[2], and G. Scovazzi[2,3]
[1]Department of Mathematical Sciences, Computational Science Program
University of Texas at El Paso, El Paso, TX, USA
[2]Department of Civil and Environmental Engineering, Duke University, Durham, NC, USA
[3]Department of Mechanical Engineering and Material Science, Duke University, Durham, NC, USA

Keywords: ALE; embedded boundary method; finite element method; shock hydrodynamics; multi-material flows; fluids-structure interaction.

ABSTRACT

We present an embedded boundary method (EBM) in the arbitrary Lagrangian-Eulerian (ALE) computational fluid grids for multi-material flow computations. Such an EBM-ALE procedure proves to be advantageous in numerical simulations of the interaction between multiple fluids and structures, and multi-material shock hydrodynamics. In both scenarios, mesh motion for fluids is desired to either follow the structural motion (fluids/structure interaction) or to enhance the resolution near shock fronts automatically (shock hydrodynamics). And the proposed methodology allows us to capture the material-interface between adjacent immiscible fluids on the morphing grid implicitly, hence capturing large interface motions and topological changes.

The methodology is first described using the two-fluid scenario (two fluid materials occupy the same computational domain and share the same mesh), where the method is characterized by the following features: (1) a level set method to capture the material interface implicitly as the zero contour of the level set function, (2) a ghost value procedure to enforce the transmission condition at the embedded material interface and to handle phase changes, and (3) any preferred explicit flow solver for a single fluid on ALE grids. In this talk, we consider two different procedures to define the ghost values, namely constant extrapolation and multi-material Riemann solutions – the former is robust and easy to implement for almost all equations of state, whereas the latter produces more physical solutions but requires more computation effort. Furthermore, the single-fluid solver we choose to demonstrate the methodology is a monolithic finite element method for ALE flow computations of compressible inviscid fluids; whereas in principal any explicit ALE flow solver can be adopted.

Several theoretical aspects of the methodology will be discussed, which includes: comparison between the two ghost value construction procedures using benchmark multi-phase flow problems, extension from first-order ghost values to second-order ones via a positivity-preserving extrapolation approach, and quantitative assessment of the conservation properties. Finally, we discuss extensions of EBM-ALE to more than two fluid materials using the projection level set method and to a structure-liquid-gas interaction application by coupling the liquid-gas mixture with the structure via a partitioned coupling procedure.

Back

Dual Domain Material Point Method and Multivelocity Formulation

Applied to Sweeping Wave Impact and Plastic Spallation

Duan Z. Zhang and Christopher C. Long

T-3 Fluid Dynamics and Solid Mechanics Group, Theoretical Division,
Los Alamos National Laboratory,
Los Alamos, NM 87545
dzhang@lanl.gov

Dual domain material point (DDMP) method [1] is an advanced version of the material point method capable of simulating large deformation of history-dependent materials. To consider the fluid-solid interaction, in this work we combine the DDMP method with the multivelocity formulation to study sweeping detonation wave impact on a tantalum plate. The explosive, its reaction product gas, and the surrounding air are described using the Eulerian method by a single velocity field, which is computed using the finite volume method on the mesh. The Jones-Wilkins-Lee (JWL) equation of state is used to model the reaction product gas.

The tantalum plate is modeled using the tensile plasticity (TEPLA) model [2-3] and is described using both the Lagrangian method by the material points and the Eulerian method on the mesh nodes. This velocity field is solved using the DDMP method to track the history-dependent large plastic deformation, pore growth, and material failure. For numerical stability, the plastic pore growth is solved implicitly. The interaction between the reaction product gas and the solid is modeled by a drag model between the phases. Because of the use of the multivelocity formation and the material point method, no special treatment for the gas-solid interfaces is needed.

Our numerical results are compared with experiment [4]. The comparison suggests that the history-dependent nature of the plasticity is well-represented by the DDMP method. Before strain softening of the material, the numerical results compare well with the experiment and converge upon mesh refinements. However, the calculated spall velocity is found to be mesh dependent, indicating a need for a strain softening model for the metal.

References

[1] D. Z. Zhang, X. Ma, P. T. Giguere, Material point method enhanced by modified gradient of shape function, Journal of Computational Physics 230 (2011) 6379–6398.

[2] F. L. Addessio, J. N. Johnson, Rate-dependent ductile failure model, Journal of Applied Physics 74 (1993) 1640–1648.

[3] Q. H. Zuo, J. R. Rice, An implicit algorithm for a rate-dependent ductile failure model, Journal of Applied Physics 104 (2008) 083526.

[4] Gray, G.T., Hull, L.M., Livescu, V., Faulkner, J.R., Briggs, M.E., Cerreta, E.K., Influence of sweeping detonation-wave loading on shock hardening and damage evolution during spallation loading in tantalum, EPJ Web of Conferences 26 (2012) 02004.

This work was performed under the auspices of the United States Department of Energy. The financial support for this work is provided by the ASC Program, and the Next Generation Code (NGC) project, and the Joint DOD/DOE Munitions Technology Development Program.

Back

A Positivity-Preserving Finite Volume Scheme for Diffusion Equations on Polyhedral Meshes and its Application in Electrostatic Particle-In-Cell Simulation

Qiang Zhao, Guangwei Yuan and Zupeng Jia

Institute of Applied Physics and Computational Mathematics, Beijing 100094, China
(zhaoq@iapcm.ac.cn)

Keywords: polyhedral meshes, positivity-preserving scheme, diffusion equations, electrostatic particle-in-cell.

ABSTRACT

In this paper, we give a new cell-centered finite volume scheme for diffusion equation on polyhedral meshes and prove it is positivity-preserving. Based on harmonic average point, we design a new locally explicit weighted method to calculate intermediate unknowns, including the vertex and face unknowns. Our scheme is applicable for distorted meshes with cell-faces being non-plane, and suitable for diffusion problems with discontinuous coefficient. Numerical examples verify the convergence and positivity of numerical solution of our scheme. As an application, electric potential and fields are derived from the derived finite volume scheme in electrostatic particle-in-cell simulation. The problem of current collection by cylindrical Langmuir probes in collisionless plasmas is used for validation.

References

[1] A Shuai Wang, Xudeng Hang, Guangwei Yuan, “A positivity-preserving pyramid scheme for anisotropic diffusion problems on general hexahedral meshes with nonplanar cell faces”, Journal of Computtational Physics, 371,pp.152-167, 2018.

[2] J.Droniou, C.L.Potier, “Construction and convergence study of schemes preserving the elliptic local maximum principle”, SIAM J.Numer. Anal. 49(2):459-490, 2011

[3] L.Chang, G.Yuan, “An efficient and accurate reconstruction algorithm for the formulation of cell-centered diffusion schemes”. J.Comput. Phys., 231(20):6935-6952, 2012.

[4] Nikolaos A. Gatsonis, Anton Spirkin, “A three-dimensional electrostatic particle-in-cell methodology on unstructured Delaunay-Voronoi grids”, J. Comput. Phys., 228:3742-3761, 2009.

Back

Abstracts of poster presentations

An Arbitrary Lagrangian-Eulerian DG Method on Triangular Grids

Jayesh Badwaik[†]
[†] Institut für Mathematik, Universität Würzburg (badwaik.jayesh@gmail.com)

Keywords: Conservation Laws; ALE methods; DG methods; Euler Equations;

ABSTRACT

We present a single step, explicit in time discontinuous Galerkin scheme on two dimensional simplex grids using the arbitrary Lagrangian-Eulerian approach for conservation laws in two dimensions. The grid is moved with a velocity which is close to the local fluid velocity. This considerably reduces the numerical dissipation in the Riemann solvers and provides automatic mesh adaptation. The time integration is performed using ADER-type approach where a local predictor is first computed in each cell following by the actual update of solution to the next time level. Such an approach is computationally more efficient than Runge-Kutta schemes. In such an approach, the quality of the mesh can deteriorate over time, and we use a combination of mesh velocity correction algorithms and local mesh repair algorithms to maintain the quality of the mesh. We show that we are able to maintain good mesh quality for long periods of simulation. The local nature of the algorithms allow the method to be embarrassingly parallel.

For discontinuous solution, standard TVD/TVB limiters are implemented which perform much better on moving grids than static grids. If we use a numerical flux which resolves stationary contact waves, then we capture moving contact waves exactly. Second, third and fourth order methods are developed and shown to give optimal convergence rates on a smooth test case. Several other test cases are provided to demonstrate the accuracy of the proposed scheme for advection and Euler equations in two dimensions. The method can be extended in a very similar way to the third dimension.

The work has been done jointly with Praveen Chandrashekar and Christian Klingenberg.

Investigating the effects of hot electron generation from laser-plasma interactions

K. Bennett[†]**, T. Goffrey**[†] **and T. D. Arber**[†*]
[†] Centre for Fusion Space and Astrophysics, University of Warwick
(k.bennett@warwick.ac.uk)

Keywords: shock hydrodynamics; multi-material hydrodynamics; ALE methods; Laser-plasmer interactions;

ABSTRACT

Due to the required laser intensities and plasma conditions in laser-fusion experiments, kinetic laser plasma interaction instabilities (LPI) occur in all such schemes. These LPIs alter the temporospatial characteristics of laser absorption and create populations of energetic (hot) electrons. Measuring the characteristics of these hot-electrons is of critical importance as they determine whether the fusion fuel is preheated – potentially precluding ignition. To study the effects of these hot electron populations in a range of plasma conditions, we have implemented a laser ray-tracing model into the Odin code, a radiation-hydrodynamics ALE code developed at the University of Warwick. We have also added a model for the generation and tracking of hot electron populations due to LPIs. We present early results from this model and comparisons with an experimental campaign carried out on the Omega laser facility.

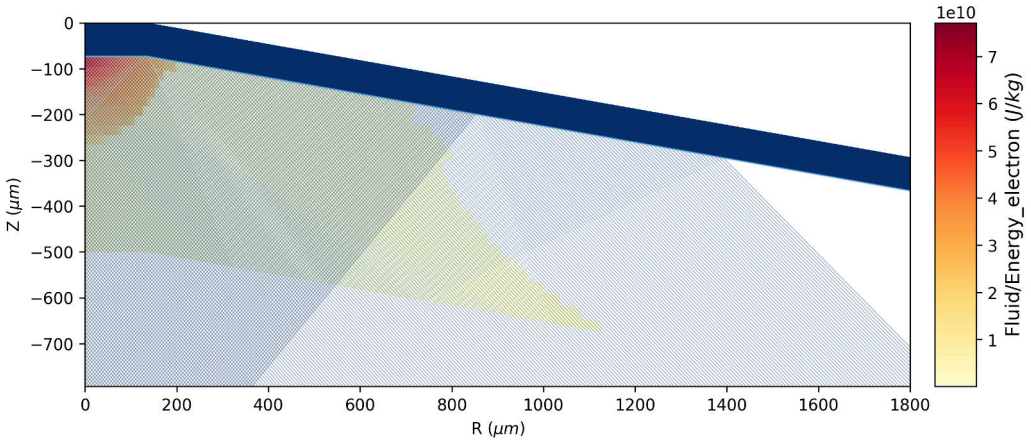


Figure 1: Electron energy of ablated plasma due to laser rays incident on a conical target.

Back

3D cell-centered Lagrangian second order scheme for the numerical modeling of hyperelasticity system

J. Breil[†*], **G. Georges**[‡] **and P.-H. Maire**[†]
[†] CEA CESTA, 15 Avenue des Sablières, CS 60001, 33116 Le Barp Cedex, France
(jerome.breil@cea.fr)
[‡] Michelin, 63040, Clermont-Ferrand, France

Keywords: Lagrangian methods; Hyperelasticity; Cell-centered scheme; Generalized Riemann Problem; Multi-dimensional.

ABSTRACT

The work proposed here is the development of the 3D cell-centered Finite Volume EUCCLHYD [1] scheme applied to the hyperelasticity system. This study is the 3D extension of the work [2] with the difference that we are working with the left Cauchy-Green tensor B instead of the deformation gradient F which enables to work in a fully updated Lagrangian formalism. The second order extension of this scheme is proposed using a MUSCL procedure combined with a GRP approach. The limitation of the tensor fields is done in a component-wise manner. Moreover, the complete GRP (Generalized Riemann Problem) procedure is proposed in the case of Neo-Hookean compressible solids. The scheme is validated on several test cases introducing small as well as large deformations. In particular, good results are found on the non trivial problems of oscillating and twisting beams (Figure 1).

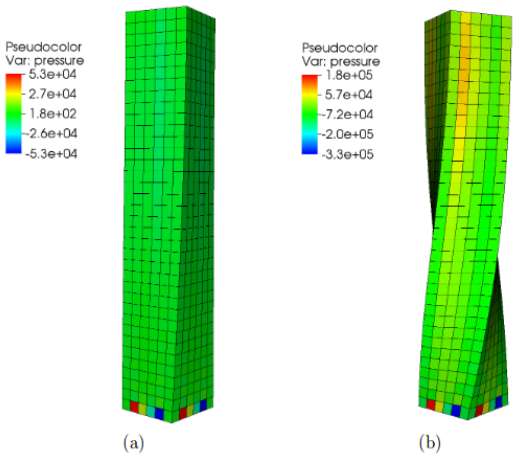


Figure 1: Twisting column - First (a) and Second order (b) solutions - Beam shape and pressure field at time t=0.1s on a ($6 \times 6 \times 36$) cells meshes.

References

[1] J. Breil, G. Georges and P.-H. Maire, "Second-order extension in space and time for a 3D cell-centered Lagrangian scheme", *Computers & Mathematics with Applications*, 2018.

[2] G. Kluth and B. Després, "Discretization of hyperelasticity on unstructured mesh with a cell-centered lagrangian scheme", *Journal of Computational Physics*, 229, pp. 9092–9118, 2010.

Back

Recovering discrete Rankine-Hugoniot conditions on uneven meshes with anti-diffusive schemes: application to the 1D compressible Euler equations

R. Chauvin[†], S. Guisset[†] and A. Llor[†]
[†] CEA, DIF F-91297 Arpajon, France
(remi.chauvin@cea.fr, sebstien.guisset@cea.fr, antoine.llor@cea.fr)

Keywords: Progressive meshes; shock waves; Godunov schemes; hydrodynamics; anti-diffusive methods

ABSTRACT

It is shown, in a simple one dimensional setting, that standard Godunov-type solvers and classical staggered schemes completely fail in capturing isolated shock waves on uneven meshes. This is due to the fact that the numerical viscosity of such schemes varies with the cell size leading to a loss of the discrete Rankine-Hugoniot conditions. In order to overcome these issue, several anti-diffusive numerical schemes are presented and compared. Such schemes are expected to recover the Rankine-Hugoniot condition since no numerical diffusion is involved. Numerical results are presented confirming that hybrid Godunov-anti-diffusive strategies can be very effective when studying the propagation of shock waves on meshes with geometrically varying 1D meshes.

Back

Portage+Tangram: Update on Scalable Multi-Material Remapping

G. Dilts[†], R. Garimella[†], A. Herring[†], E. Kikinzon[†], C. Malone[†], N. Ray[†], M. Shashkov[†], D. Shevitz[†] and J. Velechovsky[†]
[†] Los Alamos National Laboratory
{gad,rao,angelah,kikinzon,cmalone,nray,shashkov,shevitz,velechovsky}@lanl.gov

Keywords: multi-material remapping; interface reconstruction; ALE methods; mesh-free methods.

ABSTRACT

We will present recent updates to the flexible, scalable and customizable multi-material remapping package called *Portage* and its companion interface reconstruction package called *Tangram*.

Portage is a hybrid parallel remapping framework that can be used in a wide range of applications requiring transfer of field data between two simulations, two physics packages or two discretizations (meshes or particle swarms). Applications can use the supplied remapping drivers as-is or they may choose to write a completely customized driver uniquely suited to their application. Like *Portage*, *Tangram* is a hybrid parallel, flexible interface reconstruction package that can be easily used in multi-material applications. *Tangram* has in-built VOF and MOF [1] interface reconstruction methods in 2- and 3-dimensions but can also be extended with other methods. Both *Portage* and *Tangram* can be interfaced easily with client applications through a lightweight interface to the client's mesh and state data.

Previously, we presented results of single-material mesh-mesh remapping and particle-particle remapping. In this update we present several important updates to remapping capabilities in *Portage* and interface reconstruction capabilities in *Tangram*. In particular we discuss and present results for the following topics:

- VOF and MOF reconstruction in 2- and 3-dimensions
- Distributed multi-material remapping [2]
- Repair of fields when not all of the source mesh is covered by the target mesh and vice-versa
- Remapping of fields between subdomains of each mesh so that fields from one subdomain in the mesh do not "bleed" into an adjacent domain with disparate properties

We will also describe how *Portage* and *Tangram* are being successfully used in applications.

References

[1] Dyadechko, V. and Shashkov, M. "Reconstruction of multi-material interfaces from moment data," *J. of Comp. Physics*, v 227, n 11, pp. 5361–5384, 2008.

[2] Kucharik, M. and Shashkov, M. "One-Step hybrid remapping algorithm for multi-material arbitrary Lagrangian Eulerian Methods," *J. of Comp. Physics*, v 231, n 7, pp. 2851–2864, 2012.

Back

Non-diffusive radiation transport and non-ideal Magnetohydrodynamics on arbitrary structured meshes.

T. Goffrey[†*], **K. Bennett**[†], **K. McGlinchey**[‡] **and T. D. Arber** [†]

[†] Centre for Fusion Space and Astrophysics, University of Warwick
(t.goffrey.1@warwick.ac.uk)

[‡] Department of Physics, Imperial College London

Keywords: multi-material hydrodynamics; Lagrangian methods; ALE methods; Radiation Transport; Magnetohydrodynamics

ABSTRACT

Odin is a multi-material, structured mesh, arbitrary Lagrangian Eulerian code developed by the University of Warwick and collaborators over the last decade. The aim of the Odin project is to provide the UK laser-plasma community with a dedicated independent modelling capability to design laser-fusion experiments. Physics packages include diffusive and non-diffusive radiation transport, non-ideal MHD (resistive diffusion, Nernst advection, Biermann battery), isotropic and anisotropic thermal conduction and laser ray tracing. I will present an overview of the implementation and benchmarking of the core radiation-magnetohydrodynamics algorithm, focusing on methodology for non-diffusive transport and non-ideal MHD terms on arbitrary structured meshes.

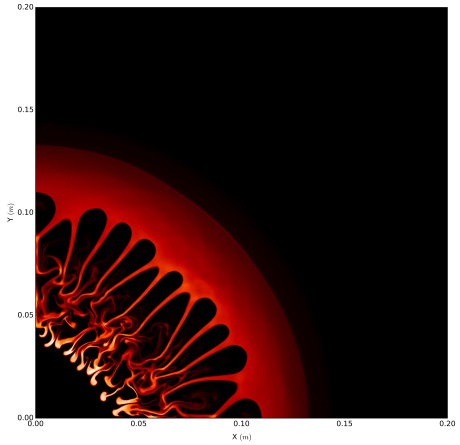


Figure 1: Odin modelling the stagnation phase of a dense imploding shell. The inner interface had a 5% sinusoidal perturbation applied.

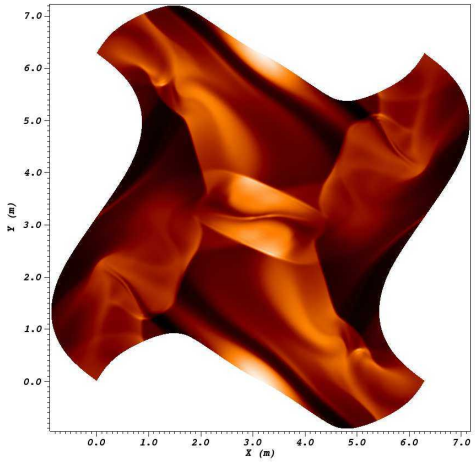


Figure 2: Density plot of the Orszag-Tang MHD vortex problem calculated with Odin in a mixed Lagrangian-Eulerian calculation.

Back

Coupling Laser Physics to Radiation-Hydrodynamics

B. M. Haines[†], K. S. Anderson[*], W. W. Dai[†], D. E. Keller[*], J. A. Marozas[*], and P. W. McKenty[*]
[†] Los Alamos National Laboratory (bmhaines@lanl.gov)
[‡] Laboratory for Laser Energetics, University of Rochester

Keywords: Radiation hydrodynamics, Mesh generation methods, Data transfer between meshes

ABSTRACT

In order to accurately model implosion hydrodynamics in a radiation-hydrodynamics code, it is essential to include accurate accounting for energy deposition physics. In inertial confinement fusion (ICF), energy deposition profiles and energy transport have a strong impact on the development and evolution of hydrodynamic instabilities [1]. Nevertheless, accurately modeling laser beam propagation in radiation-hydrodynamics codes presents unique challenges associated with disparate resolution requirements, the potential to seed spurious noise in highly unstable systems, and computational expense.

We discuss new a method for coupling laser ray-tracing physics to a radiation hydrodynamics code, developed in the process of implementing laser physics [2] into the xRAGE radiation hydrodynamics code [3, 4]. Traditionally, computational laser ray-tracing is performed on the radiation-hydrodynamics mesh. This exacerbates ray noise and computational expense, since these meshes are typically optimized for the hydrodynamics. We have developed a mesh generation and evolution strategy that addresses the unique requirements of the laser ray-trace in a separate mesh, enabling performance enhancements and strategies to reduce noise seeded by the discretization of beams into computational rays. In addition, we have employed several methods to ensure that spurious mesh imprinting is minimized. These involved optimizing the laser and radiation-hydrodynamics meshes as well as interpolation between them and requires the use of an exact initialization method for the radiation-hydrodynamics mesh. These techniques have enabled efficient computation of laser-driven implosions and other experiments with minimal introduction of spurious noise.

References

[1] B. M. Haines et al. “Detailed high-resolution three-dimensional simulations of OMEGA separated reactants inertial confinement fusion experiments” *Physics of Plasmas*, 23, 072709, 2016.

[2] J. A. Marozas et al. “Wavelength-detuning cross-beam energy transfer mitigation scheme for direct drive: Modeling and evidence from National Ignition Facility implosions”, *Physics of Plasmas*, 25, 056314, 2018.

[3] M. Gittings et al. “The rage radiation-hydrodynamic code”, *Computational Science & Discovery*, 1(1), 015005, 2008.

[4] B. M. Haines et al. “High-resolution modeling of indirectly driven high-convergence layered inertial confinement fusion capsule implosions”, *Physics of Plasmas*, 24, 052701, 2017.

Back

On High-order Finite Difference Algorithm for Compressible Multi-material Flows

Zhiwei He[1], Baolin Tian[1,2], Li Li[1] and Yousheng Zhang[1,2]

[1] Institute of Applied Physics and Computational Mathematics, Beijing, China
(he_zhiwei@iapcm.ac.cn)
[2] Center for Applied Physics and Technology, Peking University, Beijing, China

Keywords: multi-material interficial flow, non-conservative production term, high-order finite difference method, WENO, local characteristic decompostion.

ABSTRACT

This talk systematically analyzes and proposes the numerical mechanism of non-physical pressure oscillation at the interface when calculating the multi-material flow problem by the high-order finite difference method (HOFDM) (component-wise; characteristic-wise) and the corresponding consistent numerical algorithms. The results show that: (1) The pressure oscillations at the interface is essentially caused by the inconsistency between the numerical viscosity and the state equation used in the numerical interface region. For the general nonlinear state equations and multi-material mixed state equations, the traditional high-porder finite difference method will inevitably produce non-physical numerical oscillations at the interface. (2) In the HOFDM, oscillations are due to the incompatibility of the point-wise splitting of eigenvalues in flux vector splitting and the inconsistency of component-wise nonlinear difference discretization among equations of mass, momentum, energy, and even fluid composition for multi-material flows. This paper presents a general solution to solve this problem—the consistent discretization principle (including: consistency of vector flux vector splitting methods, nonlinear difference discretization and non-conservative equations describing the interface evolution). (3) Using local characeristic decomposition (that is, using the characteristic-wise finite difference method), the inconsistency disccussed above can be effectively avoided. However, the non-conservative equation still needs a specific consistent discretization approach. Through theoretical derivation, this paper gives a general framework for non-conservative product terms in this non-conservative equation. The relevant numerical tests verify the correcteness of the above analysis, and verifies the reliability of the proposed algorithms.

Fig. 1 shows the interface shape in the late stage of a two-dimensional Richtmyer–Meshkov instability problem. From the results, we can see FC-WENO5 cannot maintain a smooth interface shape owing to the generation of the errors in velocity and pressure. There are obvious disturbances across the interface, causing it to acquire a sawtooth appearance. In contrast, the

Back

present algorithm yields a high-quality result without spurious oscillations. These results show that the present algorithm not only has the ability to maintain the equilibria, but also includes sufficient and approximate numerical dissipation for the strong shock and rarefaction waves.

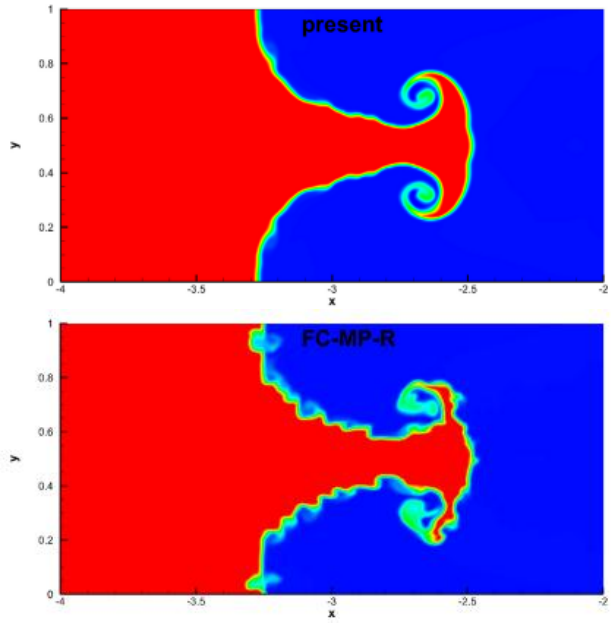


Figure 1: Density fields of the two-dimensional Richtmyer–Meshkov instability problem.

References

[1] Z.-W. He, Y.-S. Zhang, X.-L. Li, L. Li, B.-L. Tian, ”Preventing numerical oscillations in the flux-split based finite difference method for compressible flows with discontinuities”, Journal of Computational Physics, 300, pp: 269–287, 2015.

[2] Z.-W. He, Y.-S. Zhang, X.-L. Li, B.-L. Tian, ”Preventing numerical oscillations in the flux-split based finite difference method for compressible flows with discontinuities, II”, International Journal for Numerical Methods in Fluids, 80, pp: 306–316, 2016.

[3] Z.-W. He, L. Li, Y.-S. Zhang, B.-L. Tian, ”Consistent implementation of characteristic flux-split based finite difference method for compressible multi-material gas flows”, Computers & Fluids, 168, pp: 190–200,2018.

A Moving Discontinuous Galerkin Method with Interface Condition Enforcement for Incompressible Flows with Surface Tension

A. Kercher[†*], **A. Corrigan**[†], **D. Kessler**[†] **and D. Mott**[†]
[†] Laboratories for Computational Physics and Fluid Dynamics, Naval Research Laboratory

Keywords: surface tension; incompressible; multi-material hydrodynamics; moving discontinuous Galerkin method; interface condition enforcement; interface-tracking.

ABSTRACT

The Moving Discontinuous Galerkin Method with Interface Condition Enforcement (MDG-ICE), developed by the current authors [1, 2], is formulated for incompressible, multi-material, flows with surface tension. Interface forces, such as surface tension, are naturally incorporated into the MDG-ICE weak formulation, which enforces the conservation law and interface condition separately and treats the grid as a variable in order to detect and fit a priori unknown interfaces. Thus, in contrast to the discontinuous Galerkin (DG), continuous Galerkin (CG), and finite difference (FD) discretization methods, MDG-ICE can incorporate a surface force, via interface condition enforcement, and maintain a sharp interface, via grid movement, throughout the evolution of the flow.

In this work, the MDG-ICE formulation for incompressible flows with surface tension is described and used to numerically simulate the motion of buoyant bubbles in an immiscible multi-material flow while maintaining sharp interfaces, avoiding both numerical dissipation and oscillations in the solution. The numerical solutions will be compared to experimental results and previous numerical studies in order to access the accuracy and stability of the purposed method.

In previous work, it was shown that MDG-ICE can be used to detect and fit a priori unknown discontinuities, without introducing low order errors, in both steady and unsteady flows, for low ($p \leq 1$) and high ($p \geq 2$) order polynomial degrees, and in arbitrary dimensions ($d \leq 4$). Furthermore, MDG-ICE has been used to accurately fit curved interface geometry. For the case of a Mach-3 bow shock, MDG-ICE solutions using using $p1/p2$ super-parametric and $p = 2, 3$ isoparametric elements were shown to obtain optimal order convergence upon grid refinement. For the case of Burgers accelerating shock, MDG-ICE was used to accurately compute the evolving shock trajectory, represented by the curved spacetime interface topology, thus fitting the shock throughout the entire spacetime domain.

References

[1] A. Corrigan, A. Kercher, and D. Kessler. A moving discontinuous Galerkin finite element method for flows with interfaces. Technical Report NRL/MR/6040–17-9765, U.S. Naval Research Laboratory, December 2017.

[2] A. Corrigan, A. Kercher, and D. Kessler. A moving discontinuous Galerkin finite element method for flows with interfaces. *International Journal for Numerical Methods in Fluids*, 89(9):362–406, 2019.

Back

Recent Developments in the High Order Finite Element Hydrodynamics Code BLAST

R. A. Anderson, V. A. Dobrev, Tz. V. Kolev, R. N. Rieben, V. Z. Tomov and D. A. White

Lawrence Livermore National Laboratory
(anderson110@llnl.gov, dobrev1@llnl.gov, tzanio@llnl.gov, rieben1@llnl.gov, tomov2@llnl.gov, white37@llnl.gov)

Keywords: ALE hydrodynamics; finite element methods; high-order methods; adaptive mesh refinement; mesh optimization.

ABSTRACT

BLAST is a high-order finite element ALE hydrodynamics research and development code which implements the high order finite element methods described in [1] and is based on the open source finite element software library, mfem [2]. We review some recent developments in the code including improvements in the numerical methods, physics capabilities and performance on modern computer architectures.

The high-order ALE hydrodynamics formalism in BLAST was recently extended to support 3T radiation-hydro coupling and problems with spherical symmetry. We also developed a matrix-free formulation for computing the finite element based hyperviscosity and are exploring new conservative and multi-rate time integrators for coupled physics. New algorithms for unstructured adaptive mesh refinement and high-order mesh optimization have been added to the code.

We also discuss the high performance computing advantages that high-order methods provide for the case of parallel strong scaling for large problems of a fixed size and present our latest work in using GPUs to accelerate the compute intensive low level kernels of the Lagrangian algorithm, including their implementation in the Laghos miniapp, see 1 and [3].

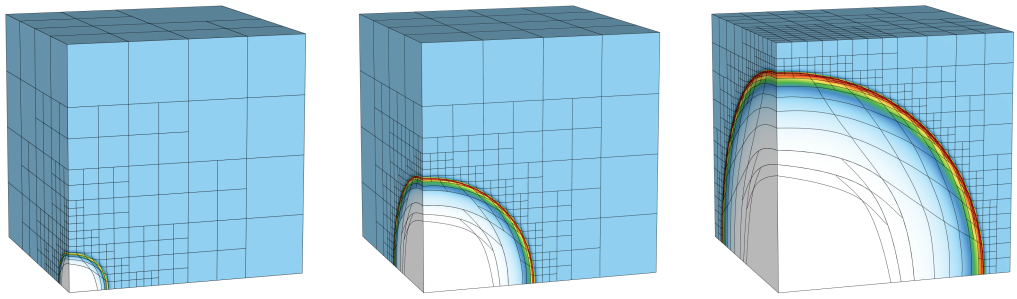


Figure 1: Dynamic adaptive mesh refinement for the high-order finite element discretization of the Sedov problem in the Laghos miniapp.

References

[1] R. A. Anderson, V. A. Dobrev, Tz. V. Kolev, R. N. Rieben and V. Z. Tomov, "High-Order Multi-Material ALE Hydrodynamics", *SIAM Journal on Scientific Computing*, (40) 2018, pp. B32-B58.

[2] MFEM: Modular finite element methods library, https://mfem.org.

[3] Laghos: Lagrangian high-order solver miniapp, https://github.com/CEED/Laghos.

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344, LLNL-ABS-768381

Back

Reducing Diffusion of Remapping by Non-Polynomial Function Reconstructions

M. Kuchařík[†] and R. Loubère[‡]
[†] FNSPE, Czech Technical University in Prague (kucharik@newton.fjfi.cvut.cz)
[‡] IMB, University of Bordeaux (raphael.loubere@u-bordeaux.fr)

Keywords: Arbitrary Lagrangian-Eulerian methods; remap; function reconstruction; diffusion control; THINC.

ABSTRACT

Remapping is one of essential steps of indirect ALE methods, conservatively transferring fluid quantities between computational meshes after mesh rezoning. At discontinuities, it is known to produce unphysical overshoots, which are in practice reduced by various techniques, such as limiters [1], a posteriori repair [2], FCT [3], or MOOD [4], generally increasing diffusion of the remapped values. Here, we present a new remapping technique, avoiding diffusion by non-polynomial function reconstruction, trying to represent the discontinuity in the cell by steep (but still continuous) anti-diffusive THINC function [5, 6]. This conservative reconstruction allows to position the discontinuity inside the cell such that neither limiter nor other bound-enforcing mechanism is needed, and sharp interface is preserved. Several typical numerical examples are shown to demonstrate properties of the method.

References

[1] T. J. Barth. Numerical methods for gasdynamic systems on unstructured meshes. In C. Rohde D. Kroner, M. Ohlberger, editor, *An introduction to Recent Developments in Theory and Numerics for Conservation Laws, Proceedings of the International School on Theory and Numerics for Conservation Laws*, Berlin, 1997. Lecture Notes in Computational Science and Engineering, Springer. ISBN 3-540-65081-4.

[2] M. Kucharik, M. Shashkov, and B. Wendroff. An efficient linearity-and-bound-preserving remapping method. *Journal of Computational Physics*, 188(2):462–471, 2003.

[3] D. Kuzmin, R. Lohner, and S. Turek, editors. *Flux Corrected Transport: Principles, Algorithms, and Applications*. Scientific Computation Series. Springer-Verlag New York, LLC, 2005.

[4] G. Blanchard and R. Loubere. High order accurate conservative remapping scheme on polygonal meshes using a posteriori MOOD limiting. *Computers & Fluids*, 136:83–103, 2016.

[5] Z. Sun, S. Inaba, and F. Xiao. Boundary variation diminishing (bvd) reconstruction: A new approach to improve godunov schemes. *Journal of Computational Physics*, 322:309–325, 2016.

[6] X. Deng, B. Xie, R. Loubere, Y. Shimizu, and F. Xiao. Limiter-free discontinuity-capturing scheme for compressible gas dynamics with reactive fronts. *Computers & Fluids*, 171:1–14, 2018.

The Authors acknowledge support from the Czech Science Foundation project 18-20962S, the EUROfusion project CfP-AWP17-IFE-CEA-01, the European Regional Development Fund project CZ.02.1.01/0.0/0.0/16_019/0000778, and the Czech Ministry of Education project RVO 68407700.

Back

High-order interface representation in THINC method

R. Kumar[1], L. Qian[2] and F. Xiao[1]
[1]Department of Mechanical Engineering, Tokyo Institute of Technology, Japan
(xiao.f.aa@m.titech.ac.jp)

[2]College of Materials Science and Technology, Nanjing University of Aeronautics and Astronautics, Nanjing, China

Keywords: Interface reconstruction, VOF, THINC, level set

ABSTRACT

THINC (Tangent of Hyperbola for INterface Capturing) method is a geometric/algebraic VOF (Volume of Fluid) method to compute moving interface. The THINC reconstruction mimics a volume fraction field by an essentially continuous function in which the interface is represented by a surface of lower dimensionality. The geometrical properties of the interface surface can be formulated by a polynomial, so-called surface polynomial, and then processed through algebraic steps, which means that using higher order surface polynomials for representing the interface does not substantially increase the algorithmic complexity.
We have devised several THINC schemes using quadratic and higher-order surface polynomials. Efforts have been made to extract the geometrical information of the moving interface from different approaches, such as least square, THINC/level set coupling, THINC/scaling, etc. Fig.1 shows the reconstructed surface using the 1st, 2nd and 4th order polynomials.

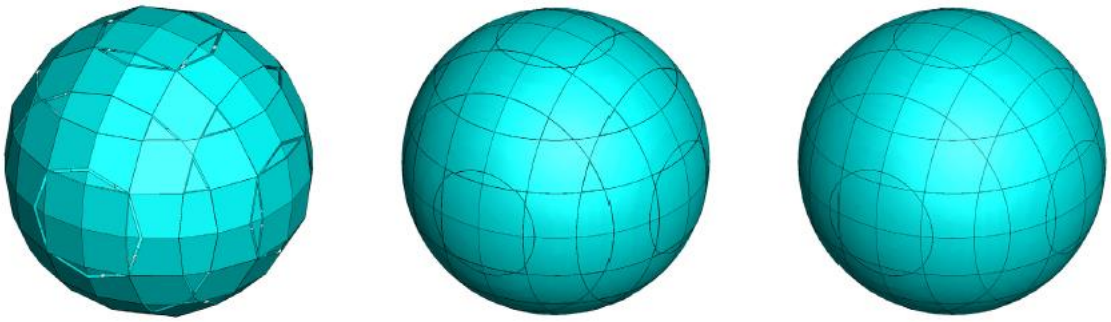


Figure 1: Reconstructions of a spherical surface by the 1st (a), 2nd (b) and 4th (c) order polynomial representations.

References

[1] L.Qian, Y.Wei and F.Xiao, “Coupled THINC and level set method: A conservative interface capturing scheme with high-order surface representations”, Journal of Computational Physics, 373, 284-303(2018).

Back

A Lagrangian Discontinuous Galerkin Hydrodynamic Method for Elastic-Plastic Solid Dynamics

E.J. Lieberman[†*], X. Liu[†], N.R. Morgan[†], D.J. Luscher [‡] and D.E. Burton[†]
[†] X-Computational Physics Division; Los Alamos National Laboratory
(elieberman3@lanl.gov)
[‡] Theoretical Division; Los Alamos National Laboratory

Keywords: Lagrangian Methods; Hydrodynamics; Discontinuous Galerkin; Solid Dynamics; Analytic Solutions; Shocks.

ABSTRACT

We present a new multidimensional high-order Lagrangian discontinuous Galerkin (DG) hydrodynamic method that supports hypoelastic and hyperelastic strength models for simulating solid dynamics with higher-order elements. We also present new one-dimensional test problems that have an analytic solution corresponding to a hyperelastic-plastic wave. A modal DG approach is used to evolve fields relevant to conservation laws. These fields are approximated high-order Taylor series polynomials. The stress fields are represented using nodal quantities. The constitutive models used to calculate the deviatoric stress are either a hypoelastic-plastic, infinitesimal strain hyperelastic-plastic, or finite strain hyperelastic-plastic model. These constitutive models require new methods for calculating high-order polynomials for the velocity gradient and deformation gradient in an element. The plasticity associated with the strength model is determined using a radial return method to with a J_2 yield criterion and perfect plasticity. The temporal evolution of the governing equations is achieved with the total variation diminishing Runge-Kutta (TVD RK) time integration method. A diverse suite of 1D and 2D test problems are calculated. The new 1D piston test problems, which have analytic solutions for each elastic-plastic model, are presented to demonstrate the formal accuracy of the various models with linear and quadratic polynomials in the new Lagrangian DG method. 2D test problems, such as the Taylor anvil problem in Figure 1, are calculated to demonstrate the stability and robustness of the the new Lagrangian DG method on multidimensional problems with high-order elements and quadratic polynomials.

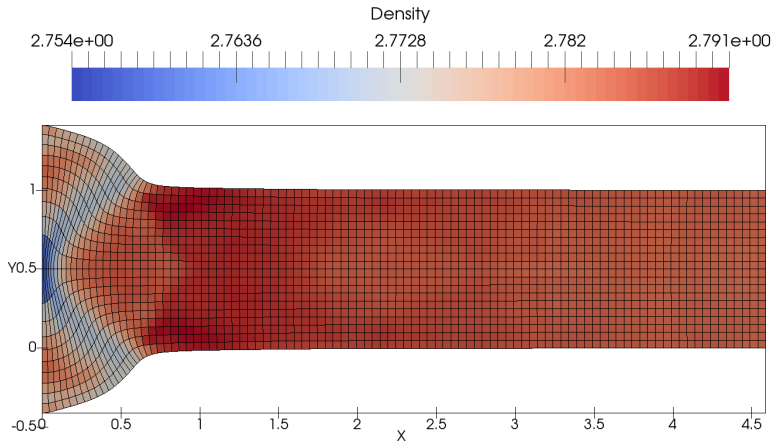


Figure 1: Cell average density in Taylor anvil problem with quadratic polynomials and curvilinear elements.

The authors acknowledge the help and discussion provided by Karlene Maskaly and the support of NNSA through the LDRD program at Los Alamos National Laboratory (LDRD Project: 20170051DR). The Los Alamos release number is LA-UR-19-20376.

Back

A Lagrangian Discontinuous Galerkin Hydrodynamic Method for Reactive Materials

E.J. Lieberman[†*], X. Liu[†], N.R. Morgan[†] and D.E. Burton[†]
[†] X-Computational Physics Division; Los Alamos National Laboratory
(elieberman3@lanl.gov)

Keywords: Lagrangian Methods; Hydrodynamics; Discontinuous Galerkin; Reactive Materials; Shock-to-Detonation.

ABSTRACT

We present a new multidimensional high-order Lagrangian discontinuous Galerkin (DG) hydrodynamic method that supports multiphase, programmed burn and reactive burn models. A modal DG approach is used to evolve fields relevant to conservation laws. These fields are approximated high-order Taylor series polynomials. The mass fraction of reacted materials is represented using a nodal quantity. The Davis reactant and product equations of state are used with pressure-temperature equilibrium to perform the multiphase modeling. A subcell method is used to determine reaction times for individual nodes within a cell for the programmed burn model. The Scaled Unified Reactive Front (SURF) reactive burn model is used to determine the reaction rate at individual nodes, with various adaptions made to the model so that it may benefit from the high-order method. The temporal evolution of the governing equations is achieved with the total variation diminishing Runge-Kutta (TVD RK) time integration method. Both 1D and 2D shock-to-detonation test problems are presented to demonstrate the accuracy and robustness of the reactive material models within the high-order method. The reactive burn model is of particular importance to test due to its sensitivity to mesh resolution. As such, the results of the discontinuous Galerkin hydrodynamic method are compared to those of the staggered grid hydrodynamic method, as in Figure 1, to determine the influence the high-order method has on the sensitivity.

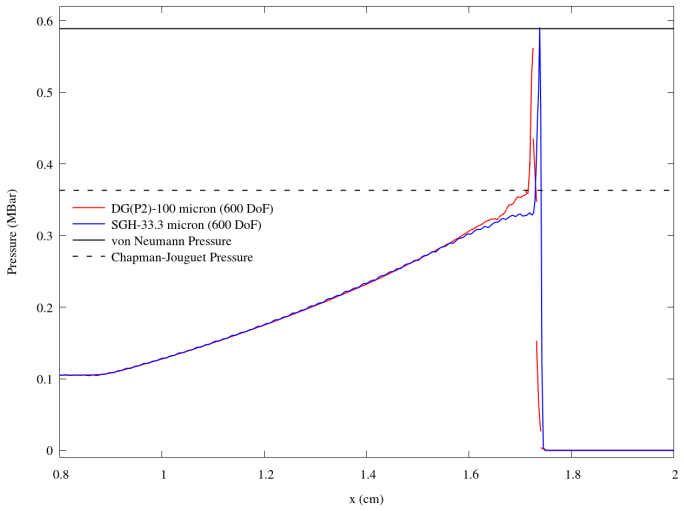


Figure 1: The pressure fields from the quadratic discontinuous Galerkin method and the staggered grid hydrodynamic method for a 1D shock-to-detonation problem using matching degrees of freedom.

The authors acknowledge the help and discussion provided by Karlene Maskaly, D.J. Luscher, Carl Johnson and Matt Price and the support of NNSA through the LDRD program at Los Alamos National Laboratory (LDRD Project: 20170051DR). The Los Alamos release number is LA-UR-19-20376.

Back

A hermite WENO-based limiter for a Lagrangian discontinuous Galerkin method

Xiaodong Liu[1], **Nathaniel R. Morgan**[1] **and Donald E. Burton** [1]
[1]X: Computational Physics Division, Los Alamos National Laboratory
(xliu@lanl.gov, nmorgan@lanl.gov, burton@lanl.gov)

Keywords: Hermite WENO, Lagrangian, discontinuous Galerkin, characteristic fields

ABSTRACT

We present a hermite WENO-based limiter in the context of Lagrangian discontinuous Galerkin (DG) hydrodynamic method [1] for solving the two-dimensional gas dynamic equations on unstructured hybrid meshes. The physical conservation laws for the specific volume, momentum and total energy are discretized using a DG method based on linear Taylor expansions. The nodal velocity, and the corresponding forces, are explicitly calculated by solving a multidirectional approximate Riemann problem. In addition to the cell average information, hermite WENO utilizes valuable yet handily high-order derivative information to keep WENO reconstruction stencils in the von Neumann neighborhood. In order to achieve better non-oscillatory qualities, the hermite WENO limiter is used with a local characteristic field decompositions. This new Lagrangian DG hydrodynamic method conserves mass, momentum, and total energy. Results from a suite of test problems are presented to demonstrate the robustness and expected second-order accuracy of this new limiter.

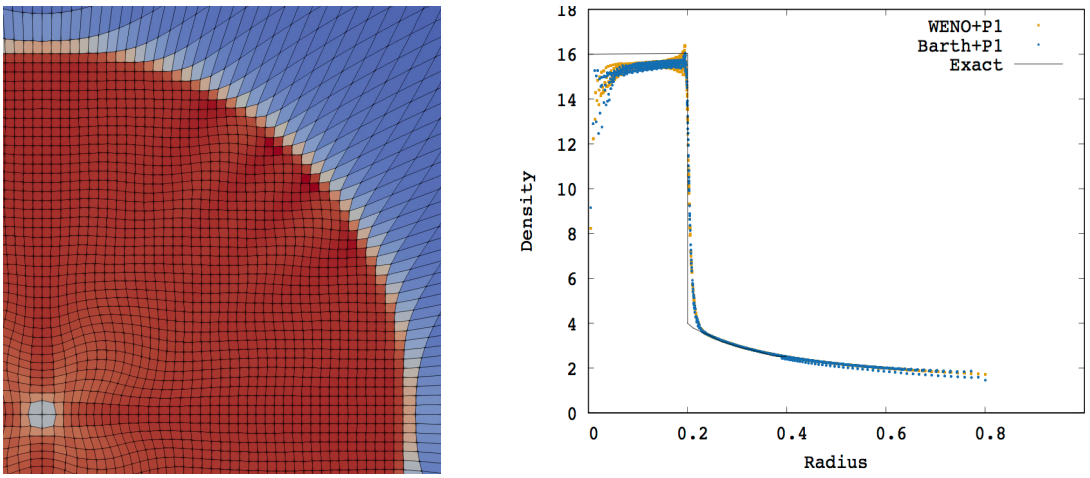


Figure 1: The results for Noh using hermite WENO.

References

[1] X. Liu, N. Morgan and D. Burton, “A Lagrangian discontinuous Galerkin hydrodynamic method”, Computers & Fluids, 163, pp.68-85, 2018.

We gratefully acknowledge the support of the Laboratory Directed Research and Development (LDRD) program at Los Alamos National Laboratory. The release number is LA-UR- 19-21978.
.

Back

Using the SMG scheme to study Rayleigh-Taylor instability growth in solids

Gabi Luttwak[†]
[†] Dynamic 123D, consulting, Haifa, Israel (gabi@dy123d.com)

Keywords: Lagrangian methods; ALE methods; multi-material ALE methods

ABSTRACT

Raleigh-Taylor instability (RTI) occurs while a less dense fluid is accelerating a denser one. Under gravity the material strength damps and prevents RTI formation in solids. However, at higher accelerations RTI will prevail. The Staggered Mesh Godunov (SMG) scheme [1] for Lagrangian and ALE hydrodynamics is applied to study the effect of yield strength on the RTI growth. A test problem is set up which extends for solids a well known test for RTI growth in fluids [2]. The influence of material strength and acceleration on RTI growth is investigated. The SMG scheme is well fitted to study RTI development as it is robust even in Lagrangian mode, due to its natural mesh stabilizing effect which damps the hourglass instability. It can handle larger deformations in its ALE and multi-material MMALE modes. The SMG scheme employs frame-invariant slope limiters. The convex hull based VIP limiter is used for vectors [3] and oriented Bounding Box based limiter for the stress tensor [4]. This way, we prevent numerical effects of symmetry breaking to interfere, while following the RTI growth. The test case can serve to estimate the sensitivity of the scheme to its parameters and mesh. In Figure 1 we compare Lagrangian and MMALE calculations at T=0.28μs, with g=-100m/s^2,and yield strength Y=1.0Gpa.

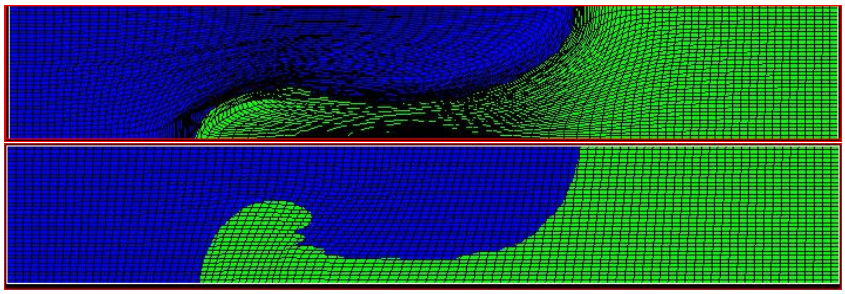


Figure 1: Comparing Lagrangian (upper) and MMALE (lower) calculations; T=0.28, g=-100, Y=1.0

References

[1] G. Luttwak and J. Falcovitz, "Staggered Mesh Godunov (SMG) Schemes for Lagrangian Hydrodynamics", *Shock Compression of Condensed Matter-2005, Furnish M. D. et al. editors*, pp. 339–342, 2006.

[2] R. Loubere , P.H. Maire , M. Shashkov , J. Breil , S. Galera , "ReALE A reconnection based ALE method", *Journal of Computational Physics*, 229, pp. 4724–4761, 2010.

[3] G. Luttwak and J. Falcovitz, "Slope limiting for vectors: A novel vector limiting algorithm", *International Journal for Numerical Methods in Fluids*, 65, pp. 1365–1375, 2010.

[4] G. Luttwak, "On the extension of monotonicity to multidimensional flows", 7^{th} *Int. Conf. on Num. Methods for Multi-Material Fluid Flow (MULTIMAT 2015), Wurzburg, Germany, 2015, Manuscript, http://dy123d.com/gabilut files/papers/monotonicity_in_multidim.pdf*

Back

A 2D/3D High-Order Finite Element Library in C++

Jacob Moore[†‡] **and Nathaniel Morgan**[†]
[†] Los Alamos National Labs (moore_j@lanl.gov, nmorgan@lanl.gov)
[‡] Mechanical Engineering, Mississippi State University

Keywords: High Order Finite Element; Serendipity Space; C++.

ABSTRACT

We discuss the creation and implementation of a generalized library of mathematical functions for both 2D and 3D linear, cubic, and quadratic serendipity elements as well as function for creating stable arbitrary ordered elements. This element library can be used for research and development of both continuous [1, 2] and discontinuous [3] finite element methods for solving a diverse range of partial differential equations. The code has a range of functions for calculating quantities that are commonly used in finite element methods such as the gradient of a basis function, the Jacobi matrix, the inverse Jacobi matrix, the determinant of the Jacobi matrix, and a physical position inside the element to name a few examples. The library also supports both Gauss-Legendre and Gauss-Lobatto quadrature rules up to 8 quadrature points in each coordinate direction. The examples and discussions will focus on Lagrangian solid mechanics and dynamics, but the element library can be used for a diverse range of applications applications.

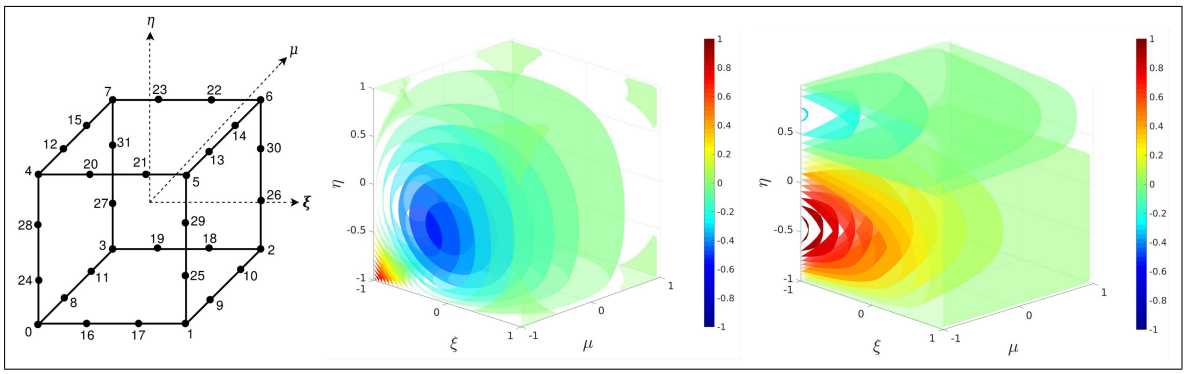


Figure 1: The nodal numbering scheme for the cubic Hex32 element (left) and the basis functions plotted for a corner node (mid) and an edge node (right).

References

[1] D. Flanagan, T. Belytschko, A uniform strain hexahedron and quadrilateral with orthogonal hourglass control, International journal for numerical methods in engineering 17 (5) (1981) 679–706.

[2] V. Chiravalle, N. Morgan, A 3d finite element ALE method using an approximate Riemann solution, International Journal for Numerical Methods in Fluids 83 (8) (2017) 642–663.

[3] X. Liu, N. R. Morgan, D. E. Burton, A Lagrangian discontinuous Galerkin hydrodynamic method, Computers & Fluids 163 (2018) 68–85.

We gratefully acknowledge the support of the ASC ATDM program at Los Alamos National Laboratory. LA-UR-19-21699

Back

Anti-diffusive methods for multiphase flows with exchange phenomena at the interfaces

V. Mahy[1], R. Motte[2], F. De Vuyst[3], C. Fochesato[4] and M. Peybernes[4]

[1]CMLA, CNRS UMR 8536, ENS CACHAN, F-94235 Cachan, France (vincent.mahy@cmla.ens-cachan.fr)

[2]CEA, DAM, DIF, F-91297 Arpajon, France (renaud.motte@cea.fr)

[3]LMAC EA 2222, UTC, Sorbonne Universités, 60200 Compiègne, France (florian.de-vuyst@utc.fr)

[4]CEA, DEN, DTN/SMTA/LMAG, Cadarache, F-13108 Saint Paul-lez-Durance, France (christophe.fochesato@cea.fr, mathieu.peybernes@cea.fr)

Keywords: anti-dissipative transport scheme, interface tracking methods, exchange models.

ABSTRACT

Anti-dissipative transport schemes have known an increasing interest for interface capturing problems and multi-component compressible flows [1, 2, 3, 4] during the past years. Their simplicity of implementation and natural extension to 3D computations make them attractive alternative methods compared to interface tracking methods like VOF. They also present advantages for High Performance Computing on multicore/manycore architectures [5]. However, they still know accuracy issues and interfaces instabilities in some cases. In addition, during interactions between phases, additional modeling questions arise. Indeed, taking into account a modeling defined for a sharp interface in a diffuse setting is not obvious since we cannot rely on equilibrium hypotheses. In fact, the exchange surface is no longer naturally defined (neither its position nor its surface).
This work is aimed at improving both stability and accuracy issues of compressive interface capturing methods. We present a "shape-preserving" local extremum diminishing explicit conservative advection scheme that takes into account some local geometrical properties of the interface. Then this method is evaluated and adapted to the treatment of exchange models (especially for the thermal conduction between two phases in temperature imbalance).

References

[1] Després, B., Lagoutière, F., "Contact discontinuity capturing schemes for linear advection and compressible gas dynamics". SIAM Journal of Scientific Computing 16, 479–524 (2001).

[2] Després, B., Lagoutière, F., Labourasse, E., Marmajou, I., "An anti-dissipative transport scheme on unstructured meshes for multi- component flows". International Journal on Finite Volumes 7, 30–65 (2010).

[3] Faucher, V. and Kokh, S., "Extended Vofire algorithm for fast transient fluid-structure dynamics with liquid-gas flows and interfaces", J. Fluids and Structures 39 (2013) 102–125.

[4] Bernard-Champmartin, A., De Vuyst, F., "A low diffusive Lagrange-remap scheme for the simulation of violent air-water free-surface flows", Journal of Computational Physics, Vol. 274, pp 19–49 (2014).

[5] Gasc, T., Peybernes, T., Poncet, P., De Vuyst, F., "Performance modeling & prediction of second-order staggered Lagrange-remap Hydrodynamics solvers: modeling, measurements & validation", GAMNI, Mécanique des fluides numérique, IHP Paris, 5-6 feb 2015, DOI:10.13140/2.1.4313.6802 (2015).

Back

Towards Isotropic Transport with Co-Meshes

C. Paulin, E. Heulhard de Montigny and A. Llor
CEA, DAM, DIF, F-91297 Arpajon, France, (christina.paulin.ocre@cea.fr)

Keywords: transport; numerical diffusion; isotropy; mesh imprinting; modified equation.

ABSTRACT

Transport is the central ingredient of all numerical schemes for hyperbolic partial differential equations and in particular for hydrodynamics. A major artifact produced by numerical transport is mesh imprinting [1]. Though mesh imprinting is inevitable, its anisotropy can be modulated and is thus amenable to significant improvements.
Motivated by the development of hydro-schemes for ICF (Inertial Confinement Fusion, [2]), the GEEC (Geometry, Energy and Entropy Compatible, [3]) approach has been developed. The transport operator is the key element in the GEEC formalism, but its current discretization displays a significant anisotropic behavior. Upgrading to higher order introduces complexities in the quasi-symplectic design of the scheme due to corner fluxes, without actually much improvement to the second order (a quasi industrial standard). The aim of the present work is to improve isotropy before upgrading the transport operator to second order, which is done with an enlarged first order upwind stencil.
We suggest a new definition of stencils by taking into account second nearest neighbors (across cell corners) and call the resulting strategy "co-mesh approach". In order to derive an accurate stencil, the modified equation [4] is used to study numerical dissipation and to determine the combination of initial stencil and co-mesh stencil leading to minimal anisotropy.
The co-mesh approach leads to improved isotropy for first order upwind transport, as it can be observed in Figure 1. Further investigations will analyze criteria to optimize isotropy. For reasons of simplicity the co-mesh strategy is introduced on usual 2D Cartesian grids. Extension to deformed quadrangular structured meshes and 3D grids is currently in progress.

Figure 1: Representation of numerical diffusion on the transport of a "delta" function (four cells at the bottom left corner) along directions $\vec{v} = (\cos(\theta), \sin(\theta))^t$, for $\theta = 0$, $\pi/8$ and $\pi/4$; usual upwind scheme (left) and co-mesh upwind scheme (right); transport over a radius of $96h$ (where h is the spatial discretization step), on a 128×128 grid, in 192 iterations;

References

[1] T.B. Lung, P.L. Roe. "Toward a reduction of mesh imprinting", *International Journal for Numerical Methods in Fluids*, 450–470, 2014.

[2] B. Zohuri. "Inertial Confinement Fusion Driven Thermonuclear Energy", Springer, 2017.

[3] T. Vazquez-Gonzalez. "Conservative and mimetic numerical schemes for compressible multiphase flows simulation", Université Paris-Saclay, 2016, PhD dissertation.

[4] R.F. Warming, B.J. Hyett. "The modified equation approach to the stability and accuracy analysis of finite-difference methods", *Journal of computational physics*, 159–179, 1974.

Back

An approximate Riemann solver for non-conservative hyperbolic systems

A. Serezhkin[†], **I. Menshov**[† ‡]
[†] All-Russia Research Institute of Automatics, ROSATOM Company (VNIIA) ul. Sushchevskaya, 22,127055 Moscow, Russia (aaserezhkin@gmail.com)
[‡] Keldysh Institute for Applied Mathematics, Russian Academy of Sciences (KIAM RAS) Miusskaya sq., 4, 125047 Moscow, Russia (menshov@kiam.ru)

Keywords: non-conservative hyperbolic systems; Riemann Problem solution; Eulerian methods.

ABSTRACT

We propose a new method to approximately solve the self-similar initial value Riemann problem for the hyperbolic system of quasi-linear equations in general non-conservative form. The method developed is based on the idea of path integration in the phase space developed by Dal Maso, Pares et al. We introduce an approximate wave structure (a set of discontinuities arising due to break-up of initial discontinuity) in accordance with the set of eigenvalues of the Jacobian matrix and propose the method for choosing appropriate paths connecting perturbed parameters on both sides of these discontinuities. The waves are classified into two groups: shock-type and fan-type, and the path across the discontinuity is constructed depending on its type. The method is then to iteratively sweep forward and backward the wave structure until the values in the unperturbed zones given with these iterations converge to given initial values of the Riemann problem considered. Once converged, this method yields the set of wave velocities and perturbed parameters in the domains between the waves. We show that for the case of conservative systems the proposed method allows to obtain the exact solution of the Riemann problem with any desired precision. For non-conservative systems, the method gives rather good approximation of the solution which maintains some important features of the exact solution, e.g., contact discontinuities in elastoplastic models. The proposed approximate Riemann solver is implemented in the finite volume discretization with standard Godunov averaging procedure. The scheme obtained is applied to and validated on several benchmark problems related to different systems (gas dynamics, elastoplastics, two-phase flows). Results are compared with alternative numerical methods.

References

[1] G. Dal Maso, P.G. LeFloch and F. Murat, “Definition and weak stability of nonconservative products”, *J. Math. Pures Appl.*, 74 (1995) 483548.

[2] M. L. Munoz-Ruiz and C. Pares, “Godunov method for nonconservative hyperbolic systems”, *M2AN*, Vol. 41, No 1, 2007, pp. 169185.

Back

Low-dissipation high-order finite volume fluxes for compressible mixing with heat release

GS Sidharth[†]

[†] Methods and Algorithms, Los Alamos National Laboratory (sidgs@lanl.gov)

Keywords: shock hydrodynamics; multi-material hydrodynamics; Eulerian methods;

ABSTRACT

Mixing of multiple gas species with heat release encounters strong variable-density effects, both inertial and dilatational. Since the mixing processes in flows of relevance are often dominated by instability-driven vortical stirring, low-dissipation methods are important for coarse-grained (large-eddy) simulations of these flows. Accurate representation of small-scale features is critical to physics-based subgrid models.

Presence of sharp interfaces in species that mix, and of intermediate reaction products that reside at these interfaces, requires adequate numerical dissipation for stable advection. However, species mass dissipation (and associated momentum dissipation) causes numerical dissipation of vorticity as well, suppressing stirring and consequently affecting heat release. Stable but accurate stirring of scalar fields therefore requires non-trivial low-dissipation techniques. This issue is compounded when coupled with shock-capturing and handling of large spatio-temporal variations in thermodynamic properties of the fluid.

We work within a finite-volume method with high order polynomial reconstruction of fluxes. The interfaces are diffused. Linear scaling limiters [2] are employed on high order fluxes to ensure boundedness of scalars. Shock/contact sensor enabled novel numerical dissipation forms are explored systematically for 2D test cases with shocks, vortical stirring and heat release. Emphasis is placed on avoiding spurious oscillations in mass-fraction and temperature fields while conserving species mass, momentum and total energy.

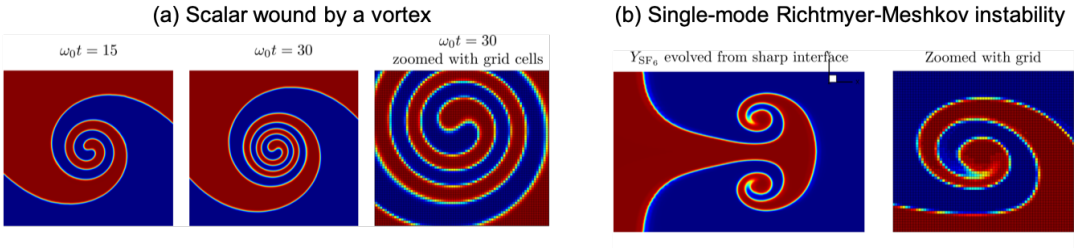


Figure 1: Numerical tests with scaling limiters and low-dissipation fluxes scalar evolution by (a) isentropic vortex, and (b) shock-deposited vorticity. [1]

References

[1] GS Sidharth, "On variable-density subgrid effects in turbulent flows", University of Minnesota, 2018

[2] PK Subbareddy, A Kartha and GV Candler, "Scalar conservation and boundedness in simulations of compressible flow", *Journal of Computational Physics*, 348, pp. 827–846, 2017.

Back

High order IMEX deferred correction scheme for multiphase flows

D. Torlo[†] and R. Abgrall[†]
[†] Institut für Mathematik, Universität Zürich, Switzerland
(davide.torlo@math.uzh.ch, remi.abgrall@math.uzh.ch)

Keywords: multiphase flows; high order; deferred correction; residual distribution; IMEX scheme.

ABSTRACT

This work aims to solve the 7 equations Baer and Nunziato multiphase flows model in the formulation of [3] with high order of accuracy. It consists of 3 equations, i.e., density, momentum and energy (Euler equations) of the two phases and one for the mass fraction. The closure equation of states of the two phases is given by the stiffend gas EOS. With respect to usual Euler equations, coupling terms play a important role in these equations. There are, indeed, non–conservative terms and stiff source terms. In particular, the stiff source terms are lead by two parameters λ, μ which represent the rate at which the two pressures and velocities are coinciding. To deal with the stiff source terms an IMEX (implicit–explicit) method is applied, to prevent instabilities brought by these terms, considering their time discretization as implicit, while the conservative flux and the non–conservative terms are kept explicit.

To get a high order accurate scheme in space and time the deferred correction iterative scheme (DeC) is applied in combination with the residual distributions (RD) schemes [1]. The first is a time integration method inspired by the Picard–Lindelöf theorem, which combines two formulations: $\mathcal{L}^1$ easy to solve but not so accurate (the IMEX scheme) and $\mathcal{L}^2$ difficult to be computed, but high order (a full implicit discretization). Through an iterative procedure with few steps, it converges to the high order solution we are interested in. Residual distributions are a class of high order schemes with compact stencil, easy to code and can recast many other well known schemes.

This work is a continuation of a preliminary work on kinetic schemes with a similar approach but different IMEX scheme in [2].

References

[1] R. Abgrall, "High Order Schemes for Hyperbolic Problems Using Globally Continuous Approximation and Avoiding Mass Matrices", *Journal of Scientific Computing*, 73(2), pp. 461–494, 2017.

[2] R. Abgrall and D. Torlo, "Asymptotic preserving deferred correction residual distribution schemes", *ArXiV*, arXiv:1811.09284.

[3] R. Saurel and R. Abgrall, "A Multiphase Godunov Method for Compressible Multifluid and Multiphase Flows", *Journal of Computational Physics*, 150(2), pp. 425–467, 1999.

The authors acknowledge the support of ITN ModCompShock project funded by the European Union's Horizon 2020 research and innovation program under the Marie Sklodowska-Curie grant agreement No 642768.

Back

Comparison of Various Equations of State for Laser Plasma Simulations Using the HerEOS Framework

M. Zeman[†], P. Váchal[†*] and M. Holec[‡]
[†]FNSPE, Czech Technical University in Prague, Czech Republic
(zemanmi3@fjfi.cvut.cz, pavel.vachal@fjfi.cvut.cz)
[‡]Lawrence Livermore National Laboratory, U.S. (holec1@llnl.gov)

Keywords: Equation of State; Thermodynamic consistency; Helmholtz free energy; Hermite interpolation; Laser plasma simulation

ABSTRACT

At the previous MultiMat conference and in its proceedings [1] we presented the HerEOS framework - a general methodology and practical implementation of arbitrary Equations of State (EOS) evaluation for Lagrangian and ALE hydrodynamic simulations, which is based on higher-order interpolations of the Helmholtz free energy and derived quantities. While the main objectives of such a tool are to improve the thermodynamic consistency of the calculations and reduce the computational cost, it is also useful as a general interface for the employment of various EOS models in various simulation codes, allowing a simple comparison.

Now we are offering a set of examples from the simulations of real experiments in the field of laser plasma interactions, performed at facilities such as ELI Beamlines in the Czech Republic or LULI in France. In these tests, we are comparing results obtained with various EOS, such as QEOS [2], FEOS [3], BADGER [4] and SESAME [5]. A variety of combinations emerges from several possible ways of how we interpolate (state variables used, order of interpolation, resolution of interpolation tables) and other choices regarding physics (ionization, opacity) and consistency preferences. Rather than seeking an universal approach to be used in all situations, we are showing the behavior and features of particular choices in realistic simulations of experiments in the field of hydrodynamics and high energy density physics.

References

[1] M. Zeman, M. Holec and P. Váchal, "HerEOS: a Framework for Consistent Treatment of the Equation of State in ALE Hydrodynamics", *Computers & Mathematics with Applications*, 2019, In Press.

[2] R.M. More, K.H. Warren, D.A. Young and G.B. Zimmerman, "A New Quotidian Equation of State (QEOS) for Hot Dense Matter", *Physics of Fluids*, 31(10), pp. 3059–3078, 1988.

[3] S. Faik, A. Tauschwitz and I. Iosilevskyi, "The Equation of State Package FEOS for High Energy Density Matter", *Computer Physics Communications*, 227, pp. 117–125, 2018.

[4] T.A. Heltemes and G.A. Moses, "BADGER v1.0: A Fortran Equation of State Library", *Computer Physics Communications*, 183(12), pp. 2629–2646, 2012.

[5] S.P. Lyon and J.D. Johnson, "SESAME: The Los Alamos National Laboratory Equation of State Database", Technical Report LA-UR-92-3407, Los Alamos National Laboratory, 1992.

Part of this work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Back

Effects of interface treatment methods on hydrodynamic instabilities between immiscible fluids

J. Velechovsky[†*], M. Francois[†], Z. Jibben[†] and T. Masser[‡]
[†] Los Alamos National Laboratory (jan@lanl.gov)

Keywords: Eulerian hydrodynamics; slope limiter; interface steepener; Volume of Fluid method.

ABSTRACT

Eulerian and Arbiltrary Lagrangian Eulerian (ALE) hydrodynamic simulations of immiscible materials typically require an interface treatment method to reduce numerical diffusion across a material interface. The simplest method is to artificially increase a gradient of material volume fractions. This method is usually referred to as interface steepener. We demonstrate that careful manipulation of the gradient is necessary in order to preserve a correct shape of the interface while using the steepener. Volume of Fluid (VOF) with Piece-wise Linear Interface Calculation (PLIC) is another and more advanced numerical method. In PLIC, a sharp planar interfaces in multi-material cells are reconstructed in order to further reduce numerical diffusion at the interface. We compare these two interface treatment methods implemented in an Eulerian code xRage with particular attention to their effect on the development of the Rayleigh-Taylor instability and the Richtmyer-Meshkov instability. Finally, we compare these numerical effects to the physical effects of surface tension on these instabilities. LA-UR-19-21390.

Registered participants:

Remi Abgrall
Jason Albright
Paola Bacigaluppi
Jayesh Badwaik
Dinshaw Balsara
Brody Bassett
Keith Bennet
Isabelle Bertron
Pavel Bochev
Walter Boscheri
Jerome Breil
Jerry Brock
Saray Busto Ulloa
Rémi Chauvin
Yibing Chen
Florian Chevassu
Simone Chiocchetti
Vincent Chiravalle
Sidafa Conde
Andrew Corrigan
Tristan Coulange
Marta D'Elia
Alan Dawes
Stéphane Del Pino
Michael Dumbser
Nicolas Favrie
Marianne Francois
Elena Gaburro
Sergey Gavrilyuk
Andrew Giles
Tom Goffrey
Fernando F. Grinstein
Jean-Luc Guermond
Charles Gueunet
Brian Michael Haines
Hennes Hajduk
Zhiwei He
Angela Herring
Ryan Hill
Philippe Hoch
Milan Holec
Matteo Ioriatti
Kseniya Ivanova
Yuliya Kanarska
Andrew Kercher
Robert Kevis
Matej Klima
Christian Klingenberg
Tzanio Kolev
Milan Kucharik
Ronit Kumar
Dmitri Kuzmin
Thomas Leroy
E.J. Lieberman
Richard Liska
Xiaodong Liu
Na Liu
Christoph Lohmann
Raphaël Loubère
Elizabeth Lovegrove
Hong Luo
Gabi Luttwak
Ian MacDonald
Pierre-Henri Maire
Robert Managan
Tomislav Maric
Igor Menshov
Douglas Miller
Jacob Moore
Jim E. Morel
Nathaniel Morgan
Renaud Motte
Robert Nourgaliev
Britton Olson
Michael Owen
Christina Paulin
Marica Pelanti
Ilya Peshkov
Mathieu Peybernes
Michael Powell
Barbara Re
William Rider
Robert Rieben
Evgeniy Romenskiy
Francesco Lohengrin Romeo
Christopher Rousculp
Richard Saurel
Thierry Schwoertzig
Alexey Serezhkin
John N Shadid
Mikhail Shashkov
GS Sidharth
David Sidilkover
Daniil Svyatskiy
Petr Sváček
Joanna Szmelter
Maurizio Tavelli
Ferdinand Thein
Nicolas Therme
Baolin Tian
Vladimir Titarev
Svetlana Tokareva
Ignacio Tomas
Vladimir Tomov
Davide Torlo
Eleuterio Francisco Toro
Sergey Utyuzhnikov
Pavel Vachal
Jan Velechovsky
Douglas Woods
Feng Xiao
Qinghong Zeng
Duan Zhang
Qiang Zhao