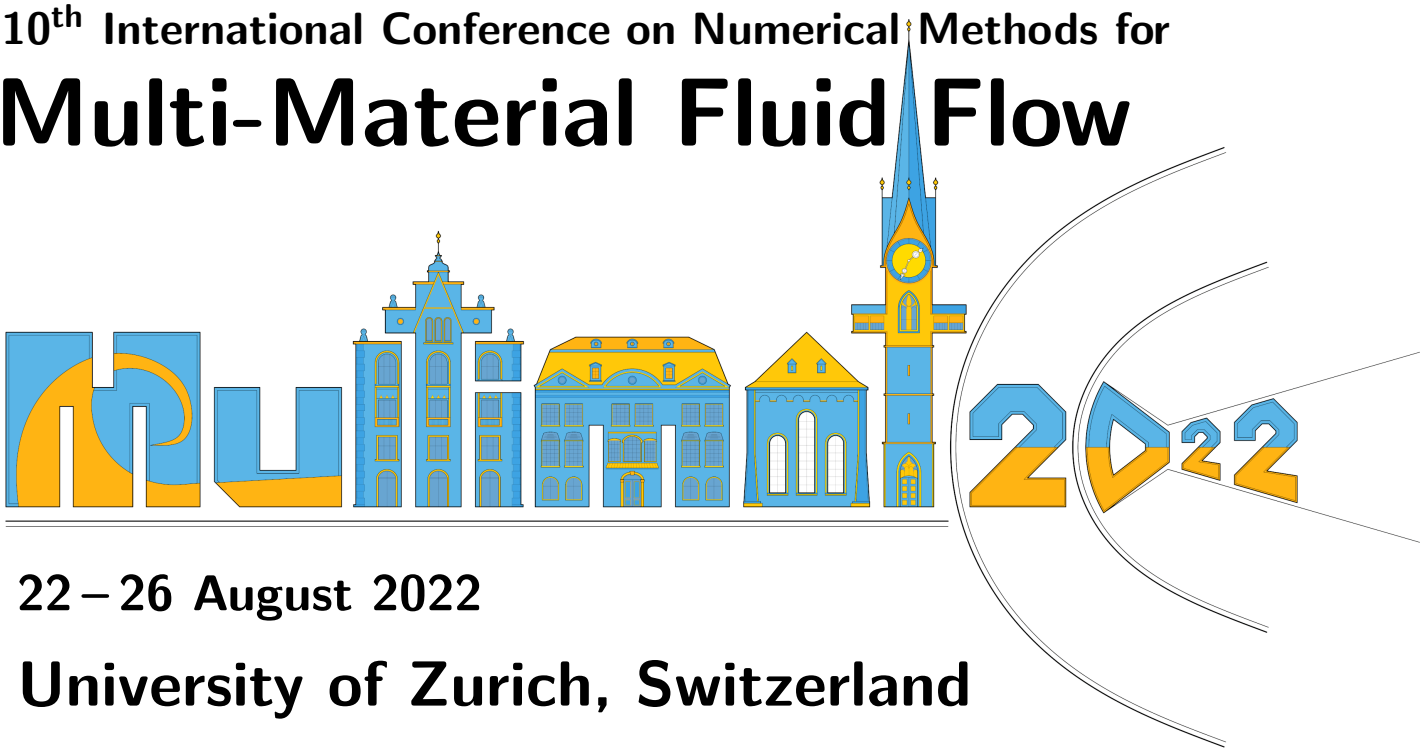
10th International Conference on Numerical Methods for

Multi-Material Fluid Flow



22 – 26 August 2022

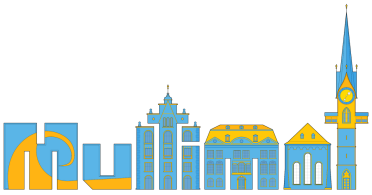
University of Zurich, Switzerland

Book of Abstracts

Organizers:

Rémi Abgrall, Elena Gaburro, Franziska Robmann

"*Behind every result is a new challenge*"



This conference has been supported by:

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Sandia National Laboratories (USA, New Mexico)

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Welcome to MultiMat 2022!

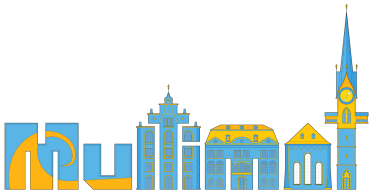
We are very pleased to welcome you to MultiMat 2022, *the 10th International Conference on Numerical Methods for Multi-Material Fluid Flows*, held at the University of Zurich in Switzerland. Switzerland lies at the heart of Europe, and the cosmopolitan city of Zurich, nestled between a crystal clear lake and an idyllic mountain landscape, offers many opportunities from cultural events, arts and history to natural beauties and good cuisine.

MultiMat 2022 builds on the success of previous MultiMat conferences: *Trento* in 2019, *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 118 abstracts, which have been carefully reviewed by the members of the scientific committee. There will be 53 talks, 15 additional talks in thematic minisymposia, and more than 20 poster presentations, given by international researchers coming from *Belgium, Canada, Czech Republic, Denmark, Finland, France, Germany, Israel, Italy, Japan, Mexico, Morocco, Russia, Switzerland, the United Kingdom, and the United States of America*. Unfortunately our friends from *China*, whose abstracts were accepted, could not come.

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, 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 and numerical methods for complex constitutive models.

We would really like to thank the scientific committee, our sponsors and in particular *all the participants* for coming to MultiMat 2022 and to be physically *here*! We wish you a very pleasant stay in Zurich and many enriching scientific and personal interactions during the conference!

Elena & Rémi



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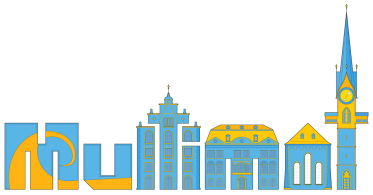

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MultiMat 2022 Venue

MultiMat 2022 takes place at the **Irchel Campus** of the **University of Zurich** (the GPS coordinates of the venue are: 47.397N 8.55E)

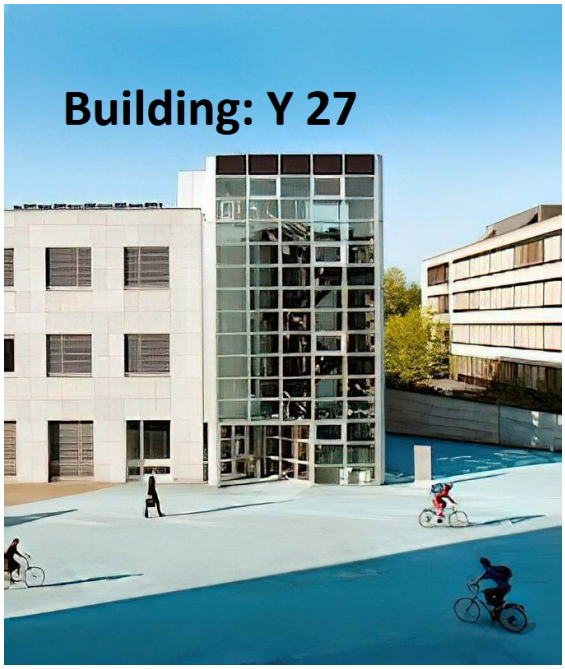
Registration is on Sunday from 17:00 to 19:30 in the building Y27

MultiMat 2022 talks: building Y15, room G-40, 9:00 – 18:00

MultiMat 2022 thematic minisymposia: building Y27, room H-25, 14:30 – 18:00

Welcome reception: Lichthof building Y24, G-100, on Monday from 18:30

Poster party: Lichthof building Y24, G-100, on Tuesday from 18:30



Social dinner: SORELL HOTEL Zürichberg, on Wednesday from 19:00
Orellistrasse 21, 8044, Zürich (30 minutes from the University)

Monday, 22 August 2022

08:00 – 09:00 **REGISTRATION** (∗)

09:00 – 09:30 **OPENING: Organizers and Stephan Neuhauss (vice-dean of the Mathematisch-Naturwissenschaftliche Fakultät of the University of Zurich)**

Chair: R. Loubère

09:30 – 10:00 **Walter Boscheri**
A 3D ADER MOOD FV method for updated Lagrangian hyperelasticity on unstructured grids

10:00 – 10:30 **Nathaniel Morgan**
On a 3D Lagrangian nodal discontinuous Galerkin method

10:30 – 11:00 **David Sidilkover**
Spurious vorticity in Lagrangian and Eulerian methods

11:00 – 11:30 **COFFEE BREAK**

Chair: W. Boscheri

11:30 – 12:00 **Bastien Manach-Pérennou**
Cell-centered Lagrangian scheme for multi-material flows with pressure equilibration

12:00 – 12:30 **Barbara Re**
An interpolation-free strategy to describe connectivity changes within the ALE framework

12:30 – 13:00 **Elena Gaburro**
Direct ALE DG schemes on Voronoi grids with topology changes and deferred mesh optimization

13:00 – 14:30 **LUNCH**

Chair: M. Owen

14:30 – 15:00 **Fernando Grinstein**
Transition and Multiphysics in 3D ICF Capsule Implosions

15:00 – 15:30 **Pierre Anguill**
A low mesh-constraints monotone scheme for the diffusion operator on general polyhedral meshes

15:30 – 16:00 **Emmanuel Labourasse**
An asymptotic preserving method for the linear transport equation on general meshes

Thematic Minisymposium: Structure preserving schemes

Chair: D. Kuzmin

Christian Klingenberg
Structure preserving numerical methods in a multi-scale context

Andreas Rupp
Bound-preserving flux limiting schemes for DG with applications to the Cahn–Hilliard equation

Thomas Paula
Robust modification of the discrete eqs method for multi-phase flow with interface capturing

16:00 – 16:30 **COFFEE BREAK**

Chair: M. François

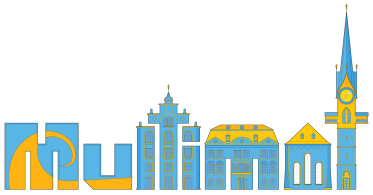
16:30 – 17:00 **Michael Dumbser**
On Thermodynamically Compatible Schemes for Continuum Mechanics

17:00 – 17:30 **Simone Chiocchetti**
Semi-implicit schemes with efficient finite rate stiff relaxation for compressible two-phase flow and plasticity

17:30 – 18:00 **Sergey Gavrilyuk**
A theoretical model of Leidenfrost's temperature

from 18:30 **WELCOME RECEPTION**

(∗) The **MAIN REGISTRATION** takes place on **Sunday 21** (17:00 – 19:30)



Tuesday, 23 August 2022

08:15 – 09:00 REGISTRATION

Chair: L. Krivodonova

09:00 – 09:30 **Bruno Després**
Interface reconstruction and development of VOFML

09:30 – 10:00 **Doug Miller**
Feature Preserving Interface Reconstruction and Tracking Using Piecewise Circular Facets with Cusps

10:00 – 10:30 **David Henneaux**
Enforcing Interface Coupling Conditions within a DG Sharp Interface Method (Viscous Gas-Liquid Flows)

10:30 – 11:00 **Daniel White**
Design Optimization of Richtmyer-Meshkov Instabilities

11:00 – 11:30 COFFEE BREAK

Chair: R. Rieben

11:30 – 12:00 **Matthew J. Zahr**
High-Order Implicit Shock Tracking for Flows with Interfaces

12:00 – 12:30 **Evan Bursch**
Radiation Hydrodynamics Modeling With High-Order Implicit Shock Tracking

12:30 – 13:00 **Jean-Luc Guermond**
Invariant-domain preserving high-order IMEX schemes

13:00 – 14:30 LUNCH

Chair: V. Perrier

14:30 – 15:00 **Riccardo Dematté**
A diffuse interface approach for multi-material simulations of condensed phase explosives

15:00 – 15:30 **Stephen Millmore**
A Multi-Physics Methodology for Four States of Matter

15:30 – 16:00 **Pavel Bochev**
Formulation and computation of partitioned schemes with nonconventional models

Thematic Minisymposium: Numerical methods for complex models

Chair: M. Zahr

Michele Giuliano Carlino
ADER scheme for incompressible Navier-Stokes on Overset grids with compact transmission condition

Jan-Phillip Bäcker
Level Set Extrapolation of Immersed Boundary Data in Unfitted FEM for Deformable Interfaces

Gerardo Hernández-Duenas
A new two-dimensional blood flow model with arbitrary cross sections

16:00 – 16:30 COFFEE BREAK

Chair: S. Chiocchetti

16:30 – 17:00 **Lilia Krivodonova**
An Arbitrarily High-Order Moment Limiter for the Discontinuous Galerkin Method

17:00 – 17:30 **Jose Castillo**
High-Order Mimetic Finite Differences on Non-trivial Geometries

17:30 – 18:00 **Andrés M. Rueda-Ramírez**
Subcell limiting strategies for the DGSEM

Thematic Minisymposium: Numerical methods for complex models

Chair: S. Gavrilyuk

Jens Keim
A Relaxation Formulation of the Navier-Stokes-Korteweg Equations

Firas Dhaouadi
A hyperbolic reformulation of the Navier-Stokes-Korteweg system

Duan Zhang
Fluid Mediated Particle Interactions Studied Using the Nearest Particle Statistics

from 18:30 POSTER PARTY

Wednesday, 24 August 2022

08:30 – 09:00 **REGISTRATION**

Chair: S. Del Pino

09:00 – 09:30 **Pierre-Henri Maire**
Entropy stable and positivity preserving schemes for multidimensional hyperbolic systems. Part I: theory

09:30 – 10:00 **Raphaël Loubère**
Entropy stable and positivity preserving schemes on unstructured grid. Part II: multidimensional validation

10:00 – 10:30 **Junming Duan**
High-Order Accurate Entropy Stable Adaptive Moving Mesh Methods

10:30 – 11:00 **Hennes Hajduk**
On the need for enforcing discrete entropy inequalities for scalar conservation laws and hyperbolic systems

11:00 – 11:30 **COFFEE BREAK**

Chair: P. Bochev

11:30 – 12:00 **Stéphane Del Pino**
Entropy stability analysis for semi-Lagrangian cell-centered schemes

12:00 – 12:30 **Eric J. Tovar**
Robust second-order approximation of the compressible Euler Equations with an arbitrary equation of state

12:30 – 13:00 **Dmitri Kuzmin**
New Limiters and Entropy Fixes for Discontinuous Galerkin Methods

13:00 – 13:30 **Alexiane Plessier**
Implicit semi-Lagrangian schemes for compressible gas dynamics

13:30 – 15:00 **LUNCH**

FREE AFTERNOON

Some suggestions:

Kunsthaus Zürich: Sammlung Emil Bührle
Major and beautiful collection of French paintings
Wednesday free admission to the collection for all visitors

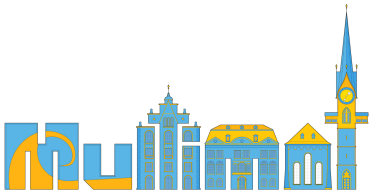
Clock and Watch Museum Beyer
Clock and watch collection, ancient and antique treasures. Entry CHF 10

Uetliberg – Top of Zürich
Uetliberg is Zürich's own mountain
Stunning view of the city and the lake

Lake cruises
Mini, short or long lake cruises on the lake of Zürich

from 19:00 **SOCIAL DINNER**

SORELL HOTEL Zürichberg
Orellistrasse 21, 8044, Zürich
(Note that it can take 30 minutes to reach the place
both from the conference venue and the city center)



Thursday, 25 August 2022

08:30 – 09:00 REGISTRATION

09:00 – 09:30 **Robert Rieben**
Multimaterial ALE remap with interface sharpening using high-order matrix-free finite element methods

09:30 – 10:00 **Rao Garimella**
Accurate remapping from 3D to 2D meshes for Multiphysics Simulations

10:00 – 10:30 **Matěj Klíma**
A three-dimensional cell-centered Lagrangian Lax-Wendroff HLL hybrid scheme

10:30 – 11:00 **Igor Menshov**
Interface capturing methods for heterogeneous multiphase flows

Chair: B. Re

11:00 – 11:30 COFFEE BREAK

11:30 – 12:00 **Mike Owen**
An SPH damage model appropriate for variable resolution

12:00 – 12:30 **Jason M. Pearl**
SPH for high-density ratio multi-material flows

12:30 – 13:00 **Ilya Peshkov**
An SPH method for the unified model of continuum mechanics

Chair: N. Morgan

13:00 – 14:30 LUNCH

Thematic Minisymposium: Interfaces

14:30 – 15:00 **Brody R. Bassett**
Dynamic Coupling of SPH and the FEM

15:00 – 15:30 **Paul Tsuji**
Embedded Meshes with Smoothed Particle Hydrodynamics

15:30 – 16:00 **Marianne François**
On exascale computing, Tusas and phase field method for solidification problem

Chair: I. Peshkov

Britton Olson
An immersed boundary method for gas-solid interface and multi-material flow in the presence of shocks

Pierson Guthrey
Complex Multi-Material Shock Interactions Using Moving DG with Interface Condition Enforcement

Shambhavi Nandan
Sharp Interface Capturing in Multi-Material Flows with an Accurate Diffuse Interface Method

Chair: B. Després

16:00 – 16:30 COFFEE BREAK

16:30 – 17:00 **Ian MacDonald**
Extension of the Interface Aware SubScale Dynamics (IA-SSD) closure model to 3D

17:00 – 17:30 **Andy Barlow**
A new fracture model based on Interface Aware SubScale Dynamics (IA-SSD) closure model

17:30 – 18:00 **Philippe Hoch**
High-order composite multi-dimensional FV schemes on unstructured meshes

Chair: P.-H. Maire

Thematic Minisymposium: Radiation hydrodynamics

Sébastien Guisset
A colocalized scheme for three-temperature grey diffusion radiation hydrodynamics

Brian Haines
An iterative algorithm for solving the nonlinear heat transport equations

Alexander Farmakalides
A Computational Multi-physics Approach for Whole System Fusion Reactor Simulations

Chair: I. Menshov

Friday, 26 August 2022

08:30 – 09:00 **REGISTRATION**

Chair: M. Dumbser

09:00 – 09:30 **Dinshaw S. Balsara**
High Order Adaptive Mesh Refinement (AMR) for Divergence Constraint-Preserving Schemes

09:30 – 10:00 **Tuan Anh Dao**
A nodal-based high-order nonlinear stabilization for finite element approximation of magnetohydrodynamics

10:00 – 10:30 **Jan Nikl**
High-order Curvilinear Finite Element Magnetohydrodynamics

10:30 – 11:00 **Maria Chrysanthou**
Mathematical and Computational Assimilation for Plasma Boundary Physics and Fusion Reactor

11:00 – 11:30 **COFFEE BREAK**

Chair: N. Nikiforakis

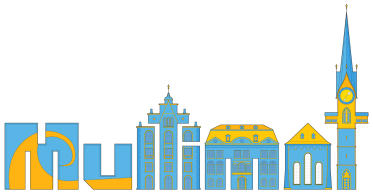
11:30 – 12:00 **Marco Petrella**
On the modeling of non-mixing compressible twophase flow

12:00 – 12:30 **Vincent Perrier**
A multiscale numerical scheme for the simulation of dispersed multiphase flows

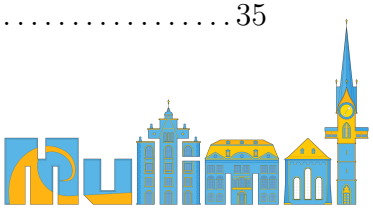
12:30 – 13:00 **Kevin Schmidmayer**
Modelling interactions of waves with diffused interfaces

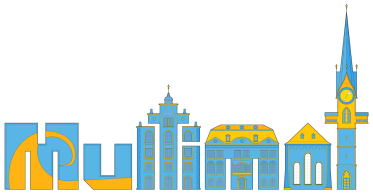
13:00 – 14:30 **CLOSING LUNCH WITH DESSERT**

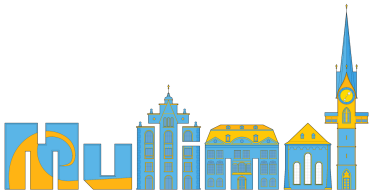
FREE DISCUSSION

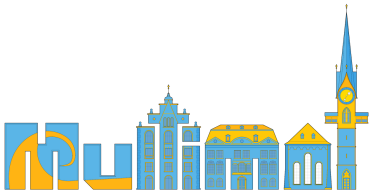


Abstracts of oral presentations

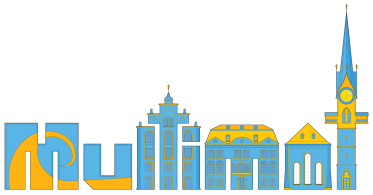








Abstracts of poster presentations



A low mesh-constraints monotone scheme for the diffusion operator on general polyhedral meshes

P. Anguill[†], **X. Blanc**[‡], **E. Labourasse**[†*]

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Keywords: Finite Volume, radiative transfer, asymptotic analysis, computational transport, monotone anistotropic diffusion, unstructured meshes.

ABSTRACT

In this talk, a new method for the 3D numerical resolution of the diffusion operator with a finite volume discretization is presented. The resulting scheme is positive, convergent and consistent. This approach has already been undertaken in 2D in [Blanc and Labourasse, 2016]. The resulting scheme is more than an extension to 3D of [Blanc and Labourasse, 2016]. New ideas are brought in with the objective of making the method even more robust, and thus able to give accurate results on 3D cells deformed by Lagrangian hydrodynamics.

In a synthetic way, the properties of this new method are :

- Conservation;
- Convergence;
- Positivity (in the sense that the unknown remains positive under the same conditions as for the continuous problem) ;
- Reduced stencil (for parallelization by domain decomposition);
- Finite volumes on the primal mesh (greatly facilitates the coupling to hydrodynamics).
- Non-symmetric diffusion matrix ;
- Non-linear scheme (in the sense that we have to solve a discrete non-linear problem, even if the continuous problem is linear).

The non-linearity constraint is acceptable because the problems we solve are intrinsically nonlinear and that the non-linearities of the scheme and of the problem can be solved concomitantly, with a low overhead. We show numerical examples including with coupling to the cell-centered hydrodynamics, to illustrate the efficiency of the scheme.

References

[Blanc and Labourasse, 2016] Blanc, X. and Labourasse, E. (2016). A positive scheme for diffusion problems on deformed meshes. *ZAMM - Journal of Applied Mathematics and Mechanics / Zeitschrift für Angewandte Mathematik und Mechanik*, 96(6):660–680.

High Order Adaptive Mesh Refinement (AMR) for Divergence Constraint-Preserving Schemes

Dinshaw S. Balsara[†]

[†] Physics and ACMS, University of Notre Dame (dbalsara@nd.edu)

Keywords: Adaptive Mesh Refinement, Divergence Constraint, WENO-like reconstruction

ABSTRACT

Adaptive mesh refinement (AMR) is the art of solving PDEs on a mesh hierarchy with increasing mesh refinement at each level of the hierarchy. Accurate treatment on AMR hierarchies requires accurate prolongation of the solution from a coarse mesh to a newly-defined finer mesh. For scalar variables, suitably high order finite volume WENO methods can carry out such a prolongation. However, classes of PDEs, like computational electrodynamics (CED) and magnetohydrodynamics (MHD), require that vector fields preserve a divergence constraint. The primal variables in such schemes consist of normal components of the vector field that are collocated at the faces of the mesh. As a result, the reconstruction and prolongation strategies for divergence constraint-preserving vector fields are necessarily more intricate. In this paper we present a fourth order divergence constraint-preserving prolongation strategy that is analytically exact. Extension to higher orders using analytically exact methods is very challenging. To overcome that challenge, a novel WENO-like reconstruction strategy is invented that matches the moments of the vector field in the faces where the vector field components are collocated. This approach is almost divergence constraint-preserving; so we call it WENO-ADP. To make it exactly divergence constraint-preserving, a touch-up procedure is developed that is based on a constrained least squares (CLSQ) based method for restoring the divergence constraint up to machine accuracy. With the touch-up, it is called WENO-ADPT. It is shown that refinement ratios of two and higher can be accommodated. An item of broader interest in this work is that we have also been able to invent very efficient finite volume WENO methods where the coefficients are very easily obtained and the multidimensional smoothness indicators can be expressed as perfect squares. We demonstrate that the divergence constraint-preserving strategy works at several high orders for divergence-free vector fields as well as vector fields where the divergence of the vector field has to match a charge density and its higher moments. We also show that our methods overcome the late time instability that has been known to plague adaptive computations in Computational Electrodynamics.

A new fracture model based on Interface Aware SubScale Dynamics (IA-SSD) closure model

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[‡] Computational Physics Group, AWE (phil.barton@awe.co.uk)

Keywords: shock hydrodynamics, multi-material hydrodynamics, Lagrangian methods, ALE methods. Fracture,

ABSTRACT

The Interface Aware SubScale Dynamics (IA-SSD) closure model was initially developed to improve the robustness of multimaterial cells and to provide a framework for introducing additional interface physics into multimaterial cells. It was initially developed for gas dynamics in [1], extended to void closure in [2] and extended to solids and void opening in [3]. In this work as well as using IA-SSD to model material interfaces it is used as part of a fracture model to simulate the opening and closing of cracks. The method uses a continuum damage model model to determine when critical damage has occurred in a cell and macroscale fracture initiates. A zero volume fracture of void is added to any cell that has reached this critical damage threshold. The IA-SSD closure model is then used to evolve the multimaterial cell and determine whether the crack will grow. If the volume fraction of the void is very small (typically $< 1.0 \times 10^{-6}$) at the end of the remap step the new void component is deleted. Test problem results will be presented demonstrating the new fracture modelling capability.

References

[1] A. Barlow, M. Klima and M. Shashkov, "Constrained optimization framework for Interface-aware subscale dynamics closure models for multimaterial cells in Lagrangian and arbitrary Lagrangian-Eulerian hydrodynamics", *Journal of Computational Physics*, 276 (2014), pp. 92–135.

[2] A. Barlow, M. Klima and M. Shashkov, "Constrained optimization framework for Interface-aware subscale dynamics closure models for voids closure in Lagrangian Hydrodynamics" *Journal of Computational Physics*, 371 (2018), pp. 914–944.

[3] M. Klima, A. Barlow, M. Kucharik and Shashkov, "An interface-aware sub-scale dynamics multimaterial cell model for solids with void closure and opening at a all speeds", *Computers and Fluids*, 208 (2020), 104578.

Dynamic Coupling of SPH and the FEM

Brody R. Bassett[†], **Robert N. Rieben**[†] **and J. Michael Owen**[†]

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Keywords: smoothed particle hydrodynamics, finite element methods, multi-material hydrodynamics.

ABSTRACT

The goal of this work is to combine the Smoothed Particle Hydrodynamics (SPH) code Spheral [1] and the Finite Element Method (FEM) code BLAST [2] such that the problem runs in FEM until converting specified elements to SPH for computational or physics considerations. The finite element method and smoothed particle hydrodynamics have been combined previously, including using the Spheral code [3] and using a similar coupling method to the one proposed here [4]. The novelty of the approach here is in the dynamic conversion of cells from the FEM to SPH particles that engages under chosen criteria, similar to how ALE conditions initiate relaxation of the mesh. The SPH particles are initialized directly from the mesh.

Some initial results for the Noh problem in X-Y geometry are shown in Figs. 1 and 2. The mesh is first initialized in BLAST as normal, following which a uniform distribution of points with number equal to the number of quadrature points is created in each cell (Fig. 1); practically, this is done by defining a uniform quadrature with uniform weights in each element and initializing the SPH particles at these positions, which ensures that the mass of the SPH particles is consistent in cells of similar size and density. The results show good agreement at $t = 0.6$ between SPH and FEM (Fig. 2).

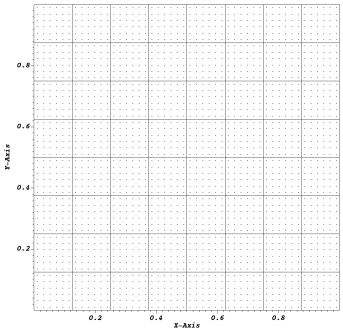

Figure 1: SPH initialization.

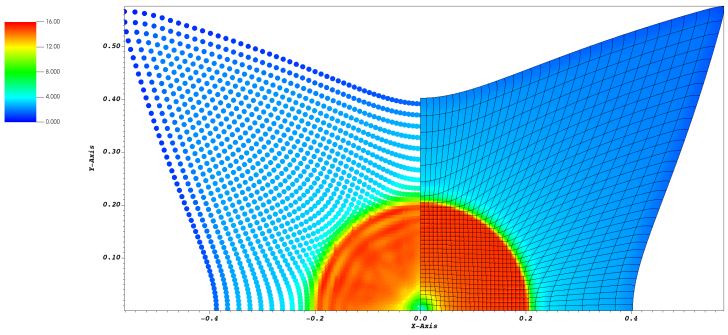

Figure 2: Mass density for SPH (left) and FEM (right).

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Formulation and computation of partitioned schemes with non-conventional computational models.

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Key Words: *partitioned schemes, reduced order models, Lagrange multipliers*

Partitioned methods for multiphysics applications allow independent solution of computational models for each constituent component, thereby increasing computational efficiency of the simulation. This efficiency can be further increased by utilizing reduced order modeling (ROM) on select subdomains. In this talk we present formulation and analysis of new partitioned schemes, which extend the approach in [1] and [2] to couplings of combinations of conventional Finite Element (FEM) and ROM sub-models. We describe the approach in the context of a model interface problem which couples a ROM with a conventional finite element method and then extend the scheme to the case of coupling a ROM with a ROM. The proper orthogonal decomposition (POD) approach is implemented to construct a low-dimensional reduced basis on half the domain and solve the subdomain problem in terms of this basis using POD/Galerkin projection. The solutions on each half of the domain are coupled using a Lagrange multiplier representing the interface flux. The multiplier at the current time step can be expressed as an implicit function of the state solutions through a Schur complement. As a result, application of an explicit time integration scheme decouples the subdomain problems, allowing their independent solution for the next time step. We show numerical results that demonstrate the proposed method's efficacy in achieving both ROM-FEM and ROM-ROM coupling.

Disclaimer. This paper describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the U.S. Department of Energy or the United States Government. SAND2021-14413 A.

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A 3D cell-centered ADER MOOD Finite Volume method for solving updated Lagrangian hyperelasticity on unstructured grids

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Keywords: hyperelasticity, Lagrangian schemes, unstructured meshes, ADER.

ABSTRACT

In this talk, we present a conservative cell-centered Lagrangian Finite Volume scheme for solving the hyperelasticity equations on unstructured multidimensional grids. The starting point of the present approach is the cell-centered FV discretization named EUCCLHYD and introduced in the context of Lagrangian hydrodynamics. Here, it is combined with the *a posteriori* Multidimensional Optimal Order Detection (MOOD) limiting strategy to ensure robustness and stability at shock waves with piecewise linear spatial reconstruction. The ADER (Arbitrary high order schemes using DERivatives) approach is adopted to obtain second-order of accuracy in time. This strategy has been successfully tested in a hydrodynamics context and the present work aims at extending it to the case of hyperelasticity. Here, the hyperelasticty equations are written in the updated Lagrangian framework and the dedicated Lagrangian numerical scheme is derived in terms of nodal solver, Geometrical Conservation Law (GCL) compliance, subcell forces and compatible discretization. The Lagrangian numerical method is implemented in 3D under MPI parallelization framework allowing to handle genuinely large meshes. A relatively large set of numerical test cases is presented to assess the ability of the method to achieve effective second order of accuracy on smooth flows, maintaining an essentially non-oscillatory behavior and general robustness across discontinuities and ensuring at least physical admissibility of the solution where appropriate. Pure elastic neo-Hookean and non-linear materials are considered for our benchmark test problems in 2D and 3D. These test cases feature material bending, impact, compression, non-linear deformation and further bouncing/detaching motions.

We will also present the extension of this scheme for solving a unified first-order hyperbolic formulation of continuum fluid and solid mechanics [2], namely the Godunov-Peshkov-Romenski (GPR) model. We demonstrate the accuracy and robustness of the scheme on a wide spectrum of material responses covered by the unified continuum model that includes inviscid hydrodynamics, viscous heat conducting fluids, elastic and elasto-plastic solids in multidimensional settings. The scheme provably respects the stiff relaxation limits of the continuous model at the fully discrete level, thus it is asymptotic preserving.

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Radiation Hydrodynamics Modeling With High-Order Implicit Shock Tracking

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Keywords: radiation hydrodynamics, shock-fitting, high-order methods, r-adaptive methods.

ABSTRACT

Traditional methods for modeling radiation hydrodynamics can present problems when encountering discontinuities. By leveraging shock tracking, an alternative method to shock capturing, we aim to generate a mesh such that element faces align with shock surfaces and other non-smooth features to perfectly represent them with the inter-element jumps in the solution basis, e.g., in the context of a finite volume or discontinuous Galerkin (DG) discretization. These methods lead to high-order approximations of high-speed flows and do not require nonlinear stabilization or extensive refinement in non-smooth regions because, once the non-smooth features are tracked by the mesh, the high-order solution basis approximates the remaining smooth features.

In this talk, we we demonstrate the viability of radiation hydrodynamics modeling using the High-Order Implicit Shock Tracking (HOIST) method [1, 2] that re-casts the geometrically complex problem of generating a mesh that conforms to all discontinuity surfaces as a PDE-constrained optimization problem. The optimization problem seeks to determine the flow solution and nodal coordinates of the mesh that simultaneously minimize an error-based indicator function and satisfy the discrete flow equations. A DG discretization of the governing equations is used as the PDE constraint to equip the discretization with desirable properties: conservation, stability, and high-order accuracy. By using high-order elements, curved meshes are obtained that track curved shock surfaces to high-order accuracy. The optimization problem is solved using a sequential quadratic programming method that simultaneously converges the mesh and DG solution, which is critical to avoid nonlinear stability issues that would come from computing a DG solution on an unconverged (non-aligned) mesh. The method is used to solve several well-known problems in radiation hydrodynamics including subsonic Marshak waves and radiation shock solutions.

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Level Set Extrapolation of Immersed Boundary Data in Unfitted Finite Element Methods for Deformable Interfaces

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Keywords: fictitious domain, immersed boundary, unfitted finite element method, level set, diffuse interface, ghost penalty, extension velocity.

ABSTRACT

We explore a new way to handle flux boundary conditions imposed on level sets [1]. The proposed approach is a diffuse interface version of the shifted boundary method (SBM, [3, 4]) for continuous Galerkin discretizations of conservation laws in embedded domains. We impose the interface conditions weakly and approximate surface integrals by volume integrals. The discretized weak form of the governing equation has the structure of an immersed boundary finite element method. A ghost penalty term (cf. [2]) is included to extend the weak solution into the external subdomain. The calculation of interface forcing terms requires (i) construction of an approximate delta function and (ii) extrapolation of embedded boundary data into quadrature points. We accomplish these tasks using a level set function, which is given analytically or evolved numerically using the algorithm developed in [5]. A globally defined averaged gradient of this approximate signed distance function is used to construct a simple map to the closest point on the interface. The normal and tangential derivatives of the numerical solution at that point are calculated using the interface conditions and/or interpolation on uniform stencils. Similarly to SBM, extrapolation back to the quadrature points is performed using Taylor expansions. The same strategy is used to construct ghost penalty functions and extension velocities. Computations that require extrapolation are restricted to a narrow band around the interface. Numerical results are presented for elliptic, parabolic, and hyperbolic test problems, which are specifically designed to assess the error caused by the numerical treatment of interface conditions on fixed and moving boundaries.

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ADER scheme for incompressible Navier-Stokes equations on Overset grids with a compact transmission condition

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Keywords: Overset Grid, Chimera Mesh, Finite Volume, Incompressible Navier-Stokes equations.

ABSTRACT

In the present work, a second order Finite Volume (FV) approach is proposed for the solution of Navier-Stokes equations for incompressible fluids over an overset configuration of meshes. In particular, an overset grid (or chimera mesh) [1] is a composition of meshes allowing to overcome the problem of the geometrical adaptation of the computational domain with a unique block of mesh. These meshes overlap each other and can move and deform during the simulation.
The Navier-Stokes equations are solved through a projection method (*Chorin-Temam*). For this reason, two different solvers are presented for the nonlinear unsetady Advection-Diffusion (AD) problem (i.e. the *prediction* of the intermediate velocity field) and the steady diffusive problem (namely the Poisson problem for the pressure in the *projection* phase).
The AD problem is numerically solved by properly adapting the prediction-correction ADER method on chimera meshes [2]. First, the motion equation for the overlapping mesh is solved in order to evolve the overset grid between two consecutive discrete times t^n and t^{n+1}. Then, through an isogeometric approach, a *local predictor solution* of AD problem is found by knowledge of the solution at time t^n. Successively, by treating the time variable as a particular spatial direction, the AD problem is written in a hyperbolic form. Finally, in a space-time FV frame and through a Local Lax-Friederichs flux along the boundary of space-time cells by exploiting the local predictor solution, the *corrected* velocity field at time t^{n+1} is recovered.
For the Poisson equation, the FV approach involves the approximation of the normal pressure gradient along the edges of each mesh cell. In particular, if the cell is not at the overlapping zone, the normal gradients along the edges are approximated by properly combining the gradients along two consecutive cells and two consecutive vertexes; otherwise the normal gradients of the cell is built as a weighted expansion of pressures in the neighbouring cells by minimising a proper convex functional [3].

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High-Order Mimetic Finite Differences on Non-trivial Geometries

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Keywords: mimetic difference operators, curvilinear grids, overlapping grids, high-order methods.

ABSTRACT

Mimetic finite-differences (MFD) are based on mimetic discrete operators, which are analogs of the differential operators: divergence, gradient, and curl, used to describe continuum problems, with successful implementations in the fields of fluid and solid mechanics.

Recent developments have focused on employing MFD to solve challenging problems by targeting partial differential equations (PDEs) with rough coefficients, jump discontinuities, and highly nonlinear problems. However, the use of MFD on irregular geometries has not been studied in detail.

We present two approaches to account for irregular geometries that cannot be handled efficiently in Cartesian coordinates. The first approach is the extension of our mimetic operators to curvilinear coordinates, and the second one is solving the problem using overlapping grids. This last technique focuses on dividing the problem domain into sub-regions using structured curvilinear grids that overlap. Due to the modeling flexibility of overlapping grids, they are used on problems that involve the simulation of complex and moving geometry.

In this research, we incorporate the curvilinear mapping transformation and the overlapping grids method into the mimetic framework. We present numerical results for linear and nonlinear problems to demonstrate the effectiveness of our schemes.

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Semi-implicit schemes with efficient finite rate stiff relaxation for compressible two-phase flow and plasticity

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Keywords: Finite-rate stiff relaxation sources; Baer–Nunziato equations; Diffuse interface; Viscous compressible multiphase flow; Material failure; Semi-implicit Finite Volume schemes; Surface tension.

ABSTRACT

Recently, several works [2, 3, 4] have been devoted to the development and numerical solution of a unified model for continuum mechanics (often called GPR, after Godunov, Peshkov, and Romenski) that can describe elasto-plastic solids and viscous or inviscid fluids with the same set of hyperbolic PDEs, rather than several PDE systems of different nature, such as the mixed hyperbolic-parabolic Navier–Stokes equations. Other physical effects that are conventionally modelled by means of equations involving second derivatives, such as surface tension forces [1], can be reformulated (from first principles) along the same lines, as first-order-hyperbolic PDEs.

In this talk, we present a semi-implicit, semi-analytical methodology aimed at accurately resolving the several different time-scales (from flow convection, acoustics, stiff relaxation processes) found in the above mentioned *unified model of continuum mechanics*, and in *compressible multiphase flow models of the Baer–Nunziato family*, with applications to visco-plasticity, crack propagation and material failure in solids, as well as to viscous multiphase fluid flows with surface tension.

We showcase the resolution and efficiency of the scheme with simulations of viscous two-phase flow with surface tension involving billions of degrees of freedom carried out at the HLRS in Stuttgart.

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Mathematical and Computational Assimilation for Plasma Boundary Physics and Integrated Fusion Reactor Simulations

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Keywords: magnetohydrodynamics (MHD), multi-material interactions, diffuse interfaces, void modelling, tokamak reactors.

ABSTRACT

This work is concerned with the implementation of computational multi-physics algorithms for the whole-system simulation of nuclear fusion reactors. The objective is to account for all regions of the reactor (plasma, vacuum and confinement vessel) within the same simulation and in a Cartesian frame of reference, which represents a significant departure from current (segregated solutions on physics-driven mesh alignment) approaches on both counts [1]. A key element of this methodology is the discretisation of topologically complex rigid boundaries as well as material and state of matter interfaces. The former implies mesh generation in the conventional CFD sense, while the latter is discretisation on both sides of the material or matter interface.

A critical element for accurate tokamak simulations is the correct and physical representation of the vacuum vessel as well as the effect of the electromagnetic properties of the confinement vessel. In this presentation, we will discuss how this is achieved through the implementation of a novel diffuse interface finite volume method [2] for the solution of the MHD equations for transient case studies, involving resistive walls and regions of true vacuum. The effect of the presence of perfectly conductive and resistive boundary conditions on the flow of the plasma inside a confinement vessel is also investigated by means of a modified rigid body ghost fluid method, which takes into account the finite resistivity of an arbitrary electromagnetic rigid body. All simulations are performed using fully explicit high-order finite volume methods, whose shock-capturing characteristics are highly favourable for the simulation of violent processes, such as vertical displacement events within tokamak reactors.

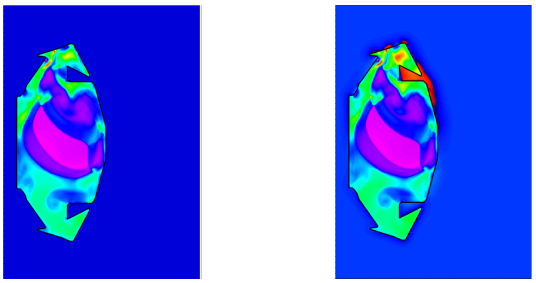

Figure 1: Magnetic field component profile for perfectly conductive wall (left) and resistive wall (right) within the ST40 fusion reactor geometry.

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A nodal-based high-order nonlinear stabilization for finite element approximation of magnetohydrodynamics

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Keywords: MHD, stabilized finite element method, artificial viscosity, residual based shock-capturing, high order methods

ABSTRACT

We propose a robust nodal artificial viscosity stabilization for finite element approximation of magnetohydrodynamics (MHD) that is high-order accurate, parameter-free, and simple to implement.

First, we motivate the new stabilization technique on scalar conservation laws using linear finite elements. The proposed method satisfies the discrete maximum principle while no *ad-hoc* parameters or mesh-size variables are invoked, as opposed to the conventional maximum principle preserving methods, e.g., upwind or Lax-Friedrichs methods. Compared to edge-based or cell-based approaches, nodal-based viscosity is simpler to store and cheaper to calculate, and is more localized in higher-order polynomial spaces. Then, the finite element residual is used to make the method high-order in space. We extend the method to solve the MHD equations. At the PDE level, we show that the added viscous regularization term is consistent with the thermodynamics [1]. At the fully discrete level, the method **contains no parameters**, is **nodal-based**, is **high-order** for smooth solutions, and has **shock-capturing** capability. The time discretization can be done by any strong-stability-preserving explicit scheme. Several challenging benchmarks are investigated, some of which are demonstrated in Figure 1.

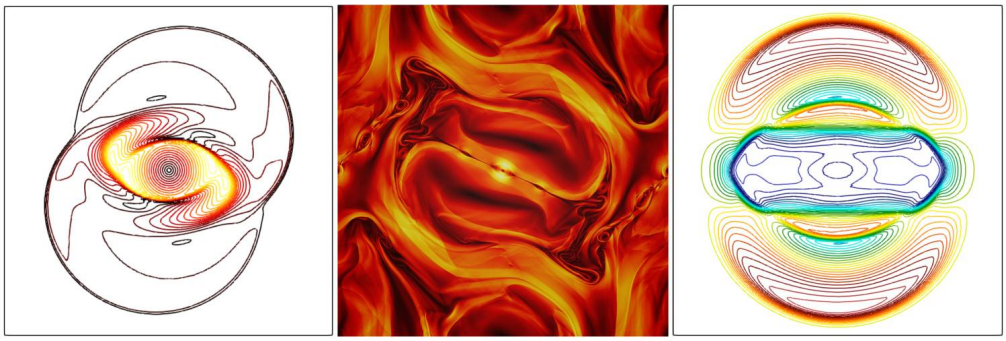

Figure 1: Residual-based viscosity finite element solutions to several popular MHD benchmarks. From left to right: mach number of the MHD rotor problem, magnetic solution of the Orszag-Tang problem, magnetic solution of the MHD Blast problem. See [2] and references therein.

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Entropy stability analysis for semi-Lagrangian cell-centered schemes

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Keywords: shock hydrodynamics, entropy stability, Lagrangian methods.

ABSTRACT

We present an optimal bound to the calculation of the time step that ensures entropy stability of finite-volume semi-Lagrangian schemes to approximate compressible gas dynamics. This condition is derived in the case of Mie-Grüneisen equation of states in dimensions 1, 2 and 3, for both the Glace [1, 2] and the Eucclhyd [3] schemes.

By construction, finite-volume methods are naturally conservative. However, consistency (and weak-consistency) can be more difficult to establish, especially in dimension greater than one. In the case of explicit schemes, the stability is generally the consequence of imposing a constraint that limits the time step δt with regard to the numerical solution at time t^n and the mesh size.

In the case of semi-Lagrangian cell-centered schemes, stability constraints of the form $\delta t < C_{CFL} \min_j \frac{\delta x_j}{c_j}$ have been expressed in [4, 5] in 1d and in [1] in 2d. The index j denotes a generic cell, δx_j a characteristic length and c_j the local sound speed.

In this presentation we will first demonstrate that in the semi-Lagrangian context, stability conditions of the form $c\delta t/\delta x < 1$ are neither necessary nor sufficient. Then we will establish a new time step constraint that ensures entropy-stability. We will provide a few numerical experiments and comment the obtained results. Finally we will discuss the overall approach.

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A diffuse interface approach for multi-material simulations of condensed phase explosives in direct contact

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Keywords: Diffuse interface formulation, condensed phase explosives, hierarchical adaptive mesh refinement, multi-dimensional root-finding algorithm.

ABSTRACT

In this work we present a new diffuse interface formulation and an associated algorithm for the simultaneous multi-material numerical simulation of condensed phase explosives in direct contact with each other. Examples include composite rate-stick (i.e. involving two explosives in contact) problems and interaction of shock waves with chemically-active particles in condensed-phase explosives. There are several formulations which address the compliant or structural response of confiners and particles due to detonations, but the direct interaction of explosives remains a challenge for most models and algorithms. The proposed formulation addresses this problem by extending the conservation laws and mixture rules of an existing hybrid augmented-Euler/multi-phase formulation [1] (suitable for solving problems involving the coexistence of reactants and products in an explosive mixture and its immiscible interaction with inert materials) to model the interaction of multiple explosive mixtures. An algorithm for the solution of the resulting system of partial differential equations is presented, which includes a new robust method for the retrieval of the densities of the constituents of each explosive mixture. This is achieved by means of a multi-dimensional root-finding algorithm which employs physical as well as mathematical considerations in order to converge to the correct solution. The algorithm is implemented in a hierarchical adaptive mesh refinement framework and validated against results from problems with known solutions. Additional case studies demonstrate that the method can simulate the interaction of detonation waves produced by military grade and commercial explosives in direct contact, each with its own distinct equation of state and reaction rate law.

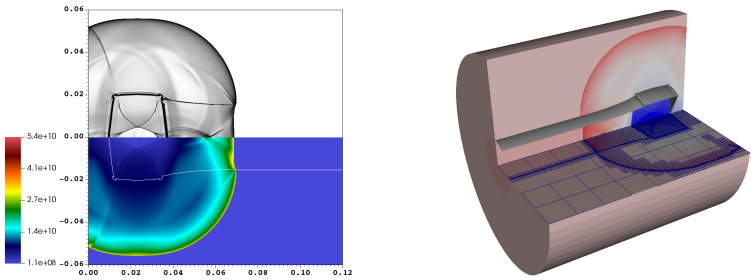

Figure 1: Numerical solutions for a four equation of state rate stick problem [2]. The figure illustrates the pressure field and density-based mock Schlieren plot (left) as well as the three- dimensional density field and the distribution of AMR grids (right).

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Interface reconstruction and development of VOFML

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Keywords: interface reconstruction, VOF, Machine Learning.

ABSTRACT

Interface tracking and interfaces reconstruction is still arguably a bottleneck in hydro-fluid simulations [2]. Volume of Fluids (VoF) methods [3] offer the possibility of flux design in combination with interface reconstruction. Recently new methods [4] emerged based on Machine Learning techniques and Machine Learning softwares. Initially these methods were developed for viscous fluids modeled with Navier-Stokes equations.

We address VOFML (that is VOF developed within a ML technology) methods trying to follow the attempt [1] which is centered on Euler equations for compressible non viscous fluids discretized on a Cartesian mesh with a Lagrange+remap scheme. Our overall objective is to design new VOFML schemes by using datasets with enhanced accuracy and to explore various scenarii in terms of dataset construction and optimization algorithms. A typical result is proposed in Figure 1 where it is visible that VOFML achieves in some cases an accuracy which is equal or superior to some standard algorithms of the discipline. We will review the principles of this methodology together with a recent new algorithm for T-junction. This new method can be based on a VOFML technique for two fluids.

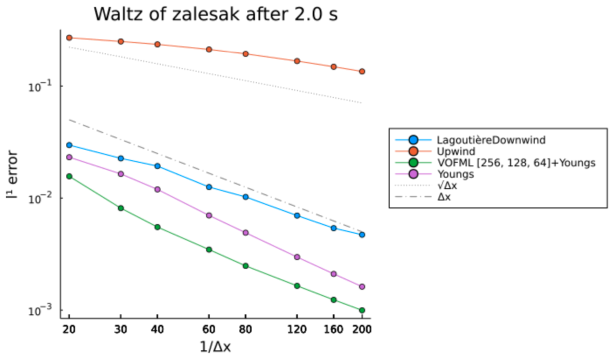

Figure 1: Convergence error for the Zalezak Waltz.

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A hyperbolic reformulation of the Navier-Stokes-Korteweg system

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Keywords: multiphase flows, diffuse interface, hyperbolic equations, high-order methods.

ABSTRACT

We present a novel first-order hyperbolic reformulation of the Navier-Stokes-Korteweg system, based on the Godunov-Peshkov-Romenski model of continuum mechanics[1], combined with an augmented Lagrangian approach[2], allowing to cast the nonlinear dispersive Euler-Korteweg equations into a first-order hyperbolic system. The latter method is based on a classical penalty method used to approximate the gradient terms in the Lagrangian by a new set of independent variables, for which suitable closure equations are sought. The governing equations for the new introduced degrees of freedom admit curl-free constraints which must be taken into account in order to obtain stable numerical solutions. Thus, we employ here a thermodynamically compatible generalized Lagrangian multiplier (GLM) approach [3], similar to the GLM divergence cleaning introduced by Munz *et al.* [4] for the divergence constraint of the magnetic field in the Maxwell and MHD equations.

The system of equations is solved at the aid of a high-order ADER Discontinuous Galerkin finite-element scheme with *a posteriori* subcell finite volume limiting in order to deal with shock waves, discontinuities and steep gradients in the numerical solution. We show numerical results for several standard benchmark problems, including Ostwald ripening in one and two space dimensions, diffuse and dispersive traveling wave solutions.

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Acknowledgements

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High-Order Accurate Entropy Stable Adaptive Moving Mesh Methods

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Keywords: entropy stable scheme, (multi-component) compressible Euler equations, special relativistic (magneto)hydrodynamics, adaptive moving mesh method, high-order accuracy.

ABSTRACT

The adaptive moving mesh method is a powerful tool to improve the efficiency and quality of numerical simulations with localized structures, e.g. sharp transitions or discontinuities in relatively localized regions, which often appear in the solutions in the quasi-linear system of hyperbolic conservation laws. For the governing equations of the fluid flows, the entropy condition should be respected according to the second law of thermodynamics, and it is desirable to seek the entropy stable (ES) schemes satisfying some discrete or semi-discrete entropy conditions. This talk will present the high-order accurate ES adaptive moving mesh methods for the hyperbolic systems and their applications to the 2D and 3D special relativistic (magneto)hydrodynamics [1, 2] and the (multi-component) compressible Euler equations with the stiffened equation of state (EOS) [3]. The key is the high-order discretization of the metrics introduced by the coordinate transformation and the construction of the high-order ES fluxes with the discrete metrics. We will also show the mesh iteration redistribution or adaptive moving mesh strategy built on the minimization of the mesh adaption functional. Extensive numerical tests have been conducted in [1, 2, 3] to validate the shock-capturing ability and high efficiency of our methods.

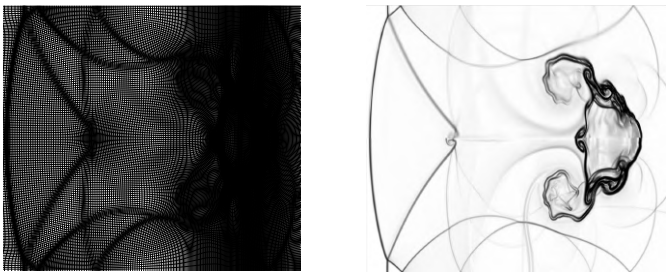

Figure 1: The shock-bubble interaction problem of the two-component Euler equations with the stiffened EOS [3]. Left: Adaptive mesh; right: schlieren image of the density obtained on 800×160 adaptive moving mesh (top half) and 2400×480 uniform mesh (bottom half).

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On Thermodynamically Compatible Schemes for Continuum Mechanics

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Keywords: first order hyperbolic formulation of continuum mechanics, thermodynamically compatible finite volume schemes, entropy inequality, energy conservation.

ABSTRACT

In this talk we discuss a new class of structure-preserving schemes for hyperbolic and thermodynamically compatible (HTC) systems with involution constraints, which have been studied for the first time by Godunov in 1961 and later in a series of papers by Godunov & Romenski. In particular, we consider the unified first order hyperbolic model of continuum mechanics proposed by Godunov, Peshkov and Romenski (GPR) that is able to describe the behavior of moving elasto-plastic solids as well as viscous and inviscid fluids within one and the same governing PDE system.
In particular, we present a new thermodynamically compatible finite volume scheme that is exactly compatible with the overdetermined structure of the model at the semi-discrete level, making use of a discrete form of the continuous formalism introduced by Godunov in 1961. A very particular feature of our new thermodynamically compatible finite volume scheme is the fact that it directly discretizes the **entropy inequality**, rather than the total energy conservation law. Energy conservation is instead achieved as a mere consequence of the scheme, thanks to the thermodynamically compatible discretization of all the other equations.
Computational results for several test cases are presented in order to illustrate the performance of the new scheme.

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A Computational Multi-physics Approach for Whole System Fusion Reactor Simulations

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Keywords: magnetohydrodynamics (MHD), multi-material interactions, mesh-generation and adaptation, IMEX schemes, tokamak reactors.

ABSTRACT

This work is concerned with the development of numerical multi-physics algorithms for the whole-system simulation of magnetically confined plasma in toroidal devices. A key area of interest is the transition of a steady-state plasma to unsteady disruption events which can lead to loss of confinement. The large disparity in spatial and temporal timescales of the physical processes involved necessitates some important considerations. Firstly, initial data for unsteady simulations must be computed from non-trivial, non-linear steady-state solutions to the underlying system of equations. Secondly, since traditional explicit schemes fail to adequately capture the inherent all-mach nature of the flow, some form of implicit treatment is required to by-pass the restrictive explicit timestep. Thirdly, uniform mesh sizing will either be too computationally demanding or will fail to capture the fine behaviours on the small scale and thus adaptive mesh generation must also be considered.

We address these issues in the development of a novel framework that will allow for feasible whole-system tokamak simulations. The objective is to account for all regions of the plasma and vessel (core, edge, and vessel wall) within the same simulation and in a Cartesian frame of reference, which represents a significant departure from current (segregated solutions on physics-driven mesh alignment) approaches on both counts [1]. A key element of this methodology is the generation of steady-state profiles, the discretisation of topologically complex rigid boundaries, and the resolution of disparate length and time scales all occurring in the same framework.

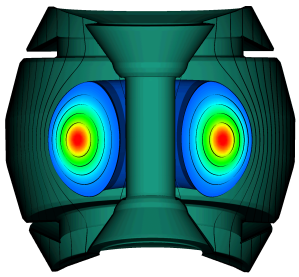

Figure 1: Equilibrium solution for the plasma density shown within the ST40 tokamak reactor geometry.

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Tusas: Toward Exascale Phase-Field Simulation

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Keywords: phase-field, solidification, exascale computing

ABSTRACT

Predictive simulation of solidification in pure metals and metal alloys remains a significant challenge in the field of materials science, as microstructure formation during the solidification process plays a critical role in the properties and performance of the solid material. The phase-field method is a common approach for quantitative modeling of dendritic growth, however extremely computationally expensive in 3D. We recently developed Tusas, a novel open-source, phase-field simulation framework based on a fully implicit parallel approach for coupled phase-field equations [1] to simulate dendritic growth 3D (Figure 1). Our phase-field method flexibly addresses multiple physical variables including composition, anisotropy, phase, temperature, orientation, and stress, fully coupled as a set of nonlinear partial differential equations on high-resolution meshes. Tusas alleviates time-scale challenges with implicit time integration, mitigates length-scale challenges with finite element spatial discretization methods, and leverages the Trilinos library and JFNK (Jacobian-free Newton-Krylov) nonlinear and GMRES (generalized minimal residual method) linear solvers for improved algorithmic efficiency and parallel scalability. Tusas' ability to scale both strongly and weakly with up to 4 billion unknowns on thousands of GPUs was demonstrated using benchmark phase-field simulations on Summit as shown in Figure 1.

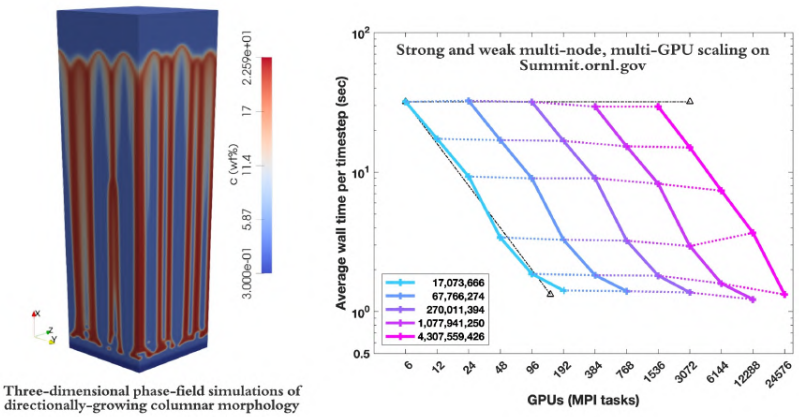

Figure 1: (left) 3D simulation snapshot showing alloy dendrite evolution using the Tusas phase-field approach. (right) Strong and weak multi-node, multi-GPUs scaling on Summit.

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High order direct ALE DG schemes on Voronoi grids with topology changes and deferred mesh optimization

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Keywords: ALE, ADER, DG, arbitrary high order in space and time, Voronoi, mesh optmization

ABSTRACT

In this talk we present a novel high order accurate direct Arbitrary-Lagrangian-Eulerian (ALE) Discontinuous Galerkin (DG) scheme with *a posteriori* subcell Finite Volume (FV) limiter, on moving Voronoi meshes that, at each time step, are *regenerated*, thus connectivity and topology changes may occur.

The Voronoi tessellation is obtained from a set of generator points moving according to a high order approximation of the local fluid velocity, combined with suitable mesh optimization techniques, that both maintain a high quality of the moving mesh and, thanks to a deferred-in-time approach to connectivity changes, reduce the occurrence of topology changes around shock and contact waves [4]. Then, the old and new elements associated to the same generator point are connected in space and time to construct the so-called space-time control volumes, whose bottom and top faces may be different polygons; also *degenerate sliver elements* are incorporated in order to *fill the space–time holes* that arise due to the topology changes [3, 2, 1]. The final ALE DG scheme is obtained by integrating a space-time conservation formulation of the governing hyperbolic PDE system over the Voronoi and sliver space–time control volumes. The obtained scheme satisfies the GCL by construction and is conservative thanks to the careful treatment of the space–time holes.

We close the presentation with a set of numerical results that proves that the novel deferred mesh optimization greatly improves the robustness of the scheme without affecting its Lagrangian character.

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Accurate remapping from 3D to 2D meshes for Multiphysics Simulations

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Keywords: Multi-physics simulations, Remapping, Dimensionality reduction.

ABSTRACT

We describe a method of remapping fields from a 3D mesh (source) to a 2D mesh (target) with accuracy guarantees and maintenance of field discontinuities across material boundaries. It is used to couple a 3D simulation to a more expensive, complex multiphysics simulation in 2D.

The method we outline performs the remapping by using particle swarms as intermediaries. The 2D target mesh is first rotated into position to align with a user-defined plane going through the 3D source mesh. Then particle swarms representing cell centers are initialized for the two meshes and the source particle fields are intialized from the corresponding cell-centers. Local Regression Estimation[1] is then used to remap fields from the source particle swarm to the target particle swarm. Finally, values from the target particles are simply copied to the 2D mesh cell centers.

Local Regression Estimation is a generalization of Moving Least Squares interpolation to simultaneously interpolate fields and their derivatives. Such direct interpolation of derivatives is much less oscillatory than estimating them using finite differences on the interpolated field. The order of accuracy of the method is controlled by the basis functions used by the Local Regression Estimator - the linear bases used here yield second-order accuracy (See Figure 1).

This method also includes a specialization called part-by-particle which minimizes bleeding or diffusion of disparate fields across material boundaries. It relies on custom support geometry for the particles called faceted support that conforms to the shape of the mesh cells.

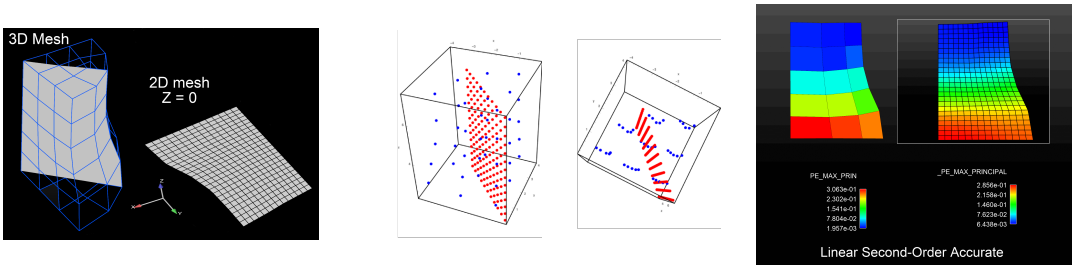

Figure 1: Remapping of max. principal stress from 3D Taylor Anvil mesh to 2D. (left) Positioning of 2D slicing plane in 3D space, (middle) two views of 3D mesh particles in blue and 2D mesh particles in red (right) Field on the slice of the source mesh and on the target mesh.

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A theoretical model of Leidenfrost's temperature

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Keywords: phase transition, film boiling, Leidenfrost temperature.

ABSTRACT

When water is projected onto a moderately heated metal plate, it spreads out, starts to boil and evaporates very quickly in a turbulent manner. Things are quite different when the metal is incandescent: the water temperature remains below the boiling temperature, divides into numerous droplets that roll, and are thrown around without boiling. This phenomenon called *Leidenfrost effect* or *film boiling*, was carefully observed in 1756 by the German physician J. G. Leidenfrost. Leidenfrost had well understood the cause of the film boiling phenomenon: there is no contact between the hot solid and water, the liquid evaporates in the vicinity of the solid and levitates on a cushion of vapor. In 1986, the film boiling phenomenon occurred in Chernobyl, and in 2011 in Fukushima, creating major nuclear accidents. The temperature above which the phenomenon occurs is called *Leidenfrost's temperature*. The reason for the existence of Leidenfrost's temperature, which is much higher than the boiling point of the liquid, is not theoretically understood. Here we prove that the Leidenfrost temperature corresponds to a bifurcation in the solutions of equations describing a dynamic evaporation of non-equilibrium liquid–vapor interface. For water, the theoretical values of the obtained Leidenfrost temperature and that of the liquid bulk, which is smaller than the boiling point of the liquid, fit the experimental results found in the literature.

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Transition and Multiphysics in 3D ICF Capsule Implosions

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Keywords: multi-material hydrodynamics; large-eddy simulation; multiphysics.

ABSTRACT

Inertial Confinement Fusion (ICF) capsules are unique with regards to hydrodynamic instabilities: the time-scales are short relative to turbulence development, so understanding the 3D transition is particularly important; 2) as the core heats, viscosity becomes important so that there is not much scale separation between the outer length scale and the viscous dissipation length scale; 3) jetting is a unique and critical phenomenon to ICF applications that arises due to Rayleigh-Taylor (RT) instability growth in a thin shell. Experiments at laser platforms such as OMEGA at University of Rochester and the National Ignition Facility (NIF) al LLNL, create a new urgency for assessing the new computational paradigms and the verification and validation of their *3D* modeling aspects in the research codes. We build on prior ICF simulations work, using *a Navier-Stokes based plasma viscosity model* in conjunction with LANL's new xRAGE HLLC hydrodynamics with *directionally unsplit algorithms and low-Mach-number correction* (LMC), enabling higher fidelity *on coarser grids* [1,2] – e.g., Taylor-Green vortex (TGV) results in Fig.1.

We simulate two ICF experiments: 1) OMEGA 50997 [3], involving an SiO_2 glass shell filled with a mixture of D_2 and ^3He and Kr impurities added to the gas, where 13.5 kJ of energy is deposited within the SiO_2 shell during 1ns, approximating the direct-drive laser absorption process in the experiment. 2) an indirect-drive NIF cryogenic capsule experiment, N170601 [4,5] requiring multi-group radiation diffusion to transport x-ray energy from the cylindrical *Hohlraum* to the target capsule. The 3D simulation model involves miscible (gas / plasma Schmidt number ~ 1) material interfaces and 3T plasma physics treatments [6]. We use relatively coarse 2D runs through onset of turbulence, followed by mapping to highly resolved 3D mesh with suitable 3D seed-perturbations [6]. We assess ILES [1,2] and *Dynamic BHR* [7] ICF predictions with the new xRAGE numerical hydrodynamics. Challenges coupling 3D hydrodynamics and multiphysics (radiation-diffusion, 3T physics, plasma viscosity and diffusivity) are discussed in this context.

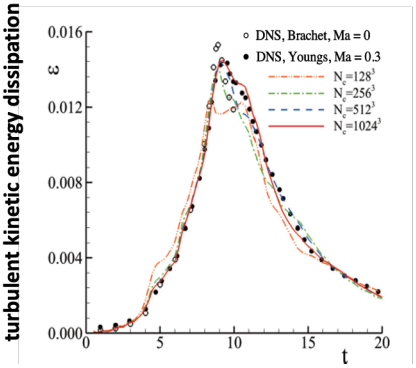

Figure 1. Turbulent KE dissipation for Ma=0.3, Re=3000 TGV [9]. LMC xRAGE capably resolves viscosity and compressibility effects.

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Invariant-domain preserving high-order IMEX schemes

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Keywords: Time integration, IMEX methods, Conservation equations, hyperbolic systems, Navier–Stokes equations, Euler equations, invariant-domains, high-order method.

ABSTRACT

We consider high-order time discretizations of a Cauchy problem where the evolution operator comprises a hyperbolic part and a parabolic part (say diffusion and stiff relaxation terms). The said problem is assumed to possess an invariant domain. We propose a technique that makes every implicit-explicit (IMEX) time stepping scheme invariant domain preserving and mass conservative. Following the ideas introduced in Part I on explicit Runge–Kutta schemes [1], the IMEX scheme is written in incremental form and, in each stage of the scheme, we first compute low-order hyperbolic and parabolic updates, followed by their high-order counterparts. The proposed technique, which is agnostic to the space discretization, allows to optimize the time step restrictions induced by the hyperbolic sub-step. To illustrate the proposed methodology, we derive three novel IMEX schemes with optimal efficiency and for which the implicit scheme is singly-diagonal and L-stable: a third-order, four-stage scheme; and two fourth-order schemes, one with five stages and one with six stages. The novel IMEX schemes are evaluated numerically on a stiff ODE system. We also apply these schemes to nonlinear convection-diffusion problems with stiff reaction and to compressible viscous flows possibly including grey radiation.

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A colocalized scheme for three-temperature grey diffusion radiation hydrodynamics.

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Keywords: colocalized Lagrangian scheme, radiation hydrodynamics, grey diffusion, discrete entropy production, plasma physics simulations.

ABSTRACT

A positivity-preserving, conservative and entropic numerical scheme is presented for the three-temperature grey diffusion radiation hydrodynamics model. More precisely, the dissipation matrices of the colocalized semi-Lagrangian scheme are defined in order to enforce the entropy production on each species (electron or ion) proportionally to its mass. A reformulation of the model is then considered to enable the derivation of a robust convex combination based scheme. This yields the positivity-preserving property at each sub-iteration of the algorithm while the total energy conservation is reached at convergence. Numerous pure hydrodynamics and radiation hydrodynamics test cases are carried out to assess the accuracy of the method. The question of the stability of the scheme is also addressed. It is observed that the present numerical method is particularly robust.

Complex Multi-Material Shock Interactions Using the Moving Discontinuous Galerkin Method with Interface Condition Enforcement

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Keywords: Shock Hydrodynamics, Implicit shock-fitting, High-order Finite Element Method, Space-time, Discontinuous Galerkin

ABSTRACT

We apply the Moving Discontinuous Galerkin Method with Interface Condition Enforcement (MDG-ICE) to the case of simulating unsteady, higher-dimensional, multi-material benchmark problems, including the cylindrical Noh and triple point shock interaction problems in order to assess the ability of MDG-ICE to overcome limitations of arbitrary Lagrangian-Eulerian (ALE) methods. MDG-ICE 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. Therefore, MDG-ICE has the ability to detect and track shocks, material interfaces, and their interaction without resorting to shock capturing or other stabilization methods. Moreover, since MDG-ICE uses a space-time formulation, it avoids the need for a remap operation that are used by ALE methods when the spatial grid becomes severely distorted. We observe that MDG-ICE avoids the undesirable phenomena of traditional ALE methods including the wall-heating phenomenon and the appearance of mixed zones.

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An iterative algorithm for solving the nonlinear heat transport equations

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Keywords: numerical methods for heat conduction, multi-material diffusion, heat transport

ABSTRACT

Radiation-hydrodynamics codes typically solve the heat transport equations using a nominally implicit approach [1] in which temperature-dependent coefficients are treated as constant during each time-step. However, plasma conductivities and heat capacities are highly sensitive to temperature, so that this approach still places highly restrictive constraints on the time-step to maintain stability. This is particularly restrictive in situations where energy is rapidly deposited into small regions containing high-Z materials next to a near-vacuum region, such as in laser-driven hohlraums – high-Z cylinders used to generate X-rays to drive inertial confinement fusion implosions – where the time-step required to achieve numerical convergence can be $< 1/100$ of the Courant condition set by the hydrodynamics.

We present an iterative method for solving the full non-linear heat transport equations [2]. Our approach is reminiscent of Anderson acceleration [3, 4]. This approach improves the convergence of iterative techniques by setting the approximate solution to be the linear combination of previous iterates that minimizes the residual. We adapt this approach by performing approximate Newton updates of each iterate, using an approximate calculation of the Jacobian in order to better account for the strong temperature dependence of the coefficients, and add an additional step to handle situations where the residual is not decreased. We use a simple test problem (Fig. 1) to show that this approach accelerates convergence compared to Picard iterations and is significantly computationally cheaper than subcycling.

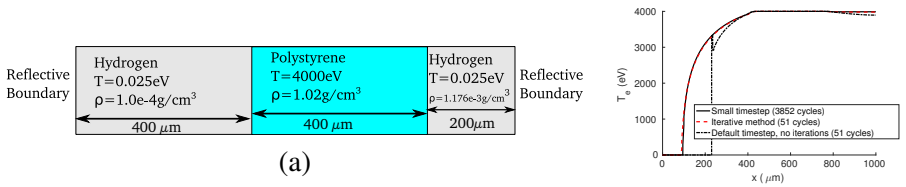

Figure 1: (a) Diagram of test problem initial conditions; (b) Test problem heat profile at $t = 3.0$ns using different solution techniques.

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On the need for enforcing discrete entropy inequalities when solving scalar conservation laws and hyperbolic systems

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Keywords: property-preserving schemes, hyperbolic conservation laws, discrete entropy inequalities, algebraic flux correction, monolithic limiting.

ABSTRACT

Following recent developments in the design of bound-preserving algebraic limiters, we investigate how to ensure entropy stability for approximate solutions of hyperbolic problems. In particular, we demonstrate the need for enforcing semi-discrete entropy inequalities by considering some scalar conservation laws, for which a sequence of approximations converges to non-entropic weak solutions [KPP07, KQdL20]. We then apply our schemes to the compressible Euler equations and related models. In this context, we also review how the incorporation of entropy viscosity affects the results of the semi-discrete methods.

Next, we elaborate on the need for additionally enforcing fully-discrete entropy inequalities [KHR22]. The reason why entropy stability in this sense is desirable, is that without this property one cannot prove Lax–Wendroff type theorems. In other words, this property is needed to be able to show that a sequence of approximations converges to the respective entropy solution of a system. Following the work of Lozano [Loz18], we observe that explicit time stepping schemes produce entropy, and, to overcome this problem, design a fully discrete explicit fix. Unfortunately, such schemes are known to reduce the convergence rate of the scheme to first order of accuracy. Thus, we design a corresponding fix for implicit time stepping schemes.

Again, we present numerical results for scalar conservation laws and the compressible Euler equations. The discussed schemes are also applicable to certain systems of balance laws, such as the shallow water equations and have been demonstrated to work well for other target discretizations. In particular, we have proposed similar bound-preserving and entropy-stable methods for discontinuous Galerkin and finite volume baseline schemes.

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Enforcing Interface Coupling Conditions within a Discontinuous Galerkin Sharp Interface Method: Application to Viscous Compressible Gas-Liquid Flows

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Keywords: Unfitted, Cut-cell, Sharp interface, High-order, Discontinuous Galerkin, Gas-Liquid Flow

ABSTRACT

Over the past decades, numerous unstructured high-order methods for solving partial differential equations have been developed, theoretically offering increased accuracy for the same computational cost when compared to standard low-order methods. However, there are several obstacles on the road to the systematic adoption of these methods for industrial applications. One of them relates to the preservation of the high-order features for low-regularity solutions, which e.g. occur in two-phase flow problems. To overcome this issue without relying on complex and time-consuming remeshing procedures, we propose an eXtended Discontinuous Galerkin (XDG) method [1, 2], based on the work of [3]. The resulting unfitted-interface discretization is particularly appealing to treat multi-material fluid flow with complex interface dynamics. The challenges associated to such flows are then shifted to the ability of the current method to (i) represent and follow the interface, (ii) sharply capture the solution discontinuities, and (iii) enforce the physical coupling conditions between the materials.

This work is particularly concerned with the last challenge, i.e. the development of coupling strategies between dissimilar materials in the context of a FEM-type cut-cell method. Of particular interest is the interaction between viscous compressible gas and liquid phases. This represents a challenging situation as both the viscous and convective fluxes need to be correctly balanced at the interface to accurately predict the mass, momentum and energy exchanges between both phases. To this end, a novel formulation has been established: state-of-the-art multiphase Riemann solvers are used to handle the convective fluxes while a weighted stabilized Nitsche's method weakly enforces the viscous jumps.

An overview of the different building blocks of our solver will first be presented. The emphasis will then be placed on explaining the novel coupling strategy specifically designed for viscous compressible two-phase flows involving phase transitions. Results about gas-liquid test cases will illustrate the ability of the current approach to achieve high-order accuracy in the presence of large contrast phase interfaces.

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A new two-dimensional blood flow model with arbitrary cross sections

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Keywords: Hyperbolic conservation and balance laws, Blood flows, High-order numerical schemes.

ABSTRACT

A new two-dimensional model for blood flows in arteries with arbitrary cross sections is derived. The model consists of a system of balance laws and it allows for variations both in the axial and in the angular directions. The system dictates conservation of mass and balance of momentum. The equations are derived from the incompressible Navier-Stokes equations. It models cross-sectional averages of fluid flows in narrow, large vessels. The main properties of the system are discussed and a positivity-preserving well-balanced second-order central-upwind scheme is presented. The merits of the scheme will be tested in a variety of scenarios. We analyze the time evolution of the blood flow under different initial conditions such as perturbations to steady states consisting of a bulging in the vessel's wall. We consider different situations given by distinct variations in the vessel's elasticity.

This work was partially supported by grant UNAM-DGAPA-PAPIIT IN112222 & Conacyt A1-S-17634 (Investigacion realizada gracias al programa UNAM-DGAPA-PAPIIT IN112222 & Conacyt A1-S-17634).

High-order composite multi-dimensional finite volume schemes on unstructured meshes

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Keywords: continuous composite nodal/edge unstructured multi-dimensional Approximate Riemann solver, high-order method, non-linear reconstruction, induced limitation.

ABSTRACT

For the approximation of multi-dimensional hyperbolic problems, we consider a general design of **composite** finite volume schemes on arbitrary unstructured meshes which are consistent and locally conservative. It offers the possibility of having numerical Approximate Riemann Solver ARS (Roe, VFFC, Rusanov, HLL(-) ...) defined at edge but also **defined at node** using extension proposed in [1].

For straight edge meshes, using some geometrical properties of normal vectors, we can associate symetric quadrature formula at arbitrary order, reproducing properties such as local conservation, and volumic equality of arbitrary cells.

Dealing for example on a one parameter family (like a θ scheme), we obtain *pure nodal* polygonal scheme, *pure edge* polygonal scheme and also *truly composite degenerate conical* scheme as special cases.

For Euler gas dynamics equation, we focus on a **non-linear reconstruction** for massic variables and propose a way to circumvent the direct velocity limitation which is not physically relevent. We show how to deduce from relation of total massic energy $E = \epsilon + \frac{1}{2}|\mathbf{U}|^2$ a limited velocity reconstruction **induced** by the direct limitation of internal massic energy ϵ.

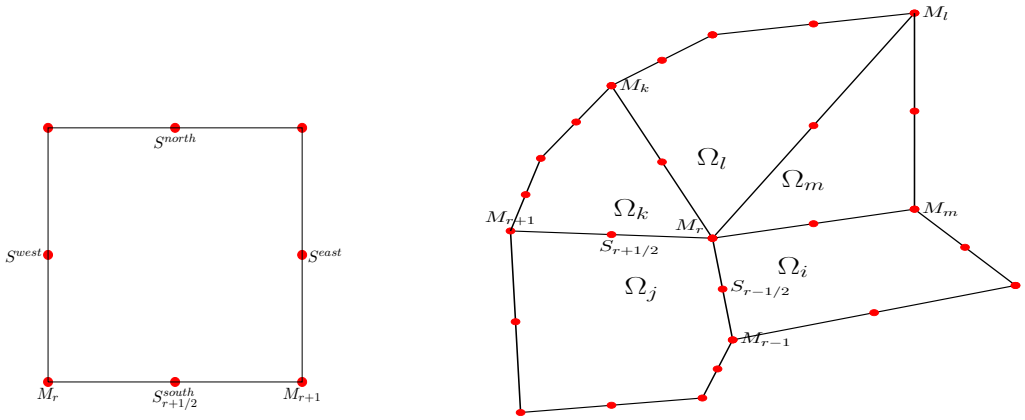

Figure 1: For all kind of mesh; structured (on left) and unstructured (on right), composite scheme exhibits two types of degree of freedom (seen like quadrature points) on cell boundary : $(\mathbf{M}_r/\mathbf{S}_{r+1/2})$ (resp. edge extremities / internal edge points).

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A Relaxation Formulation of the Navier-Stokes-Korteweg Equations

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Keywords: diffuse interface methods, multiphase flow, high-order methods.

ABSTRACT

Multiphase flow with phase transition on the pore-scale is a growing and challenging field of research. Diffuse interface approaches are promising candidates to model multiphase phenomena on the pore-scale due to their ability to deal with two-phase flow, surface tension, phase transition and complex domain topologies. A well known model which incorporates all the aforementioned physical effects is the Navier-Stokes-Korteweg-van der Waals (NSK) model [1]. However, several issues have to be faced if the numerical discretization of the NSK system is aimed. First, the non-convex bulk Helmholtz free energy induces a non-monotonous pressure function, which in turn results in mixed hyperbolic-elliptic first-order fluxes. Secondly, the gradient dependence of the underlying energy potential generates a third-order derivative in the momentum equation, which prevents the straight forward use of boundary conditions at the three-phase contact line.
In this talk, we present the non-isothermal extension of our recently presented relaxation formulation of the isothermal NSK equations [2]. The model is consistent with the Second Law of Thermodynamics and converges to the non-isothermal NSK equations for an appropriate choice of the modelling parameters. Moreover, strict hyperbolicity of the convective fluxes is guaranteed for a sufficiently large Korteweg parameter. Furthermore, we can provide thermodynamic consistent non-equilibrium boundary conditions for the fluid-solid interface, which can be specified without the requirement to solve a global elliptic equation [1] or any additional iterative procedure at the solid boundary [3].
An extension of the open-source high-order accurate CFD framework FLEXI is used for the discretization of the model. We demonstrate a very good agreement with the original NSK model in several space dimensions. The comparison is concluded by the simulation of highly dynamic 3D droplet collisions. Turning to the pore-scale, we proof our model to be consistent with the Young-Laplace law. Finally, we demonstrate the ability of our framework to handle complex domains by the simulation of a spinodal decomposition in a synthetic porous medium.

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Structure preserving numerical methods in a multi-scale context

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Keywords: compressible Euler equations with gravity, low Mach limit, asymptotic preserving schemes, well-balanced.

ABSTRACT

This lecture will focus on the compressible Euler equations, seen either as the formal limit from the Boltzmann equations or seen together with its incompressible limit. Numerical schemes that manage to follow these limits are studied together with their ability to maintain stationary solutions. We will report among other things on results from [1], [2], [3], [4].

This is joint work with among others with Wasilij Barsukow, Claudius Birke, Min Tang and Fritz Röpke.

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A three-dimensional cell-centered Lagrangian Lax-Wendroff HLL hybrid scheme

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Keywords: Lagrangian methods, cell-centered schemes, Lax-Wendroff.

ABSTRACT

Unlike many modern cell-centered methods for Lagrangian hydrodynamics that rely on nodal solvers, our recently developed scheme [1] is improving on the classical Lax-Wendroff method. The scheme is currently formulated for three-dimensional inviscid compressible flows on unstructured meshes, while earlier works have adapted the scheme for dynamics of elasto-plastic materials [2] and cylindrical geometry [3]. The predictor-corrector formulation of the Lax-Wendroff method is used which allows us to determine the mesh movement using the predicted fluid velocity centered in mesh nodes. The over-dispersion of the method in the presence of shock waves is corrected by dissipative fluxes inspired by the Harten-Lax-van Leer Riemann solver, providing artificial viscosity and artificial energy dissipation.

We demonstrate the performance of the proposed method on 3D variants of known benchmark numerical tests. The method maintains good spherical symmetry on non-conforming meshes and reduces the wall heating effect, as can be shown for example in the Noh problem (see Figure 1).

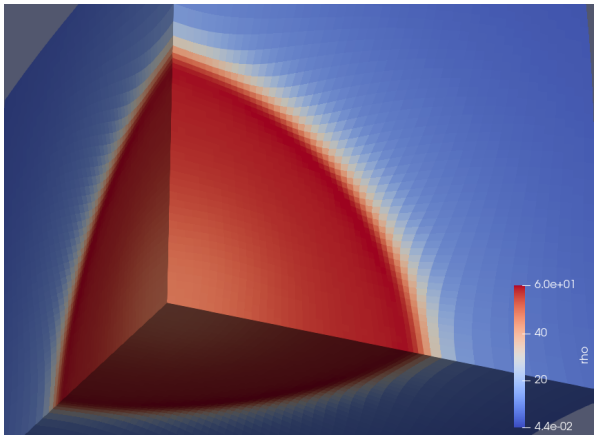

Figure 1: A spherical constant-velocity accretion shock (Noh problem), density, $t = 0.6$, 50^3 cells.

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An Arbitrarily High-Order Moment Limiter for the Discontinuous Galerkin Method

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Keywords: conservation laws; limiters; high-order methods.

ABSTRACT

We present an arbitrarily high-order limiter for the discontinuous Galerkin method on triangular meshes and its extension to nonconforming meshes that arise in adaptive computations. It limits the solution coefficients (moments) by reconstructing the slopes along a set of directions in which the moments decouple. We perform the reconstruction of the slopes on a compact stencil consisting of only eight elements, regardless of a mesh configuration. We also propose a simple algorithm to update the reconstruction stencil of elements in an adaptively refined triangular mesh. Our algorithm is implemented entirely on the graphics processing unit (GPU) and avoids race conditions. We provide numerical experiments to validate the robustness of the limiter in the presence of discontinuities and high-order accuracy on smooth solutions. Finally, we report wall clock studies to analyze the performance of the proposed limiter for the computational cost involved in setting up and executing the limiting procedure.

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New Limiters and Entropy Fixes for Discontinuous Galerkin Methods

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Keywords: nonlinear hyperbolic problems, discontinuous Galerkin methods, discrete maximum principles, entropy stability, flux correction, slope limiting.

ABSTRACT

We present a new perspective on flux and slope limiting for discontinuous Galerkin (DG) discretizations of hyperbolic conservation laws. The piecewise-constant (P_0) version corresponds to a low-order finite volume method, which is entropy stable and locally bound preserving. A piecewise-linear (P_1) or higher order DG approximation preserves these nonlinear stability properties if it is equipped with properly designed limiters. We formulate the corresponding inequality constraints and show how they can be enforced in practice. In particular, we introduce new flux limiters that ensure the validity of discrete maximum principles and cell entropy inequalities for cell averages [1, 2, 3]. Moreover, the partial derivatives of the DG-P_1 approximation are constrained using a slope limiter to ensure preservation of entropy stability and boundedness of partial derivatives in terms of low-order reconstructions. For example, the vertex-based Barth–Jespersen algorithm can be used for this purpose. We also present new slope limiters based on flux constraints and constraints for directional derivatives. The derivative-based approach makes it possible to preserve directional monotonicity in applications to problems that require different treatment of different space directions. At the flux limiting stage, the anisotropy of the problem at hand can be taken into account by using a customized definition of local bounds for inequality constraints. At the slope limiting stage, we adjust the magnitude of individual directional derivatives using low-order reconstructions from cell averages to define the bounds. In this way, we avoid unnecessary limiting of well-resolved derivatives at smooth peaks and in internal/boundary layers. The combination of direct flux limiting with slope limiting under derivative constraints produces the best results in our numerical experiments. The new methodology can be readily extended to hyperbolic systems following [4]. In the context of hp-adaptivity, optimal accuracy can be achieved by using flux/slope limiting in P_1 subcells of macroelements marked as 'troubled' by a smoothness indicator.

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An asymptotic preserving method for the linear transport equation on general meshes

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Keywords: Finite Volume, radiative transfer, asymptotic analysis, computational transport, monotone anisotropic diffusion, unstructured meshes.

ABSTRACT

This talk presents a finite-volume scheme [Anguill et al., 2022] for a linear transport equation derived from a linearization of the radiative transfer equations. This scheme has been implemented on 2D unstructured meshes, and satisfies the following properties:

- **P1** to be consistent on general meshes,
- **P2** to enforce the conservation of radiative energy,
- **P3** to be able to handle all the radiation regimes from free-streaming to diffusion (Asymptotic Preserving),
- **P4** to have the radiative energy degrees of freedom located at the centers of the elements to ensure the compatibility with the hydrodynamic scheme.
- **P5** to allow us to use the limit diffusion scheme of our choice.

As our scheme is implicit, we used a system of sub-iterations to avoid to solve a global linear system (of size equal to the cells number $\times$ directions number), while remaining stable. In addition, this sub-iterations system is acting as a fixed point loop, in order to get rid of the non-linearity of the diffusion scheme. Thanks to the properties of our diffusion scheme, we enforce the energy to remain positive in this regime, for which radiation and matter temperature are strongly coupled. We have conducted numerical 1D tests on structured and unstructured 2D meshes, which assess that the expected properties are respected. Finally, we carried out the Lattice problem test to compare our results with existing methods, in particular the Discontinuous Finite Element (DFE) discretization.

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Entropy stable and positivity preserving Godunov-type schemes for multidimensional hyperbolic systems on unstructured grid. Part II: multidimensional validation

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Keywords: Godunov scheme, Riemann solver, Entropy stable, Lagrangian-Eulerian gas dynamics.

ABSTRACT

A class of cell centered Finite Volume schemes has been introduced to discretize the equations of Lagrangian hydrodynamics on moving mesh [4]. In this framework, the numerical fluxes are evaluated by means of an approximate Riemann solver, based at the nodes of the mesh, which provides the nodal velocity required to move the mesh in a compatible manner. In this presentation, we describe the generalization of this type of discretization to hyperbolic systems of conservation laws written in Eulerian representation. The evaluation of the numerical fluxes relies on an approximate Riemann solver located at the mesh nodes. The construction of this nodal solver uses the Lagrange-to-Euler transformation introduced by Gallice [3] and revisited in [1,2] to build positive and entropic Eulerian Riemann solvers from their Lagrangian counterparts. The application of this formalism to the case of gas dynamics provides a positive and entropic finite volume scheme under an explicit condition on the time step. Moreover, this study allows us to rigorously recover the original scheme described in [5] for the Euler equations while correcting its defects. An associated MPI Finite Volume simulation code has been built in multi-dimensions for unstructured meshes. A large set of 2D/3D numerical experiments show that the proposed solver is less sensitive to spurious instabilities such as the infamous carbuncle. To further improve accuracy, the current scheme has been extended to second-order in time and space. The numerical assessment of this new method by means of representative test cases is very promising in terms of robustness. A large palette of numerical examples will assess that the obtained numerical schemes is performing appropriately. If time permits several extension will be discussed: implicitness, source terms, etc.

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Extension of the Interface Aware SubScale Dynamics (IA-SSD) closure model to 3D

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Keywords: shock hydrodynamics, multi-material hydrodynamics, Lagrangian methods, ALE methods

ABSTRACT

The Interface Aware SubScale Dynamics (IA-SSD) closure model was initially developed to improve the robustness of multimaterial cells and to provide a framework for introducing additional interface physics into multimaterial cells. It was initially developed in 2D for gas dynamics in [1], extended to void closure in [2] and extended to solids and void opening in [3]. In this work the IA-SSD closure model is extended to 3D. In addition to modelling material interfaces in 3D this capability is required for use as part of a new fracture model, where the closure model will be used to simulate the opening and closing of cracks. The new fracture capability will be the subject of another talk at this meeting. Test problem results will be presented demonstrating the new 3D IA-SSD closure model in 3D multimaterial ALE simulations.

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Entropy stable and positivity preserving Godunov-type schemes for multidimensional hyperbolic systems on unstructured grid. Part I: theoretical concepts

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Keywords: Finite Volume, Simple Riemann solver, Lagrangian and Eulerian gas dynamics.

ABSTRACT

This work describes a novel subface flux-based Finite Volume (FV) method for discretizing multi-dimensional hyperbolic systems of conservation laws over general unstructured grids. The subface flux numerical approximation relies on the notion of simple Eulerian Riemann solver introduced in the seminal work [2]. The Eulerian Riemann solver is constructed from its Lagrangian counterpart by means of the Lagrange-to-Euler mapping. This systematic procedure ensures the transfer of good properties such as positivity preservation and entropy stability [2, 1]. In this framework, the conservativity and the entropy stability are no more locally face-based but result respectively from a node-based vectorial equation and a scalar inequation. The corresponding multi-dimensional FV scheme is characterized by an explicit time step condition ensuring positivity preservation and entropy stability. The application to gas dynamics provides an original multi-dimensional conservative and entropy-stable FV scheme wherein the numerical fluxes are computed through a nodal solver which is similar to the one designed for Lagrangian hydrodynamics [3]. We also observe that the present approach relies on an approximate Riemann solver for Eulerian gas dynamics characterized by naturally ordered wave speeds contrarily to the one introduced in [4]. The robustness and the accuracy of this novel FV scheme are assessed through various numerical tests. We observe its insensitivity to the numerical pathologies that plague classical face-based contact discontinuity preserving FV formulations.

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[4] Z.J. Shen, W. Yan and G.W. Yuan, A robust and contact resolving Riemann solver on unstructured mesh, Part I, Euler method. *J.Comput. Phys.*, 2014, **268**.

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Cell-centered Lagrangian scheme for multi-material flows with pressure equilibration

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Keywords: Cell-centered Lagrangian scheme, multi-material flows, entropy dissipation, equal pressure closure.

ABSTRACT

Abstract. A cell-centered Lagrangian scheme is presented for the multi-material hydrodynamics model with equal pressure assumption. The scheme is conservative in mass, momentum and total energy while being entropic per material. This last point is critical for various engineer applications but remains in general not addressed. The entropy dissipation of each material is taken as an arbitrary portion of the global entropy dissipation hence mimicking different viscosity operators and the underlying vanishing viscosity solution. The scheme is confronted with different 1 or 2-dimensional test cases where materials have highly different equations of state. These test cases attest the robustness of the scheme and show that pressures are kept equal up to the scheme order or even strictly if an additional relaxation procedure is added.

Interface capturing methods for heterogeneous multiphase flows

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Keywords: Multi-material hydrodynamics, diffuse interface, composite Riemann problem (CRP)

ABSTRACT

Numerical simulation of multiphase flows with the interface reconstruction is considered in the framework of the non-equilibrium Baer-Nunziato (BN) type model. As it is shown in [1] this model can be used either for modeling multiphase mixtures with small inclusions of the dispersed phase in the continuum, approach without interface reconstruction or for modeling multimaterial mixtures with diffuse interface methods. In the second case it is necessary to use appropriate relaxation models and proper interface pressure and velocity closure relations.

The basic elements of the proposed approach are a simple local sub-cell reconstruction of the interface near cell faces and modeling of the relaxation processes in mixed cells with using of Composite Riemann Problem (CRP)[2]. We propose a WCRP - a generalization of the CRP solution to the non-equilibrium BN-type model. It takes into account the primary and secondary waves generation that is treated with the HLL and HLLC methods. The proposed approach does not require any artifictial relaxation parameters and makes it possible to maintain almost diffusionless contact boundary calculations.

Effectiveness and accuracy of the method proposed are demonstred on a set of banchmark problems among which are transferring interface, multimaterial Sod problems, triple point problem and shock-bubble interaction.

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Feature Preserving Interface Reconstruction and Tracking Using Piecewise Circular Facets with Cusps

J. Liu[1,2], K. Weiss[2] and J. Yao[2*] (presented by D. Miller)

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Keywords: Volume of fluids interface reconstruction; high-order-methods; ALE methods.

ABSTRACT

We show that non-diffusive volume advection in two-dimensions is achieved with several benchmark problems using a newly developed high-order volume of fluids (VOF) interface reconstruction method.

1. A new VOF interface reconstruction method using circular/corner facets (linear facets are a degenerate case of arcs). We create a circular interface facet in each mixed zone by matching neighbor volume with a hybrid Newton's-bisection method and the local solution is final. In the general case, the new VOF interface reconstruction has 3rd order accuracy and can be easily made seamless. The new method addresses intrinsic issues with Young's method such as gaps between interface facets in the case of a curved interface, and inability to define curvature or identify corners.
2. A non-diffusive volume advection scheme. In an ALE advection step, a well-defined interface can be carried over through a Lagrange step and used to compute volume distribution into a relaxed mesh. Then, an interface reconstruction step is performed to redefine the interface in the relaxed mesh. We note that the interface carried over is also a solution of interface reconstruction because all the volume fractions in the relaxed mesh are naturally matched. We provide an interface tracking method compatible with our reconstruction scheme, where it is granted to use the prior info as an initial guess to capture sub-mesh resolution features. As a result, we are able to treat multiple facets inside a single mixed cell and obtain highly accurate, non-diffusive solution for advection problems with rather coarse meshes. We show our solutions for two-dimensional incompressible flows with two materials with a) the X + O diagonal translation; b) the Zalesak rotational test; and c) the single vortex spiral test.

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A Multi-Physics Methodology for Four States of Matter

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Keywords: multi-material hydrodynamics, diffuse interface methods, sharp interface methods, magnetohydrodynamics, lightning

ABSTRACT

A numerical methodology for the simultaneous numerical simulation of four states of matter, gas, liquid, elastoplastic solids and plasma, will be presented, with applications to lightning simulations considered [1]. The distinct, interacting physical processes are described by a combination of compressible, inert, and reactive forms of the Euler equations, multi-phase equations, elastoplastic equations, and resistive MHD equations. Under the conditions of a lightning strike, the non-linear coupling between these very different materials is achieved through the recasting of the governing evolution equations into the same hyperbolic form. This allows for the solution of a single system, on a single computational grid, using shock-capturing finite volume schemes, as opposed to the finite element approach commonly employed. This approach can deal with combinations of sharp- and diffuse-interface methods to track or capture the behaviour between the materials, depending on the physics of the interface. The boundary conditions between different systems of equations, i.e. at sharp interface, are applied using mixed-material Riemann solvers, which have been derived for each pair of materials within this model.

A variety of test cases are considered, demonstrating the applicability of this approach to lightning simulations. The ability of this approach to handle complex material geometries is shown through arc attachment to aircraft fastener geometries, which hold together material panels with different material and electromagnetic properties. The use of adaptive mesh refinement to improve the resolution of complex geometric features shall also be demonstrated. Finally, in order to demonstrate the full capability of this model, a case study involving all four states of matter will be considered; a lightning strike scenario on a metal tank containing a liquid and a combustible gas.

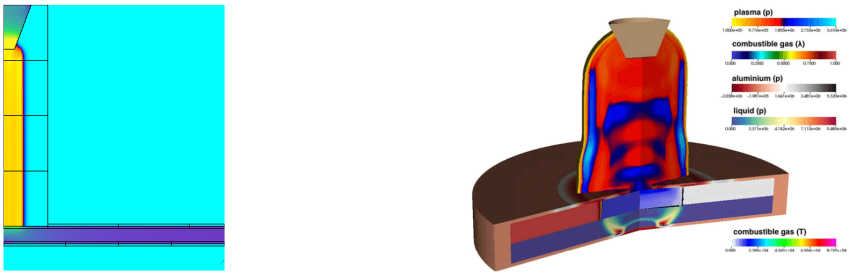

Figure 1: Left: Mesh refinement for lightning attachment. Right: Lightning strike on a metal vessel containing liquid and combustible gas

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On a 3D Lagrangian nodal discontinuous Galerkin method

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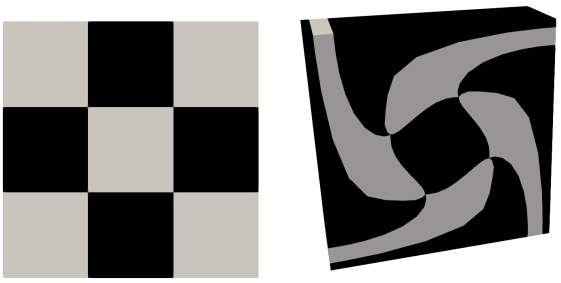
Keywords: material dynamics, high-order, Lagrangian methods, discontinuous Galerkin

ABSTRACT

We present a new 3D nodal Lagrangian discontinuous Galerkin (DG) method [1] to solve the governing equations for material dynamics using arbitrary-order hexahedral meshes that have edges that can bend and deform. The specific volume, velocity, and specific total energy fields within an element are represented by a Lagrange polynomial, which differs from modal Lagrangian DG methods that use Taylor polynomials [2, 3]. The discontinuity in the polynomials at the element surface is addressed by solving a multi-directional approximate Riemann problem at the surface vertices of the element and at additional locations along the surface. The nodal Lagrangian DG method conserves mass, momentum, and total energy. The accuracy and robustness of the new nodal Lagrangian DG method is demonstrated by simulating a suite of test problems. The result from a calculation of the Taylor Green vortex that uses a fifth-order polynomial for both the solution and the element (denoted as DG(P5)) are shown in Fig. 1.



(a) Initial mesh (b) Final mesh

Figure 1: The result from the 3D nodal Lagrangian DG(P5) method are shown for the Taylor Green vortex problem using 3x3x2 elements. A coarse mesh resolution is used to illustrate the large mesh deformation permitted by high-order meshes. The initial mesh is shown in (a) and the mesh at t=0.75 is shown in (b). The mesh is robustly deforming with the vortical flow.

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Sharp Interface Capturing in Compressible Multi-Material Flows with a Geometrically Accurate Diffuse Interface Method

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Keywords: multi-material compressible flows, Diffuse Interface Method (DIM), MUSCL reconstruction; compressive-shape preserving limiter, gradient reconstruction, MLP-UB method.

ABSTRACT

Compressible multi-material flows are encountered in a wide range of natural phenomena and industrial applications, such as supernova explosions in space, high speed flows in jet and rocket propulsion, underwater explosions, and vapor explosions in post accidental situations in nuclear reactors. In the numerical simulations of these flows, interfaces play a crucial role. A poor numerical resolution of the interfaces could make it difficult to account for the physics, such as material separation, location of the shocks and contact discontinuities, and transfer of the mass, momentum and heat between different materials/phases. Owing to such importance, sharp interface capturing remains an active area of research in the field of computational physics. To address this problem in this paper we focus on the Interface Capturing (IC) strategy, and thus we make use of a newly developed Diffuse Interface Method (DIM) called Multidimensional Limiting Process-Upper Bound (MLP-UB) [1]. Our analysis shows that this method is easy to implement, can deal with any number of material interfaces, and produces sharp, shape-preserving interfaces, along with their accurate interaction with the shocks. Numerical experiments show good results even with the use of coarse meshes.

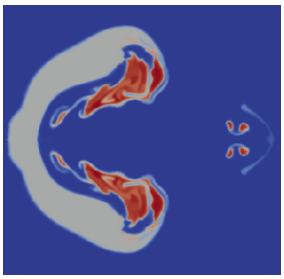

Figure 1: Evolution of the cell volume fraction for a 3-material shock concentric-bubble interaction.

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High-order Curvilinear Finite Element Magnetohydrodynamics

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Keywords: resistive magnetohydrodynamics, Lagrangian hydrodynamics, implicit magnetodynamics, high-order finite elements, curvilinear mesh.

ABSTRACT

Numerical magnetohydrodynamics is one of the major disciplines in computational fluid dynamics. The Lagrangian description is then especially suitable for rapidly expanded or compressed matter in a wide range of physical or engineering problems. However, high-order methods are typically limited only to static computational meshes due to the complexity of the model and/or lacking conservation properties. We recently proposed a conserving Lagrangian scheme for resistive MHD based on high-order curvilinear finite elements [1]. The method adopts the successful staggered-like configuration of the high-order finite elements for Lagrangian hydrodynamics, where the isoparametric mapping perfectly suits the Lagrangian approach and provides the strong mass conservation [2]. It is extended by magnetic finite elements preserving magnetic flux and divergence-free structure of the field. The consistent treatment of the magnetic field together with the methodology of an auxiliary variable for the magnetic energy [3] lead to the total energy conservation. Moreover, magnetic diffusion is solved (semi-)implicitly, providing robustness and stability to the numerical scheme. The proposed contribution reviews the design of the method and shows its properties on numerical tests and benchmarks. The ongoing and future directions of research are outlined. Relevancy to the research of plasma physics is mentioned, including dynamics of laser–target interaction, inertial confinement fusion and others.

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A suitable immersed boundary method for gas-solid interface interactions and multi-material flow in the presence of shocks using a high-order finite difference method

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Keywords: shock hydrodynamics; multi-material hydrodynamics; Eulerian methods; immersed boundary method

ABSTRACT

High-order methods offer computational advantages for resolving physical scales of motion, like those associated with turbulence and mixing [1]. A structured computational mesh simplifies high-order discretization schemes but creates complexity in how non-grid aligned features are modeled in the flow, such as rigid or solid boundaries. An immersed boundary method (IBM) is presented which is found to be suitable for a high-order compact finite difference scheme and which itself can be extended to arbitrary order. Errors and numerical convergence of the method are then compared for several test problems in 1D, 2D, and 3D. The IBM is then used to construct a multi-material algorithm which inherits many of properties of the underlying method, allows for a sharp interface between the regions, and maintains numerical stability for compact finite difference methods. The multi-material scheme is compared to the standard 4-equation model [2] on several test problems and we summarize by commenting on the advantages and disadvantages of the schemes.

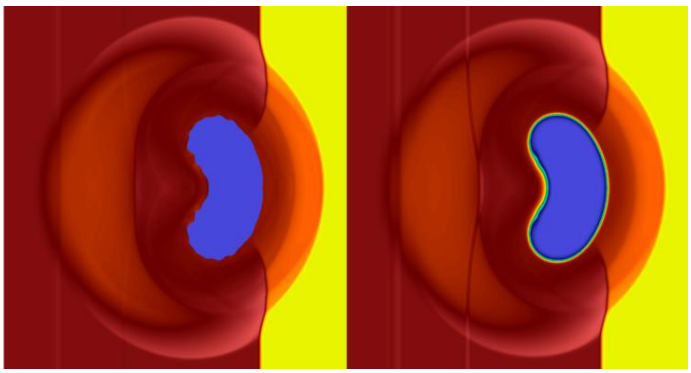

Figure 1: Contours of density for a shock-bubble interaction for (left) the proposed IBM based multi-material method and (right) the standard 4-equation, diffuse interface method.

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An SPH damage model appropriate for variable resolution

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Keywords: shock hydrodynamics, multi-material, Lagrangian methods, material failure

ABSTRACT

Smoothed particle hydrodynamics (SPH) is well suited to studying problems involving material failure and fracture due to its purely Lagrangian nature, robustness, and ability to handle arbitrarily complex topological changes in the material being modeled. The most widely used method of modeling material failure in SPH is based on the work of Benz & Asphaug [1, 2], wherein each point is randomly assigned a population of failure strains at problem initialization, which are used in combination with the instantaneous strain to evolve a damage variable on each point. However, a major limitation of the standard Benz & Asphaug model is that it implicitly assumes each point is equally likely to host any given flaw strain, which is not true if the points vary in resolution. Additionally, the storage required for the total flaw population grows as $N \log(N)$ (where N is the total number of points), and therefore as we increase problem size the memory requirements for maintaining this flaw population grows as well.

We have recently developed a new version of this algorithm which relieves both of these constraints: we assign a flaw population to each point independently based on its individual volume (allowing arbitrary variations in resolution between points), and only require storage of the minimum and maximum flaw on each point, rather than a full flaw population, removing the problem of scaling with problem size. Our new algorithm reproduces the important properties of the standard Benz & Asphaug approach, and also solves some often overlooked algorithmic issues of the standard damage model (such as the the minimum possible failure strain being deterministically specified by the volume of the part being modeled). In this talk we describe our new damage model, and show practical applications such as modeling cratering on asteroids at high-resolution near the impact site while allowing coarser resolution in the bulk of the body (fig. 1).

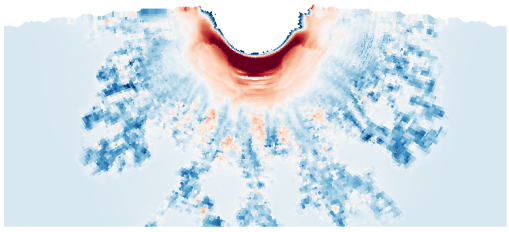

Figure 1: $y - z$ slice of mass density through a 3D model impacting a 535 kg sphere of Aluminum on 160m sphere of porous rock representing an idealized asteroid.

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A robust high-resolution modification of the discrete equations method for compressible multi-phase flow with accurate interface capturing

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Keywords: Eulerian methods, interface reconstruction methods, multiphase flows

ABSTRACT

The discrete equations method (DEM) [1] can be considered an extension of the Godunov method to multi-phase flow. It combines the solutions of pairwise Riemann problems to provide the fluxes for each phase as well as the non-conservative coupling terms between the phases. Due to its universal approach and robustness, DEM provides an excellent framework for different kinds of multi-phase flow.

However, for interface flow problems, DEM is held back by a trade-off. On the one hand, the original DEM with piecewise-constant volume fractions suffers from strong diffusion, which prevents accurate interface tracking. On the other hand, if a high-order interface reconstruction is applied, the effective cell size for wave propagation is reduced, which introduces a restrictive time-step limit.

We propose a modification, which preserves the robustness of piecewise-constant DEM for moderate time-step sizes, even if combined with high-order and highly nonlinear interface reconstruction schemes. This is achieved by a sensible combination of fluxes and non-conservative terms that effectively prevents the time-step restriction without affecting the propagation of interfaces and shock waves.

We combine our new method with a genuinely multi-dimensional THINC reconstruction [2]. The resulting scheme is very robust and captures the interface with high accuracy, even for shock-interface problems with strong interface deformation and breakup. We demonstrate its performance with simulations of shock-bubble and shock-droplet interactions, which show very good agreement with reference results from literature.

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SPH for high-density ratio multi-material flows

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Keywords: smoothed particle hydrodynamics, fluid-solid interface, multi-material hydrodynamics.

ABSTRACT

Smoothed particle hydrodynamics (SPH) is a Lagrangian mesh-free method that was originally developed to model hydrodynamic forces in astrophysical simulations [1]. The Lagrangian approach makes SPH well-suited for problems involving damage and fracture while the mesh-free nature can be beneficial for problems predisposed to mesh tangling. These advantages inspired us to attempt to apply SPH to simulate the atmospheric entry and break-up of asteroids. Traditional formulations of SPH however, contain the implicit assumptions that the density field is smooth and that mass does not vary significantly between interacting particles. When these assumptions are severely violated, as in our area of application, erroneous numerical effects can dominate the physics of interest. The most well-documented of these effects is the numerical surface tension that inhibits mixing near contact discontinuities [2]. Several modifications and reformulations of SPH have been proposed to remedy this deficiency; however, they have not been applicable to multi-material problems involving sharp contact discontinuities with disparate material properties – e.g. rarefied air interacting with porous rock.

Here we describe a density-energy SPH formulation that we have developed for this application, The method is capable of modeling the interaction of multiple materials with sharp density discontinuities, $\rho_i/\rho_j > 10^3$, arbitrary equations of state, large variations in materials properties, material strength, and damage due to brittle fracture. The method makes use of linear-corrected kernels, second-order artificial viscosity, and an artificial viscosity limiter to achieve good shock-capture and low-dissipation in smooth regions of the flow. An HLLC approximate Riemann solver partitions compression at material interfaces preventing stiff materials from becoming numerically over-compressed by interactions with pliable materials. Energy and linear momentum are conserved to machine precision using a compatible energy formulation and symmetric inter-particle forces respectively. We have validated the approach on a number of classic shock and mixing problems [3]; and we have implemented it as a solver, FSISPH, in the code Spheral++, maintained by LLNL and publicly available on github.

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A multiscale numerical scheme for the simulation of dispersed multiphase flows

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Keywords: Compressible multiphase flows, Baer & Nunziato models, Multiscale models.

ABSTRACT

The aim of this talk is to derive both a model and a numerical scheme for the approximation of multiphase models of Baer & Nunziato types[2, 7].

Such models are *averaged* models, able to both model interface flows and well mixed flows. They can be obtained by averaging Euler models following ideas developed in [3]. A new averaging method was developed in [5], based on an explicit stochastic model. We will show that the multiscale model obtained contains several known models in some limits (e.g. nonconservative and relaxation terms of [7, 5]), and also that it ensures in general all phasic entropy inequalities.

Then, we will also show that the same method can be applied at the discrete level for deriving a numerical scheme, based on the ideas of [1, 4]. This numerical scheme will be proven to ensure also positivity and all the entropy inequalities under CFL conditions that can be explicitly derived. As the model, the numerical scheme is multiscale in the sense that it depends on a parameter modeling the local topology of the flow.

Last, a simple model for the topological parameter will be discretized, and numerical results with this micro-macro model will be presented.

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An SPH method for the unified model of continuum mechanics

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Keywords: hyperbolic relaxation equations, SPH method, fluid and solid mechanics.

ABSTRACT

We present our recent results on the use of the unified model of continuum solid and fluid mechanics [1] and its discretization with a Smoothed Particle Hydrodynamics (SPH) method. Previously, the unified model was discretized using various *mesh-based* techniques including Godunov-type finite volume methods and Discontinuous Galerkin methods [1], Arbitrary Lagrangian Eulerian methods [2], a finite volume methods in the Updated Lagrangian formulation with a high-order IMEX time integrator [3], semi-implicit staggered finite volume method for low-Mach problems, thermodynamically compatible finite volume scheme.

This time we discretize the equations with a *mesh-free* technique, the SPH approach. Despite its name, the presented SPH scheme is able to deal also with solids, and thus is able to compute the solution to the unified model in both fluid and solid regimes, see Figure 1.

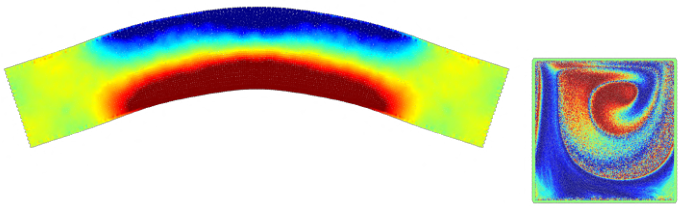

Figure 1: Solid and fluid simulation with a new SPH scheme for the unified model of continuum.

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On the modeling of non-mixing compressible twophase flow

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Keywords: twophase flow, Baer Nunziato model, Discrete Equation Method.

ABSTRACT

Compressible multiphase flow occur in many practical situations where two phases are separated by an interface. Even under the stringent simplification of neglecting mass-transfer and heat conduction, *no unique model* is generally accepted for the description of two compressible constituents.
Indeed, various twophase flow systems may appear to have very little in common, and the tendency has develop ad-hoc models, with the prominent example of the Baer and Nunziato (BN) [2] model for the description of the deflagration-to-detonation transition.
Following the guideline of physical principles fulfillment, Saurel and Abgrall proposed a new non-equilibrium model [3], which constitutes a generalization of the classical BN model to general species, describing flow fields in terms of their statistical means. One major drawback of such mathematical model is represented by the inclusion of hyperparameters, which govern the drive to equilibirium process and depend on the (unknown) microstructure-regime of the flow.
Stemming from the same averaging theory, in [1] an algorithmic procedure to simulate twophase flows was also put forward.
This latter provided two major advancements: it describes a global scheme of the Godunov type to simulate such phenomena, and allows to analyze the information about the underlying micro-structure lost when passing to the mean. Therefore, one can take the perspective of such numerical method and try to derive the hyperparameters needed for the model of [3] in the limit of vanishing resolution. Such a procedure has seen incredible achievements and goes under the name of Discrete Equation Method (DEM).
We revise the DEM, showing that such algorithmic procedure is also under-determined, in the sense that infinitely many solutions can be constructed with the same algorithm.
Nevertheless, by proving local convexity of probability coefficients, we recast the DEM into a one-parameter family of algorithms. We call this new generalization, an r-model.
We describe connection of this latter with existing models, showing its ability to interpolate between disperse and stratified flow regimes.
Refinement and perspective in the statistical sense are also described.

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Implicit semi-Lagrangian schemes for compressible gas dynamics

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Keywords: shock hydrodynamics, implicit schemes, Lagrangian methods.

ABSTRACT

The goal of this project is to deal with fluid-structure interactions in Lagrangian formalism.
To approach the equations traducing the movement of fluids, explicit schemes are traditionally used because they are easy to implement. For instance, [1] or [2] can be used for the fluid part, and [3] or [4] for the elastic part. To be stable, these schemes need to satisfy a CFL condition. In the case we are studying, the width of the structure can be very thin, and the speed of sound very high, it contributes to have such a small time step that it becomes unfavorable to use explicit methods.
To overcome this problem, the idea is to use implicit schemes. Nonetheless, some major technical difficulties appear, in particular how to prove that the scheme is well posed (the solution at the next time step exists and is unique). In this presentation, we propose a non-linear implicit scheme for the hydrodynamic part that solves multi-D compressible Euler equations in semi-Lagrangian formalism.
The presentation is articulated around three main points. First, we construct and analyze a family of non-linear implicit scheme based on the method of predictor-corrector [5]. The prediction step solves the isentropic Euler equations and the correction step corresponds to the discretization of the Euler equations with conservation of the total energy. Second, we prove the unconditionnal stability of the implicit scheme, see [6], that comes from a rewriting of the prediction step under the form:

$$\begin{cases} \text{Find } U \in \mathcal{D} \subset \mathbb{R}^n \text{ such that} \\ \nabla J(U) = AU, \end{cases} \tag{1}$$

where U is the vector of unknowns, J is a convex functional defined on the domain $\mathcal{D}$ and A is a skew-symmetric matrix of real coefficients. Hypothesis under which the problem (1) admits a unique solution will be detailed. Third, we give numerical results attesting of the precision and robustness of this implicit scheme. We should discuss the sensitivity of the method to an increased time step, the cost of computation, the use of an explicit-implicit solver in a subdomain.

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An interpolation-free strategy to describe connectivity changes within the ALE framework

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Keywords: ALE formulation, mesh adaptation, geometric conservation law, large displacement.

ABSTRACT

Numerical simulations of unsteady compressible flows generally require to deal with large deformations of the computational domain and, at the same time, to precisely represent the boundaries or the interfaces of multi-material systems. A popular approach to tackle moving boundary problems is arbitrary Lagrangian-Eulerian (ALE) framework, which permits to solve the governing equations over a deforming grid. However, the fixed-connectivity constraint that underlies standard ALE techniques limits the maximum displacement the grid nodes can undergo before entangled or bad-quality elements arise. In these situations, h-adaptation, that is grid connectivity changes such as node insertion, node deletion, or edge swapping, may help to restore grid quality, as well as to dynamically relate the grid spacing to evolving flow features. In this talk, we discuss a path-breaking strategy that is able to describe local connectivity changes within the ALE framework, thanks to a peculiar series of fictitious continuous deformations of the control volumes composing the domain, considering both finite-volume [1] and residual distribution schemes [2]. Thanks to this interpretation, the solution is mapped directly onto the adapted grid, without any explicit interpolation of the solution. Hence, the numerical properties of the underlying fixed-connectivity ALE scheme are preserved and the so-called Geometric Conservation Law (GCL) is automatically fulfilled. The absence of explicit interpolation makes easier the use of high-order BDF schemes, since the solution at previous time steps is easily recovered through the history of the indexes of the degrees of freedom. The proposed scheme is assessed by numerical simulations of moving-body problems experiencing large displacements.

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Multimaterial ALE remap with interface sharpening using high-order matrix-free finite element methods

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

ABSTRACT

We are interested in multiphysics simulations using high-order finite elements in the context of multimaterial arbitrary Lagrangian-Eulerian (ALE) hydrodynamics. For the ALE remap phase, we have relied on a method in which material volume fractions are advected in pseudo-time without any form of interface reconstruction [1]. In practice, this can lead to excessive diffusion of material interfaces. In this work, we introduce a new approach for multi-material ALE remap using high-order, matrix free techniques which incorporates a flux modification to sharpen material interfaces in a conservative manner. This approach draws inspiration from interface aware volume of fluid (VOF) methods such as [2] and [3]. In our approach, we augment our semi-discrete advection equations with a conservative flux modification which acts to sharpen material volume fraction fields based on their gradients and the transport direction. This approach requires an adaptive pseudo-time stepping technique to maintain the bounds of the remapped solution variables.

In addition, we formulate this new interface aware ALE remap method using matrix-free partial assembly techniques where globally assembled matrix operators used in the semi-discrete advection equation are no longer needed. Instead, we combine an element based, bounds preserving low order solution with a high-order DG scheme and consider both clip/scale and flux corrected transport (FCT) projection strategies for doing element wise blending of the high and low order solutions, resulting in a matrix-free FCT method for multi-material, multi-field ALE remap. We present results of our new interface aware method on 3D benchmarks running on GPUs and describe the algorithmic tailoring for the GPU that was developed.

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-833481.

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Subcell limiting strategies for the DGSEM

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Keywords: Discontinuous Galerkin Methods, Invariant Domain Preservation, Shock Capturing

ABSTRACT

We present a general family of subcell limiting strategies for high-order nodal discontinuous Galerkin (DG) schemes and apply them to the single and multi-component Euler and MHD equations. The main strategy is to construct low-order finite volume (FV) discretizations that are compatible with the high-order DG method, such that the two schemes can be seamlessly blended to guarantee additional properties, such as bounds on physical quantities (e.g., for positivity or shock capturing) and/or guaranteed entropy dissipation.

We identify four main ingredients for the implementation of this strategy, which may be combined in a flexible manner: (i) a nodal high-order DG method on Legendre-Gauss-Lobatto nodes, (ii) a compatible and robust subcell FV scheme, (iii) a convex combination strategy for the two schemes, which can be element-wise or subcell-wise, and (iv) a strategy to compute the convex blending factors, which can be either based on heuristic troubled-cell indicators, or using ideas from flux-corrected transport methods.

By carefully designing the metric terms of the subcell FV method, the resulting methods can be used on unstructured curvilinear meshes, are locally conservative, can handle strong shocks efficiently while directly guaranteeing physical bounds on quantities such as density, pressure or entropy. We further show that it is possible to choose the four ingredients to recover existing methods such as provably entropy-dissipative subcell shock-capturing approaches for Euler [1] and MHD [2], or a sparse invariant domain preserving approach [3].

We test the versatility of the presented strategies and mix and match the four ingredients to solve challenging simulation setups, such as turbulent and hypersonic Euler simulations, single and multi-component MHD problems featuring shocks and turbulence.

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Bound-preserving flux limiting schemes for DG discretizations of conservation laws with applications to the Cahn–Hilliard equation

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Keywords: discontinuous Galerkin method, maximum principle, phase-field equation, slope limiting, flux limiting, flux corrected transport.

ABSTRACT

Many mathematical models of computational fluid dynamics involve transport of conserved quantities, which must lie in a certain range to be physically meaningful. The analytical or numerical solution u of a scalar conservation law is said to be bound-preserving if global bounds $u_{\min}$ and $u_{\max}$ exist such that $u_{\min} \leq u \leq u_{\max}$ holds in the domain of definition. These bounds must be known a priori. To enforce such inequality constraints at least for element averages in the context of discontinuous Galerkin (DG) methods, the numerical fluxes must be defined and constrained in an appropriate manner. In this talk, we introduce a general framework for calculating fluxes that produce non-oscillatory DG approximations and preserve relevant global bounds for element averages even if the analytical solution of the PDE violates them due to modeling errors. The proposed methodology is based on a combination of flux and slope limiting. The (optional) slope limiter adjusts the gradients to impose local bounds on pointwise values of the high-order DG solution, which is used to calculate the fluxes. The flux limiter constrains changes of element averages so as to prevent violations of global bounds. Since manipulations of the target flux may introduce a consistency error, it is essential to guarantee that physically admissible fluxes remain unchanged. We propose two kinds of flux limiters, which meet this requirement. The first one is of monolithic type and its time-implicit version requires the iterative solution of a nonlinear problem. Only a fully converged solution is provably bound-preserving. The time-explicit version of this limiter is subject to a time step restriction, which we derive in this article. The second limiter is an iterative version of the multidimensional flux-corrected transport (FCT) algorithm and works as postprocessed correction scheme. This fractional step limiting approach guarantees that each iterate is bound-preserving but avoidable consistency errors may occur if the iterative process is terminated too early. Each iterate depends only on local information of the previous iterate. This concept of limiting the numerical fluxes is also applicable to finite volume methods. Practical applicability of the proposed flux limiters as well as the benefits of using an optional slope limiter are demonstrated by numerical studies for the advection equation (hyperbolic, linear) and the Cahn–Hilliard equation (parabolic, nonlinear) for first-order polynomials. While both flux limiters work for arbitrary order polynomials, we discuss the construction of bound-preserving slope limiters, and show numerical studies only for first-order polynomials.

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Modelling interactions of waves with diffused interfaces

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Keywords: diffuse-interface method, multiphase, compressible, interface, interaction, relaxation.

ABSTRACT

When simulating multiphase compressible flows using the diffuse-interface methods, the test cases presented in the literature to validate the modellings with regard to interface problems are always textbook cases: interfaces are sharp and the simulations therefore easily converge to the exact solutions. In real problems, it is rather different because the waves encounter moving interfaces which consequently have already undergone the effects of numerical diffusion. Numerical solutions resulting from the interactions of waves with diffused interfaces have never been precisely investigated and for good reasons, the results obtained are extremely dependent on the model used.

Precisely, well-posed models, such as the model of Kapila et al. [1], present similar and important issues when such an interaction occurs, coming from the appearance of a wave-trapping phenomenon. To circumvent those issues, we propose to use a thermodynamically-consistent pressure-disequilibrium model [2] with finite, instead of infinite, pressure-relaxation rate to overcome the difficulties inherent in the computation of these interactions. Because the original method to solve this model only enables infinite relaxation, we propose a new numerical method allowing infinite as well as finite relaxation rates.

Solutions of the new modelling are examined and compared to literature, in particular we propose the study of a shock on a water–air interface, but also for problems of helium–air and water–air shock tubes, spherical and non-spherical bubble collapses.

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Spurious vorticity in Lagrangian and Eulerian methods

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Keywords: shock hydrodynamics, Lagrangian methods, Eulerian methods.

ABSTRACT

The term *factorizable scheme* was introduced in [5] in the Eulerian framework and it signifies a numerical scheme that, unlike the standard compressible CFD methods, does not introduce non-physical coupling between the vorticity advection and acoustics factors. Such a scheme was constructed and was demonstrated to have some advantages over the standard approach (like low Mach number flow resolution, construction of fast solvers etc.). While the factorizability property is highly beneficial for the Eulerian methods, the previous expereinece shows that it is not really crucial. The standard (Eulerian) compressible CFD methods, though suffering from certain deficiencies due to the lack of this property, are routinely used in practice already for several decades.

The situation with Lagrangian methods is very different: the *factorizability* property appeats to be of the utmost importance within the Lagrangian framework. We shall consider several successful Lagrangian schemes (both staggered grids based [3] and collocated cell-centered [1, 4]) and show that all of them are *factorizable*. On the other hand, one of the early attempts to create a collocated cell-centered Lagrangian method was CAVEAT. It suffered from significant spurious vorticity production [2], leading to large errors and mesh entanglement. We shall demonstrate that the underlying numerical scheme is *not factorizable*.

A likely conclusion from this is that the *factorizability* property emerges as a key attribute of a "successful" Lagrangian method.

We shall also present two- and three-dimensinal Lagrangian versions of the original Eulerian factorizable method [5], examine their performance on test problems and discuss their links to the existing methods. A potential advantage of the proposed collocated scheme is in its simplicity.

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Robust second-order approximation of the compressible Euler Equations with an arbitrary equation of state

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Keywords: Euler Equations for gas dynamics, arbitrary equation of state, high order methods, Eulerian methods, shock hydrodynamics

ABSTRACT

This work is concerned with constructing a robust, high-order approximation of the compressible Euler equations for gas dynamics supplemented with an arbitrary or tabulated equation of state. In particular, we show how to construct a high-order graph-viscosity coefficient using an interpolated entropy pair useful when the equation of state is given by tabulated experimental data. Similarly, we construct an entropy surrogate functional that is used in a convex limiting technique that preserves the invariant domain of the system. Finally, the numerical method is then verified with analytical solutions and then validated with several benchmarks seen in the literature and laboratory experiments.

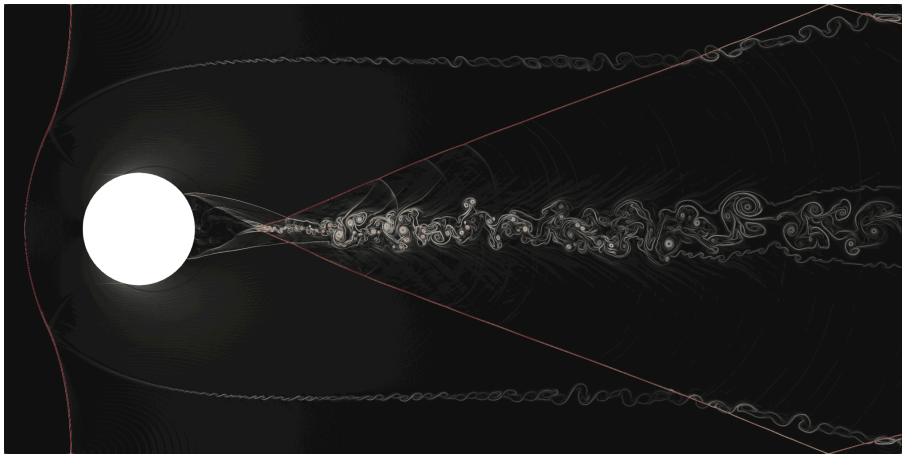

Figure 1: Mach 3 flow around a cylinder with Van der Waals equation of state.

Embedded Meshes with Smoothed Particle Hydrodynamics

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Keywords: embedded meshes, hydrodynamics, material failure, meshfree methods.

ABSTRACT

Embedded grid methods [1] couple the interaction of two overlapped meshes, where a solid Lagrangian foreground mesh is usually overlayed on top of a fluid Eulerian background mesh. These methods have been shown to work well on fluid-structure interaction problems, offering significant advantages over standard ALE (Arbitrary Lagrangian-Eulerian) techniques. The first benefit is ease of use, as a conforming mesh around the solid structure does not have to be constructed; a second benefit is that they avoid mesh tangling at the fluid/solid interface, which standard ALE mesh relaxation techniques can run into very easily. Previous works have shown analysis on the stability of the time integration and conditioning of the linear system which arises from enforcing velocity constraints at the interface of the foreground and background meshes.

Meshfree methods like Smoothed Particle Hydrodynamics have long been used to simulate problems with material strength and damage/failure. The purpose of this work is to show the hybridization of the embedded mesh technique with a meshfree SPH method for such problems, where the foreground now contains SPH particles representing the solid rather than Lagrangian finite elements. Details of the cut-cell technique and interface construction are described, and the velocity constraints are extended to handle the smoothing functions used in SPH. This technique [3] is demonstrated through the coupling of the arbitrary Lagrangian-Eulerian code ALE3D, the embedded mesh interface FEusion, and the smoothed particle hydrodynamics package Spheral [2], all codes which are developed at Lawrence Livermore National Laboratory.

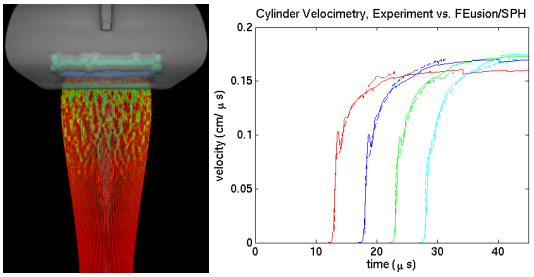

Fig. 1. Snapshot of a cylinder test simulation with embedded SPH method, and comparison of the experimental vs simulated surface velocimetry.

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Design Optimization of Richtmyer-Meshkov Instabilities

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Keywords: shock hydrodynamics; Richtmyer-Meshkov; optimization.

ABSTRACT

The Richtmyer-Meshkov Instability (RMI) occurs when a material interface is impacted by a shock. Small perturbations on the interface will grow forming either jets or bubbles depending upon the relative densities of the materials. Applications of RMI include aerospace, inertial confinement fusion, metal forming, etc. While the study of fluid instabilities is most common, we are interested in solids such as metals and plastics, with impact velocities in the 2-5 km/s range [1]. The late-time behavior is strongly dependent upon the non-linear material properties and shock tube experiments are often conducted to help develop these material models. Our application is different, we are interested in controlling the RMI by introduction of a second material interface. This second interface is parameterized, and computational design optimization is used to find a design that either suppresses or enhances the RMI.

The design optimization process relies upon accurate forward simulations of RMI. The LLNL Blast code is used for these simulations, this is a higher-order finite element Arbitrary Lagrangian Eulerian code [2][3]. Tabular equation of state data is used, along with Steinberg-Guinan strength models and a simple tensile failure model. Since we perform thousands of simulations, we cannot directly examine the results and instead need an automated computable metric to measure the RMI growth rate. This is accomplished using tracer particles that are placed on the initial interface, and the peaks and valleys can be tracked versus time. The RMI growth rate is then easily determined via the peak-to-valley distance. Finally, the designable material interface is parametrized using a piecewise cubic Hermite polynomial, the polynomial coefficients are the design variables.

Public domain machine learning software is used to determine the optimal polynomial coefficients that minimize the RMI. The machine learning algorithm determines the specific hydrodynamic simulations to be performed and iterates until some convergence criteria is achieved. The primary result is that, for our specific RMI suppression application, the optimization process yielded a design that suppresses RMI growth rate by 90%. A second application is in progress, that of increasing the RMI. The details of the algorithm and these results will be presented.

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High-Order Implicit Shock Tracking for Flows with Interfaces

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Keywords: shock-fitting, high-order methods, r-adaptive methods.

ABSTRACT

Shock tracking, as an alternative method to shock capturing, aims to generate a mesh such that element faces align with shock surfaces and other non-smooth features to perfectly represent them with the inter-element jumps in the solution basis, e.g., in the context of a finite volume or discontinuous Galerkin (DG) discretization. These methods lead to high-order approximations of high-speed flows and do not require nonlinear stabilization or extensive refinement in non-smooth regions because, once the non-smooth features are tracked by the mesh, the high-order solution basis approximates the remaining smooth features.

In this talk, we introduce the High-Order Implicit Shock Tracking (HOIST) method [1, 2] that re-casts the geometrically complex problem of generating a mesh that conforms to all discontinuity surfaces as a PDE-constrained optimization problem. The optimization problem seeks to determine the flow solution and nodal coordinates of the mesh that simultaneously minimize an error-based indicator function and satisfy the discrete flow equations. A DG discretization of the governing equations is used as the PDE constraint to equip the discretization with desirable properties: conservation, stability, and high-order accuracy. By using high-order elements, curved meshes are obtained that track curved shock surfaces to high-order accuracy. The optimization problem is solved using a sequential quadratic programming method that simultaneously converges the mesh and DG solution, which is critical to avoid nonlinear stability issues that would come from computing a DG solution on an unconverged (non-aligned) mesh. The method is used to solve several complex, two- and three-dimensional compressible flows and is shown to deliver high accuracy per degree of freedom.

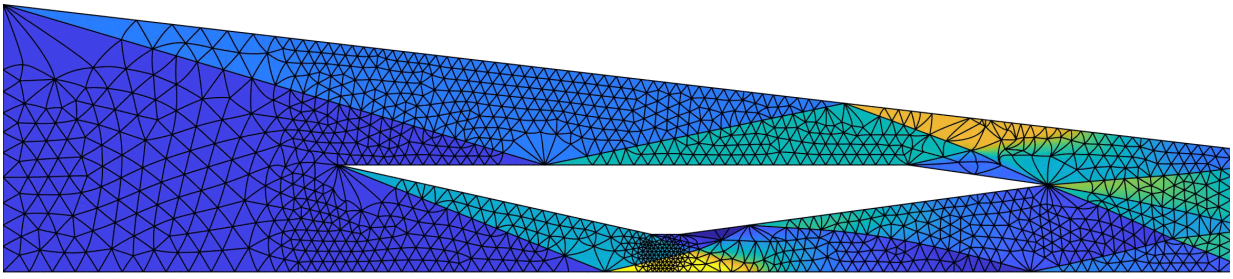

Figure 1: High-order implicit shock tracking simulation of Mach 5 flow through a scramjet.

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Fluid Mediated Particle Interactions Studied Using the Nearest Particle Statistics

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Keywords: particle-fluid-particle interactions, disperse multiphase flows

ABSTRACT

The drag force is the primary force considered for interactions between two phases. Efforts have been made to include effects of particle volume fraction, Reynolds number, and Mach number in the drag models. Recent works [1] have shown that such force models are insufficient. Effects of mesoscale particle structures need to be considered. Mesoscale structures are three-dimensional objects, while the drag force is a vector that can only be used to represent the phase interaction in a certain direction. To consider multi-particle interactions and deformation or motion of particle mesoscale structures, a stress tensor representing particle interactions is necessary. Definition of such stress has only been successful for limited cases, such as Stokes flows. The main difficulty comes from the long-range nature of the hydrodynamic interactions among the particles. Even in the dilute particle limit, the conventional pairwise interaction approximation leads to divergent integrals.

In this work, based on the ensemble phase averaging method, we introduce a relation between the ensemble average and the quantity conditional on the nearest particle [2]. Because of the rapid far-field decay of the nearest particle probability, when the quantities conditional on the nearest particle can be calculated, the relation can be used to study interactions among all the particles, not only the nearest pair, without the divergence difficulty.

This method has been used to study the particle sedimentation velocity in an isotropic uniform Stokes flows and recovered the classic results from the renormalization technique [3]. It is also found that solving for flow fields conditional on the nearest particle is more difficult than finding the flow field conditional on a particle (not necessarily the nearest) position. Results from numerical simulations should be the main tool for such study of particle interactions.

Without the divergence difficulty, we can then define a particle-fluid-particle (PFP) stress in a way similar to the potential part of the virial stress in molecular dynamics. Particle-resolved numerical simulations are performed to calculate the PFP stress for flows with finite Reynolds numbers. In the flow regime studied, this PFP stress is shown to be the macroscopic representation of the drafting–kissing–tumbling mechanism.

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Speed of sound measurements in multifluids for calibrating Eulerien two-phase fluid models.

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Keywords: Thermodynamics, Eulerien multiphase modeling, Virtual Mass, Physical acoustics.

ABSTRACT

In this talk, we first present a new and general approach to compute all the thermodynamic properties (a.k.a thermodynamic coefficients) of fluid mixtures from those of the constituants, regardless of any assumed equation of state [1]. This includes the adiabatic and isothermal speeds of sound but also thermal coefficients such as the Gruneisen and the adiabatic parameters. Secondly, we present an analysis of the different Eulerian multiphase models, regarding the predicted speed of propogation of small pertubations. For the class of two-velocity models, we show that Virtual Mass interaction terms are crucial to reproduce sound's speed measurements. Moreover these measurements can be used to completely identify the virtual mass interaction between two fluids[1]. We conclude the talk by presenting some cases of viscous multifluids models and a generalisation of the Stokes-Kirchhoff[3] attenuation and dispersion relations to multiphase flows.

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A study of LES-SGS closure models applied to a fluidized bed reactor

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Keywords: Fluidized bed reactor, LES, Turbulent Flow, SGS models

ABSTRACT

Limited supply of conventional fossil fuels and global environmental problems put stress on the renewable and clean energy technologies, among which biomass gasification is one of the most emerging technologies for the efficient utilization of biomass. Biomass gasification by fluidized bed reactors (FBR) has been found to present good prospects due to its high rates of heat and mass transfer, excellent mixing properties, and good temperature control [1]. The investigation of the hydrodynamics of fluidized beds through numerical simulations has become increasingly common [2]. The main challenge of such investigation lies in the wide range of spatial and temporal scales that need to be considered. Various processes taking place at the scale of the particle (*e.g.* drag on the particle, inter-particle collisions, heat transfer and surface reactions) can cause the macroscopic behavior to reach a variety of granular flow regimes. It is difficult to capture the complex physics of a BFR at the particle scale using a Reynolds-Averaged Navier–Stokes (RANS) model, since most of the spectral information of turbulence is lost during the time-averaging Moreover, full Direct Numerical Simulation (DNS) of FBR configuration may not be a practical solution yet. An alternate simulation strategy is a mesoscopic-scale approach based on DEM and LES that allows for a faster and more holistic study of the parameter space of FBR. However, LES is sensitive to details of its formulation because the energetics are tied to unresolved processes in the vicinity of particle region. Usage of an appropriate SGS model is an essential requirement to capture the underlying physics of the fluidized state in a proper manner. However the performance of different SGS models applied to BFR configuration has not been much reported in the literature. In the present study, we investigate the FBR flow using four SGS models, namely, static and dynamic Smagorinsky model, WALE model and Sigma model. Additional simulation without SGS model is performed. The efficacy of the SGS models is assessed by examining the detailed physics of the FBR.

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A novel implicit finite volume scheme for hypersonic steady flow problems

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Keywords: Hypersonic steady flow, Finite-Volume, Euler equations, implicit scheme.

ABSTRACT

Implicit time discretization in computational fluid dynamics to compute steady state solution of hypersonic flows was a field of researches in the 70's-80's. Since then, only few novel methods have arised but no revolution has occured. However, it is suitable to use implicit finite volume schemes to solve hyperbolic systems such as Euler equations in extreme flow conditions. Theoretically, these schemes do not suffer from timestep restrictions to guarantee stability, unlike the explicit ones. Nonetheless, CFL restrictions are still required in practice, especially for stiff numerical test cases such as high Mach number stationary flow with bow shocks around obstacles. Nowadays, the well-known Yee method [1] is commonly used to solve CFD problems the implicit way. However, there is no formal theoretical basis for systems of conservation laws [2]. Consequently, the increase in CFL is driven by several *ad-hoc* parameters depending on the test case. The purpose of this presentation is to first study the mathematical environment of classical implicit finite volume schemes and to enlight their weaknesses. Secondly, we will propose a new approach based on an appropriate change of variables supplemented by a more adequate linearization of the overall system [3]. The new method aims to be more robust and possibly more efficient regarding timestep restrictions. Numerical results will assess this study.

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A Diffuse Interface Mesh Generation Method for Multi-phase Incompressible Flows

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Keywords: Diffuse interface, mesh generation, incompressible, multi-phase, adaptive mesh refinement

ABSTRACT

This work is concerned with the representation of non-trivial rigid boundary geometries in the numerical simulation of low-speed multiphase flows. Our previous work focused on sharp interface approaches for compressible and incompressible flow problems [1, 2], with the aim to generalise the concept of mesh generation to interface capturing, which could therefore be deployed in multi-material problems [3]. Although these approaches offer robust and accurate rigid and multi-matter boundary representations, the underlying level sets have well-known issues with regard to conservation and efficacy of parallelisation. To overcome these issues but still retain the concept of material interface capturing, a diffuse interface approach was recently devised for multi-physics problems at extreme compressible and high strain-rate states [4, 5]. The original method uses flux-based explicit algorithms, so in this talk we present an extension for the solution of the incompressible Navier-Stokes equations using pressure correction-based methods. The algorithm is based on a modification of the viscous flux terms of the momentum equations to enforce a no-slip boundary condition at the solid surface, which is represented as a smooth volume-fraction field. The method is implemented in a highly parallelised adaptive mesh refinement software framework. The resulting code is validated for multi-fluid and free-surface benchmarks. Results indicate that the method is as robust and accurate as its sharp-interface counterparts, while significantly mitigating their conservation issues and demonstrating better parallel performance. This in turn greatly reduces the computational expense of studying multiphase flow phenomena at the full range of length and time scales, driving forward the understanding of the essential physics involved in the energy industry.

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Efficient Numerical Treatment of High-Contrast Composite Materials

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Keywords: high contrast; saddle point problem; robust preconditioning; Uzawa method; Lanczos method.

ABSTRACT

This talk concerns a robust numerical treatment of an elliptic PDE with high contrast coefficients. We introduce a procedure by which a discrete system obtained from a linear finite element discretization of the given continuum problem is converted into an equivalent linear system of the saddle point type. Then three different preconditioned iterative procedures are proposed for a special type of application, namely, highly conducting particles located at distances comparable to their sizes distributed in the matrix of a finite conductivity. Robust preconditioners for solving the derived saddle point problem using three iterative procedures are proposed [1]. Robustness with respect to the contrast parameter and the mesh size is justified. Numerical examples support theoretical results and demonstrate independence of the number of iterations on the contrast, the mesh size and also on the different contrasts on the particles.

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Modeling electronic viscous heating in plasmas

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

ABSTRACT

Dynamical simulations of plasma under inertial confinement fusion or high energy density physics (HEDP) conditions require the simultaneous solution of systems of equations describing compressible hydrodynamics, thermal conduction and electron-ion coupling. In particular, the equations must be supplemented with a model for computing irreversible work done on the plasma and partitioning it between the ions and electrons, such as in a hydrodynamic shock. Previously in LANL's Eulerian multiphysics code xRAGE, the shock energy was delivered solely to the ions and did not take into account the impact of electron viscosity in shock heating which can lead to an overheating of the ions. This talk will discuss the implementation of a more sophisticated model based on work done by Velikovich [1]. The newer model divides the shock energy between electrons and ions based on a ratio of their viscosities [2]. The electron viscosity becomes more dominant in high Z plasmas (Z > 7). However, the magnitude of the effect is also highly sensitive to the strength of the shock.

We systematically explore the impacts of electronic viscous heating by simulating a range of shock strengths and materials. We observe a dramatic decrease in the impact for shock strengths greater than approximately Mach 2.5. We also explore the impact on recent capsule implosions. With electronic viscous heating, we calculate a higher adiabat at peak implosion velocity which predicts that more energy is required to achieve ignition in the capsule. Thus, under certain conditions, predicting implosion conditions requires accurately partitioning shock energy between electrons and ions.

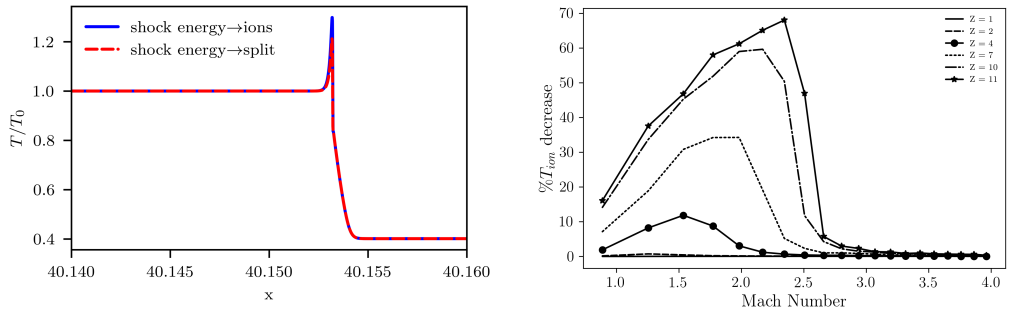

Figure 1: Temperature profile for a 1D shock with and without shock splitting (Left) and the decrease in peak ion temperature due to shock splitting at different shock strengths (Right)

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BoBa: Towards HPC implementations of tensor trains for Multiphysics

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Keywords: Lagrangian methods, Radiation hydrodynamics, Mesh Generation methods, including mesh adaptation, Advanced Discretization methods, High-order methods

ABSTRACT

We seek to introduce *information compression* directly into the discrete representation of physical field variables for multimaterial/multiphysics applications. We accomplish this by replacing conventional storage formats with data structure abstractions of *tensor trains*. A *tensor train* is a representation for vectors and matrices which has an exponential information compression rate[1], at the cost of increased computational complexity for a general random-access operation. However, this cost is offset by the structured nature of many common numerical operations found in moving-mesh and high-dimensional methods; especially linear operations in radiation transport and mesh geometry calculations in hydrodynamics methods. We discuss the development of abstraction layers which include performant libraries of operations which act on this data format. We present our work thus far for developing this storage format for (1) high-order radiation hydrodynamics, (2) Lagrangian and ALE methods, and (3) advanced GPU architectures.

Prepared by LLNL under Contract DE-AC52-07NA27344.

LLNL-ABS-835209

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Conservative remapping of material-dependent fields between possibly misaligned material regions

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Keywords: multi-material remap; conservative interpolation; multi-physics simulation.

ABSTRACT

In this work, we present an algorithm to interpolate or remap material fields between polyhedral meshes where the source and target cells are restricted to be pure, in the sense that each cell can contain a single material. It is conservative and preserves sharp material boundaries on the target mesh, even if the source and target regions delineating the same material are slightly misaligned [1]. If those material regions are aligned, then the algorithm is also linearity-preserving and bounds-preserving. For a given material, the field is recovered on the target material region from the overlapping source material region using a conservative reconstruction. A repair step is proposed to enforce conservation properties and local field bounds for the case of misaligned boundaries. No assumption is made on the topology of the input meshes. The accuracy of the algorithm is numerically assessed on several examples using our open-source library Portage [2].

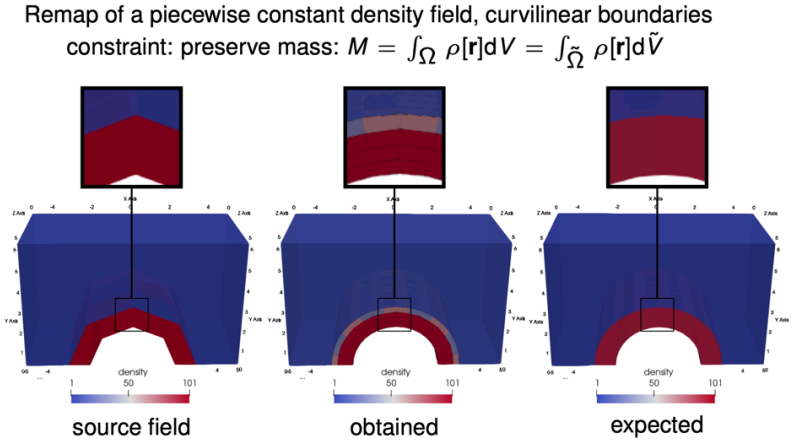

Figure 1: Problem of material field remapping between misaligned material regions.

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High-Order General-S_N Method Enabling Efficient Deterministic Transport in Hydrodynamic Simulations

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Keywords: high-order FEM; phase-space discretization; radiation hydrodynamics.

ABSTRACT

We propose a novel deterministic transport model employing a spatially varying angular coordinate system. Our generalized version of S_N angular discretization (GS_N) enables efficient high-dimensional phase-space simulations on Lagrangian hydrodynamic meshes by designing spatially dependent angular quadrature, see Figure 1, that address four critical simulation needs: (a) efficiently mitigates rays-effect often present in radiation transport in hydrodynamic simulations, (b) preserves symmetry and consequently prevents the numerical seeding of plasma instabilities (a show-stopper for standard S_N in ICF applications), (c) allows relativistic effects of radiation transport by using GS_N in fluid frame of reference, and (d) trades memory for computation by reducing the number of degrees of freedom. The latter builds on a high-order phase-space discretization in angles, energy, and space, while using GS_N in angles and adopting the adaptive mesh refinement capability to energy and space using MFEM [1].

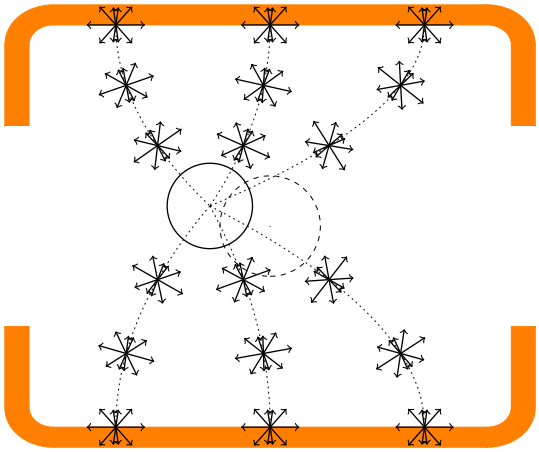

Figure 1: GS_N angular quadrature orientation following ICF capsule.

References

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

A New Fokker-Planck Acceleration Technique For Multiphysics Problems with Highly Forward-Peaked Scattering

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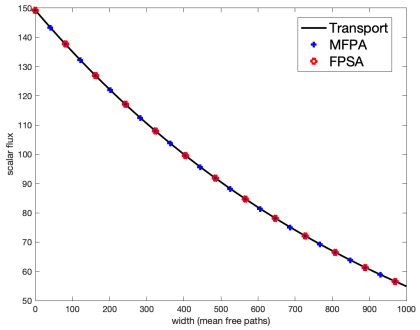
Keywords: radiation transport, multiphysics, acceleration.

ABSTRACT

This work applies a new acceleration technique known as Modified Fokker-Planck Acceleration (MFPA) [5] towards multiphysics problems with highly forward-peaked scattering. The Fokker-Planck equation, which is an asymptotic limit of the transport equation in highly forward-peaked settings, is modified and used to accelerate the linear Boltzmann equation in a high-order/low-order (HOLO) acceleration scheme. The modified Fokker-Planck (FP) equation preserves the angular flux and flux moments of the transport equation. The preservation of moments in the modified FP equation is particularly appealing for applications to multiphysics problems [1], in which the coupling between transport and the other physics can be done through the FP equation. Coupling the modified FP equation with multiphysics isolates expensive transport sweeps. A target application for MFPA is radiative transfer in clouds, where photons undergo highly forward-peaked scattering. MFPA is is coupled to a variety of radiative transfer beam problems [2, 3]. We observe up to two times speed up in wall-clock time when using this new technique compared to multiphysics coupling using the standard Fokker-Planck Synthetic Acceleration (FPSA) technique [4].



Method	Runtime (s)	Transport sweeps
Transport	5.10	5364
FPSA	0.109	8
MFPA	0.0488	4

Figure 1: Radiative results for 16 angles, 15 moments, using the Exponential Scattering Kernel

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Analytic Solution to Elastic-Plastic Piston Problem with Hardening

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Keywords: Shock Hydrodynamics, Solid Dynamics, Analytic Solutions.

ABSTRACT

We present a new analytic solution derivation for the elastic-plastic piston problem that includes hardening as part of the problem physics. The elastic-plastic piston problem is a common verification problem for solid dynamics and involves an impact on a one-dimensional (1D) solid body, producing an elastic precursor wave followed by a slower plastic shock wave. Analytic solutions for this problem have been previously derived in the cases of hypoelasticity [1] and hyperelasticity [2] with no hardening. We expand on the hypoelasticity derivation by adding a linear hardening model implemented with the Wilkins radial return (RR) method. In addition to the analytic solution derived solely from general solid dynamics, we discovered an additional analytic solution for the particular implementation of the Wilkins RR method, in which the return to the yield surface is performed in one step while the yield stress is held constant, resulting in a change in elastic behavior during plastic deformation as seen in Fig. 1. We test the convergence behavior of a Lagrangian staggered-grid hydrodynamic (SGH) method on this problem and show convergence toward the one step analytic solution when that implementation of the Wilkins RR is used. If the Wilkins RR is instead implemented with an iterative process, the results converge to the original general analytic solution.

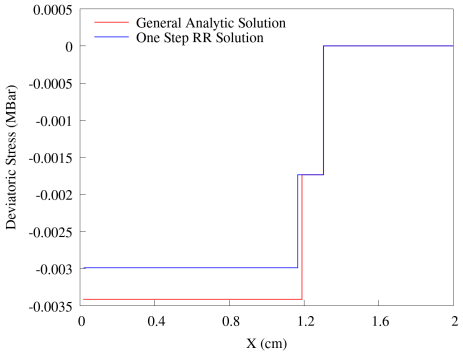

Figure 1: Analytic solutions of deviatoric stress for the elastic-plastic piston problem with linear hardening.

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Confinement Pagosa/MATCH/SURF simulation of Center Ignited Spherical Mass Explosion (CISME) experiment for study on DDT

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

ABSTRACT

PAGOSA is a powerful computational tool used in high explosive safety assessments. Using the LANL-developed Mechanically Activated Thermal CHemistry (MATCH) ignition-to-deflagration model, in conjunction with the Scaled Uniform Reactive Front (SURF) detonation model, Pagosa has successfully been used to simulate Deflagration-to Detonation Transitions (DDT), which are of utmost importance to safety considerations for conventional high explosives. To achieve a DDT event, explosive confinement is known to be a major factor and Pagosa is being used to study the effects of confinement.

Burn rate is a metric of violence in HE reaction. Burn rate has a strong dependence on confining pressure as there is positive feedback between the two: a high burn rate generates high pressure and a high pressure in turn enhances the burn rate. Moreover, experiments show that there is a jump in burn rate above a critical pressure p_c, as shown in Figure 1. This jump is due a transition from conductive to rapid convective burn: at sufficiently high pressure, burning explosive gas is forced into open cracks in the explosive, thus accelerating the burn rate. MATCH uses accumulated damage to incorporate this mechanism and thus achieve agreement with the CISME experiments. In an accompanying study, we have also shown that due to the Richtmyer Meshkov Instability (RMI), even without cracks, a solid HE (inert) can be penetrated by high pressure burning gas if the surface has small perturbation surface roughness (Fig. 1 right).

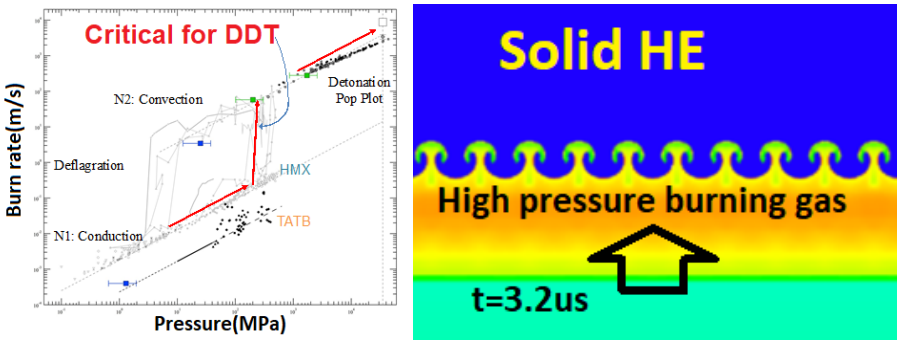

Figure 1: left: ***From L. Smilowitz and B. Henson (C-PCS, LANL);*** right: ***Forced-entry (LA-UR 21-18951) due to RMI instability for uneven surface. After t=3.2μs, the small perturbation of interface unevenness developed to mushrooms penetrating the solid HE.***

A fully conservative system for compressible immiscible fluids flow discretized by a low-diffusive interface scheme

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Keywords: shock hydrodynamics, multi-material hydrodynamics, Lagrangian methods.

ABSTRACT

In this work, we present a finite volume method (FVM) dedicated to the simulation of compressible inviscid immiscible multifluid flows. The starting point of this work is the use of the so-called five-equation Euler model [1] using stiffened gas equations of state (EOS). We have developed a second-order accurate FVM using a MUSCL slope reconstruction strategy. We have encountered strong pressure oscillations at fluid interfaces, a well-known problem referred in the literature. We suspect two possible sources of difficulty: i) the nonconservative nature of transport of the volume fraction; ii) an inconsistency (already mentioned in [3]) between pressure and internal energies at cell interfaces for flux evaluations. We therefore propose some contributions to fix these issues. We start by introducing a new variable and an additional conservation law leading to a fully conservative six-equation system which is formally equivalent to the five-equation one. Secondly we propose a formula to guarantee consistency between energy and pressure (referred to as energy consistency criterion or ECC [3]). Additionally, to get geometrically accurate fluid interfaces, the Euler solver is coupled with a low-diffusive interface method where gradient reconstructions use a genuinely multidimensional limiting process (MLP) as presented in [2]. A particular treatment is done for multifluid problems with more than two fluids: a renormalization on the volume fractions is used to ensure that the sum of volume fractions is equal to one. Finally we validate this approach on various numerical tests for two-dimensional problems, involving triple or quadruple points, and more than two materials.

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A Pure Lagrangian High-Order Hydrodynamics Method

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Keywords: shock hydrodynamics, multi-material hydrodynamics, Lagrangian methods.

ABSTRACT

High-order methods for hydrodynamics potentially offer significant improvements in robustness and physics fidelity over standard staggered-grid schemes [1]. Elsewhere they have been seen to require less ALE allowing more Lagrangian mesh motion, reduced numerical dissipation through fewer ad-hoc fix-ups and improved symmetry on meshes that are non-uniform [2]. This presentation describes the implementaton of a pure Lagrangian high-order scheme in 2D Cartesian slab geometry and is based quite heavily on our understanding of the work of [1, 2]. The purpose of our implementation is to allow us to make some in-house assessments of high-order methods on standard hydrodynamic test problems. The presentation discusses the current stage of our implementation and our future plans which include extending the scheme we have implemented to axisymmetry.

References

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Enabling interfacial flow simulations with larger time steps

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Keywords: interfacial flows, geometric Volume of Fluid; isoAdvector; interface advection; OpenFOAM.

ABSTRACT

It is well-known that geometric Volume of Fluid (VoF) methods outperform algebraic VoF methods in terms of accuracy, but are also more computationally demanding. Recently, a faster geometric VoF method, isoAdvector [1][2] was developed and implemented in the open-source Computational Fluid Dynamics (CFD) software OpenFOAM®. IsoAdvector has been used for a wide range of interfacial flow simulations including pressure swirl atomizers, breaking waves, fire-sprinklers and hydraulic jumps. A drawback of geometric VoF methods is that the modelling assumptions in their derivations generally require small time steps corresponding to interfacial Courant number, CoI, less than or close to unity. Even within this limit, accuracy is expected to deteriorate when approaching CoI ≈ 1 from below due to the gradual breakdown of the modelling assumptions.

We investigate the behaviour of isoAdvector for CoI near unity and analyse the causes of the observed errors at larger time step. We find that a main culprit is the neglect of cells that are not interface cells at the beginning of a time step, but into which the interface enters during the time step. We modify the algorithm to pass interface information on to relevant downwind cells allowing for consistent flux treatment in these cells. The result is a clear improvement in advection accuracy at large time steps without compromising efficiency. Figure 1 illustrates the improvement, comparing original and modified implementation for a pure advection test case with a disc advected in a constant velocity field at CoI = 0.9. In the presentation, we will show examples of both pure advection test cases and industrial cases and discuss possible ways to further improve the algorithm.

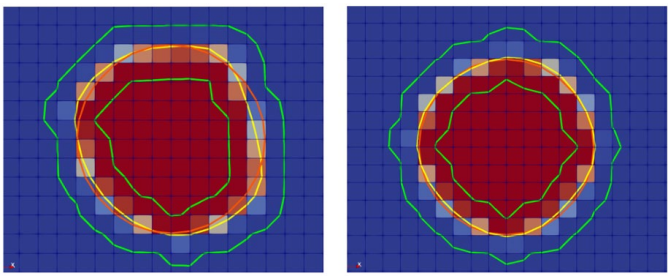

Figure 1: Volume fraction field at the final time-step of diagonally advected disc case with CoI = 0.9. Left: Original implementation. Right: Extended version. Red circle: True solution. Yellow curve: α= 0.5 contour of advected disc. Green curves: α= 0.01 and α= 0.99 contours of advected disc.

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A Dynamic Method for Detecting Shocks and Computing Their Speeds in Multi-Material Flows

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Keywords: shock hydrodynamics; multi-material hydrodynamics

ABSTRACT

Tracking the motion of shocks and computing their speeds as they propagate throughout the computational domain during hydrodynamic calculations remains a challenging unsolved problem. We present a straight-forward, cost effective approach to tracking shocks and computing their speeds in an arbitrary Lagrangian-Eulerian (ALE) framework that uses artificial viscosity [1, 2]. The method consists of two parts: shock detection and the calculation of the shock speed[3]. The shock detection algorithm operates with a cell-based tracking of a shock profile, which is based on the ratio of shock work to material work (i.e. large near shocks and near zero otherwise). During this process, the pre-shock and post-shock density and pressure and stored, which are then used to compute the shock speed based on a simple relation derived from the Hugoniot condition. Preliminary results show that this approach computes 2D oblique shock speeds at a material interface within a few percent accuracy on-the-fly (i.e. without post-processing). Additional test problems will also be presented.

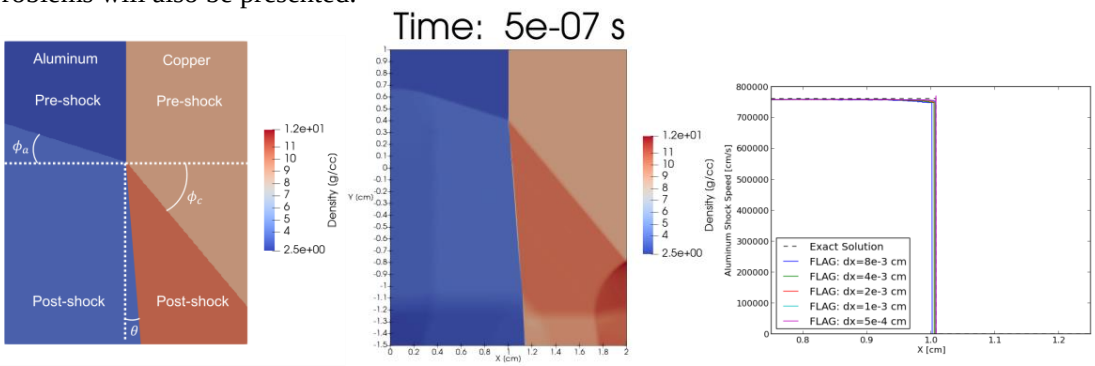

Figure 1: The initial oblique shock setup is shown on the left, and the solution after some time is shown in the center. The exact and computed shock speeds in the aluminum at Y=0.3 cm are shown (right), indicating the accuracy of the method and its convergence under mesh refinement.

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The Authors acknowledge support of the DOE ASC PEM Mix and Burn Project.

High-order monotone finite-volume schemes for 2D elliptic problems on deformed meshes

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Keywords: high order methods.

ABSTRACT

In this presentation, the problem is the following

$$\begin{cases} \alpha u - \nabla \cdot \kappa \nabla u = f & \text{in } \Omega, \\ \gamma \kappa \nabla \bar{u} \cdot \mathbf{n} + \delta \bar{u} = g & \text{on } \partial\Omega, \end{cases}$$

with $\kappa > 0, \alpha > 0, \gamma \geq 0, \delta \geq 0$ and γ and δ are not zero at the same time on the boundary edge.

We know that this equation admits a positive solution under the conditions $f \geq 0, g \geq 0$ [3]. Numerical methods preserving this property at the discrete level are called monotone or positive.

Positivity is fundamental to our applications because u can be the temperature or the concentration. We have proposed a 1D scheme [1] that preserves positivity while being high order accurate in space. This talk explains how to extend our monotone 1D scheme of any order of precision in space into 2D. We propose a family of finite volume schemes of arbitrary order. A polynomial reconstruction ensures the consistency of the fluxes.

We prove that these schemes are conservative and monotone, at the cost of the linearity of the scheme. The non-linearity is solved thanks to a fixed point. Under a stability assumption, we have also shown convergence to an order corresponding to one order less than the degree of the reconstruction. These schemes can also be symmetrized, which further induces the scheme's LMP structure [2] (Linear Maximum Preserving).

This strain of schemes is implemented in C++ in a open platform of the CEA in order to validate this approach.

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Matrix-free, high-order methods for high-performance multi-material ALE hydrodynamics on GPUs

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Keywords: ALE hydrodynamics, high-order methods, finite element methods, multimaterial, GPUs, multiphysics

ABSTRACT

MARBL is a multimaterial, multiphysics code developed at LLNL and is based on a three phase Arbitrary-Lagrangian-Eulerian (ALE) framework: evolution of physical conservation laws within a moving material (Lagrangian) frame; mesh optimization, and conservative, monotonic field remap. For each phase we employ high-order finite elements for the spatial discretizations as described in [1]. The original finite element formulations for the three phases of ALE were based on full assembly, where matrix operators used in the semi-discrete Lagrangian conservation laws, mesh optimization formulations and ALE remap terms were assembled into sparse, global matrices; then solved using parallel matrix-vector multiplication operations. Full matrix assembly scales poorly as the order of the finite element method increases and involves expensive data motion which is undesirable for GPU compute devices.

Recently, we have completed the conversion of the entire high-order finite element ALE approach used in MARBL to more computationally efficient matrix-free methods based on partial assembly, and in this talk, we review the matrix-free finite element formulation for each phase and demonstrate its computational performance in large scale 3D simulations on GPU based systems. For the Lagrange phase, this includes the force, mass and hyperviscosity operators. For the mesh optimization phase, this includes the matrix operator used in forming the non-linear objective function and applying Netwon's method to minimize it. Finally, for ALE remap we employ element-based flux corrected transport (FCT) methods which blend a low-order bounds preserving solution [2] with a high-order DG scheme using a clip/scale blending strategy resulting in a matrix-free FCT method for multi-material, multi-field ALE remap. We describe the algorithmic tailoring for the GPU that was developed for each phase and present performance comparisons between the different approaches.

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-829189.

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Numerical simulation of flow through swelling porous media

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Keywords: Porous media, Swelling, Wicking, Multiphase flow, Volume of Fluid Method,

ABSTRACT

In Engineering studies, the flow through porous media is an active subject of research due to its practical applications. The swelling of porous media as result of liquid absorption by solid matrix effects on the fluid flow through porous media. As a result, the resistance to fluid flow through porous media increases due to reduction in the porosity and permeability of porous media. The computational models of fluid flow through porous media helps to design and optimize for different engineering applications such as paper towels, industrial wicks, baby diapers, liquid composite molding processes, heat pipes, composite molding techniques, industrial filtration, hygiene products etc. The computational modelling of flow through porous media is often based on a single and multiphase assumption using Darcy's law under rigid or non-rigid conditions. While developing the computational models, assumption of rigid porous media is not always correct. If swelling effects are neglected from numerical models could lead to a serious error in the predictions from the developed computational model in terms of liquid flow front locations. Hence, it is important to include swelling effects in computational modelling and very few works attempted to model such a flow condition. Further, for the computational modelling of capillary pressure effects, the available multiphase approaches are based on the number of fitting parameters. These parameters need to be estimated analytically or measured experimentally which makes it hard to implement. The resulting computational model would not predict the flow front locations accurately if correct values of these fitting parameters are not known. In this study, a novel methodological approach is proposed which allows to account for the swelling and capillary pressure effects within the porous media. The novel combination of the Finite Volume Method and Volume of Fluid method (FVM-VOF) is used for the first-time to model the liquid absorption and swelling effects within porous media. The computational models are developed for the different flow scenarios such as flow through swelling porous media under non absorbing conditions, flow through rigid /swelling porous media under absorbing conditions. The developed computational models for each flow scenario are validated against available experimental data. The modelling framework is further extended to model the flow scenario for following applications; Liquid composite molding (LCM), industrial wicks and diapers. Different cases of flow are considered and studied critically. It is expected that the outcomes of this study would help researchers to model the capillary pressure and swelling effects accurately and efficiently. The proposed methodological framework can be used to model the flow scenarios for applications such as LCM processes, Industrial wicks, paper napkins, tissue papers, hygiene products.

Weakly Compressible Two-layer Shallow-Water Flows in General Channels

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Keywords: Hyperbolic conservation and balance laws, Non-conservative products, Numerical schemes.

ABSTRACT

We present a weakly compressible approach to describe two-layer shallow water flows in channels with arbitrary cross sections [1, 2]. The standard approach for those flows results in a conditionally hyperbolic balance law with non-conservative products while the current model is unconditionally hyperbolic. A detailed description of the properties of the model is provided, including entropy inequalities and entropy stability. Furthermore, a high-resolution, non-oscillatory semi-discrete central-upwind scheme is presented. The scheme extends existing central-upwind semi-discrete numerical methods for hyperbolic balance laws. Properties of the model such as positivity and well balance will be discussed. Along with the description of the scheme and proofs of these properties, we present several numerical experiments that demonstrate the robustness of the numerical algorithm.

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A pressure-based Baer-Nunziato model for two-phase flows governed by generic equations of state

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Keywords: Baer-Nunziato model, pressure formulation, generic equations of state, weakly compressible two-phase flows.

ABSTRACT

Within the framework of diffuse interface methods, we present a pressure-based Baer-Nunziato type model able to consider generic equations of state [1]. A special scaling is applied to the governing equations to recover the correct scaling of the pressure fluctuations in the low Mach limit. The resulting governing equations are solved using a semi-implicit finite-volume scheme that integrates implicitly the acoustic terms, and provides a robust discretization of the non-conservative terms that enforces by construction the pressure and velocity non-disturbance condition across multi-material interfaces. The proposed model can be equipped with finite-value pressure and velocity relaxation terms, which describe how the fluids are driven toward mechanical equilibrium at interfaces, and with chemical potential relaxation to include mass transfer. Each relaxation process gives rise to a system of ordinary differential equations, which is solved locally. The effects of different values of the relaxation parameters are investigated in a validation campaign.

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On Finite Element Approximation of Multiphase Flows during Glass Production Processes

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Keywords: shock hydrodynamics, multi-material hydrodynamics, Lagrangian methods.

ABSTRACT

In this paper the problem of numerical simulation of flow motion of the molten glass during the production process is discussed. 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 the float glass forming and glass blowing/pressing process shall be considered, cf. [1], [2].

First, the mathematical model describing the production of the flat glass by the float process is considered as introduced by Pilkington in the 1950s, cf. [1]. During this process the raw material is put into the furnace and melted at 1500 degrees of Celsia, homogenized in order to eliminate bubbles and then the viscous liquid flows out of the furnace through the lip part onto the melted tin bath. As the density of the glass is lower compared to the density of the tin, the melted glass forms a flowing ribbon on the melted tin. This ribbon is then transported through the stretching part to the outlet, where the flat glass is pulled out of the tin bath. Such a process is a complicated multiphisycal phenomena influenced the melted glass flow interacting with the melted tin flow significantly influenced by the by the heat transfer as the material properties depends on the widely varying temperature. One of the difficulties to be overcome are the dimensions of the computational domain (the tin bath is usually about 60 m long, but the produced flat glass height is in the range of milimeters, e.g. 2 - 20 mm). The process is further influenced by the turbulent flow of the tin, where the hot and cold zones are divided, the heat transfer by the radiation and the heaters located mainly in the stretchin area. 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, see e.g. [3]. This forming process involves extreme temperatures and large deformations and application of either Lagrangian or Arbitrary-Lagrangian-Eulerian are suitable. Here, a simplified mathematical model shall be considered and the realization of the surface tension shall be discussed. The numerical results will be presented.

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Entropy dissipation control in numerical approximations of Lagrangian hydrodynamics

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Keywords: Lagrangian hydrodynamics, Godunov methods, Random Choice methods.

ABSTRACT

One of the key points of numerical methods for solving hyperbolic systems is to provide enough numerical diffusion to correctly capture the weak physical solutions of these problems. This is closely related to the fact that the numerical schemes satisfy an entropy inequality. This guarantees that the Rankine-Hugoniot conditions are fulfilled and that the shocks are accurately resolved. With regard to gas dynamics equations physically relevant solutions have to be consistent with the second law of thermodynamics. In particular, entropy must be conserved for smooth flows.

The purpose of the present work is to address this issue in the case of cell centered finite volume discretizations dedicated to the simulation of Lagrangian hydrodynamics [2]. These methods, derived from the pioneer work of Godunov [1], rely on the resolution of approximate Riemann problems at cell interfaces in order to derive the numerical fluxes. The approximate Riemann solver is carefully designed to enforce the thermodynamic consistency and the consistency with the continuous problem. The downside of these methods is that they tend to be diffusive, even when the solution is regular, which leads to entropy inconsistency. For strong expansions, this can lead to severe inaccuracy [3].

In 1D, the flux formulation of the scheme can also be reinterpreted as the average value in the cell of the approximate Riemann solutions coming from each of its faces. This averaging process appears to be the main cause of diffusion. To overcome this difficulty, following the seminal work of [4], we derive random choice methods to compute the cell unknowns directly from the Riemann solutions. In this framework, the amount of numerical diffusion is drastically reduced since the averaging procedure is absent. It is well known that these methods are efficient when combined with the exact solution of the Riemann problem, hence employing an exact Riemann solver. On the contrary, using approximate solvers often leads to a loss of consistency and convergence. Starting from the work of Harten and Lax [5], we investigate various Riemann solvers and we try to derive key properties to build efficient schemes. This work is illustrated with various numerical results.

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Sharp Material Interfaces in xRAGE Eulerian code using Tangram Interface Reconstruction Library

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Keywords: Eulerian methods, multi-material hydrodynamics, volume-of-fluid methods.

ABSTRACT

Material interfaces move naturally with the flow. In Lagrangian simulations, each material can be therefore discretized independently avoiding numerical mixing. In contrast, Arbitrary-Lagrangian Eulerian (ALE) simulations result in the introduction of multi-material cells. In these cells, interface reconstruction is typically employed to keep materials separated. On orthogonal meshes, Eulerian simulations can be split into a set of pseudo 1D ALE simulations with continuous rezoning to the original mesh along each line for each Cartesian direction (Strang splitting) such as for the original solver in xRAGE [1]. To achieve high accuracy, discretized quantities are still reconstructed in 2D/3D space inside these pseudo 1D simulations and thus requiring fully multi-dimensional interface reconstruction. Modern Eulerian solvers do not use Strang splitting making implementation of sharp material interfaces challenging [2]. We describe these challenges and we compare these two solvers on a set of multi-material problems.

In addition to the standard Youngs' Volume-Of-Fluid (VOF) method, more accurate interface reconstructions such as Least square Volume Interface Reconstruction Algorithm (LVIRA) and Moment-Of-Fluid (MOF) are available in Tangram [https://github.com/laristra/tangram] [3]. These accurate methods not only lead to better preservation of advected shapes (see Figure 1), they also do not require as large computational stencil reducing Message Passing Interface (MPI) communication in our code.

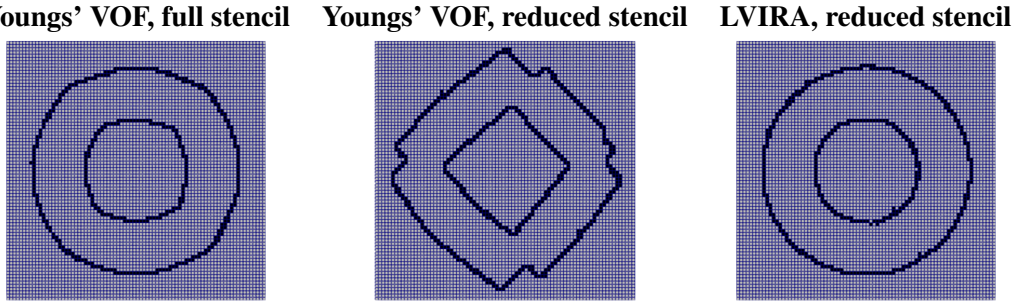

Figure 1: Originally circular interfaces after periodic advection with velocity $(1, 1/3)$ at time 6.

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Multi-Material Swept-Face Remapping in Portage

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Keywords: ALE, conservative interpolation, remapping, multi-material.

ABSTRACT

Portage is an open-source library [https://github.com/laristra/portage] for conservative interpolation (remapping) of single- and multi-material scalar data between polygonal/polyhedral meshes [1]. In addition to an accurate remap based on intersection of the two meshes, Portage also provides an approximate swept-face remap for meshes with the same topology and small displacement such as in traditional Arbitrary-Lagrangian Eulerian (ALE) hydrodynamic simulations without mesh re-connections or adaptive refinement. When the mesh displacement is very small, results of the swept-face remap are visually indistinguishable (see Figure 1) from intersection-based remapping for a single remapping step. The swept-face remap is computationally more efficient while maintaining 1) second-order accuracy is pure material regions and 2) positivity of remapped data at material interfaces [2].

However, positivity of remapped data is not guaranteed in pure material regions when using swept-face remapping even with a limited piecewise linear reconstruction. We provide an example of such situation and we discus alternative limiting strategies together with sufficient restrictions on mesh movement to preserve positivity. This is an alternative to existing positivity-preserving techniques based on the redistribution of remapped data (repair) or on corrected material fluxes.

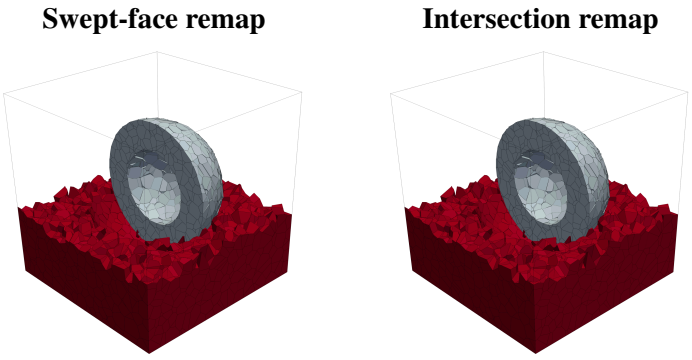

Figure 1: Remapped data colored by material indices.

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High–Resolution Simulations of Transitional Triple-Point Shock Interactions

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Keywords: shock hydrodynamics, multi–material hydrodynamics, task–based parallel computing.

ABSTRACT

This work concerns the evolution of the Ritchmyer–Meshkov instability (RMI) in a rather unconventional setting: the classic triple–point canonical problem [1]. The problem is defined here in 3D by periodically extending the out–of–plane direction. A cross section with all relevant initial conditions is given in Figure 1. The simulation includes reshock, making this a case which hasn't been studied before. The problem provides an excellent framework for studying shock induced transition as well as other instability mechanisms such as secondary baroclinic instability in a multispecies environment.

The nature of the transition to turbulence in this problem depends on initial conditions. We have analysed this dependence by running an ensemble of configurations with different initial conditions using the *Legion* programming system – a novel approach to simulating a large number of (multifidelity) simulations asynchronously. Thus we were able to quantitatively identify the most effective perturbations for promoting transition. A thorough mesh sensitivity study was performed, using 4 different meshes (in each case the grid spacing was approximately halved). Results for volume integrated TKE were shown to collapse for the finer meshes, thus demonstrating convergence.

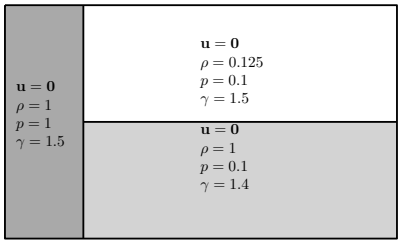

Figure 1: Initial conditions.

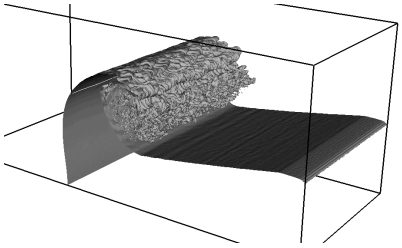

Figure 2: Mass fractions ($t < t_c$).

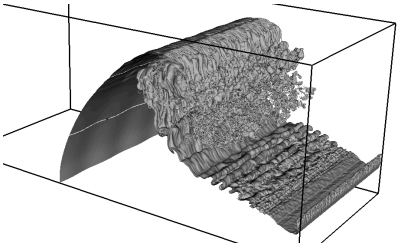

Figure 3: Mass fractions ($t > t_c$).

As an integral part of this problem, turbulent mixing is studied using two species segregated in the initial condition, using multi–component mixture transport with constant properties. The mass fractions are plotted in Figure 2 and Figure 3 for a time prior the reshock ($t < t_c$) and a time after the reshock ($t > t_c$). The effect of the difference between heat capacity ratios between the materials is also considered. A mixing indicator function is used to quantitatively measure the evolution of bulk mixing.

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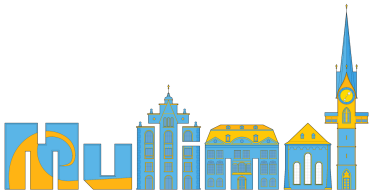

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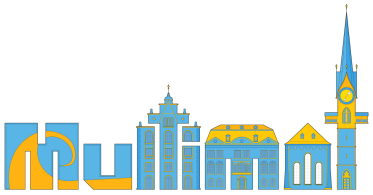

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