LA-UR-20-26469

Approved for public release; distribution is unlimited.

Title: An overview of the work in the numerical methods subteam

Author(s): Morgan, Nathaniel Ray

Intended for: Presentation to summer students

Issued: 2020-08-21

Disclaimer:

Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by Triad National Security, LLC for the National Nuclear Security Administration of U.S. Department of Energy under contract 89233218CNA000001. By approving this article, the publisher recognizes that the U.S. Government retains nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.

An overview of the work in the numerical methods subteam

Nathaniel R. Morgan

XCP-4: Continuum models and numerical methods

LANL has a rich history of developing revolutionary numerical methods

- Skyrme et. al. 1949 created the finite difference Lagrangian method with shock tracking
- Von Neumann and Richtmyer 1949 created the Lagrangian staggered grid hydrodynamic method
- Metropolis et al. 1949 created the Monte Carlo (MC) method
- Harlow 1955 created the Particle-in-cell (PIC) hydrodynamic method
- Reed and Hill 1973 created the discontinuous Galerkin (DG) method
- Shashkov et al. 1995 (and on) did pioneering work on Mimetic difference methods
- F. Brezzi, K. Lipnikov, and V. Simoncini created the virtual element method
- ... and a lot more

A focus area within XCP-4 is on creating transformative methods to solve partial differential equations (PDEs)

- Methods are developed to solve elliptic, parabolic, and hyperbolic PDEs

Fig: 3D diffusion using a Voronoi mesh with three materials and a sharp interface

Fig: Sedov blast wave

Advanced diffusion solvers are necessary to accurately simulate e.g., heat-transfer on multi-material problems

Fig: Diffusion on a Voronoi mesh with multi-material cells

Hydrodynamics methods are used to simulate compressible, shock driven flows

- Lagrangian: the mesh moves with the flow

- Eulerian: the mesh is fixed in space so material flows through the mesh

- Arbitrary Lagrangian Eulerian (ALE): the mesh moves at an arbitrary velocity ranging from being fixed (Eulerian) to moving with the flow (Lagrangian)

Contact surface methods enable mesh-mesh collision, sliding, and separation in ALE simulations

LANL leads the world in creating high-order Lagrangian discontinuous Galerkin (DG) hydrodynamic methods

- High-order Lagrangian methods are essential for high-fidelity simulations

Fig: High-order DG simulations of a PBX-9502 rate stick experiment using multiphase reactive burn

Fig: A high-order Lagrangian DG simulation of a Taylor Anvil experiment using a crystal plasticity model based on dislocation density

High-order Lagrangian methods have meshes that can bend with the flow

A. Taylor Green vortex at $t=0.75$

B. Gresho vortex at $t=0.6$

Fig: Simulations of vortical flows

High-order methods are well suited for large deformation simulations

Lagrangian DG simulation of the Gresho vortex variant

LANL leads the world in creating polytopal hydrodynamic methods

Fig: A 3D Lagrangian DG simulation of a Taylor Anvil experiment using a Voronoi mesh

Fig: A regional reconnect base ALE simulation of a notional internal confinement fusion (ICF) implosion

Numerical methods for interface-aware subscale dynamics enable accurate simulations of multi-material flows

Fig: Sharp material interfaces are used in simulations to prevent numerical diffusion

Fig: An Eulerian simulation of a multi-material vortex using sharp interfaces

Summary: work in XCP-4 seeks to create game-changing numerical methods suitable for diverse applications

Fig. The Verney test problem has a collapsing metal shell

Fig. Deformed metal rod at $t=149 \mu\text{s}$

Fig. Kidder ball is a compressing ball of gas