An overview of hydrodynamics algorithms and challenges at the NNSA Laboratories

Britton Olson, PhD
Computational Physicist and Group Leader
Weapons and Complex Integration
Lawrence Livermore National Laboratory

Chris Malone, PhD
Computational Physicist and Project Leader
X Computational Physics Division
Los Alamos National Laboratory

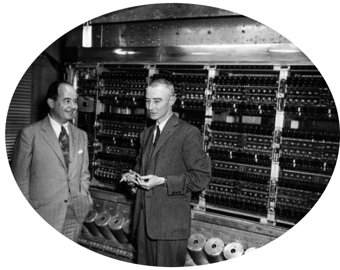
PSAAP4 Pre-proposal meeting

August 2023

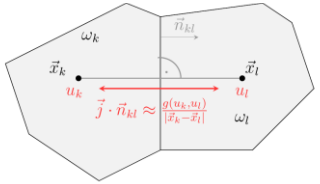
Prepared by LLNL under Contract DE-AC52-07NA27344.

Talk summary

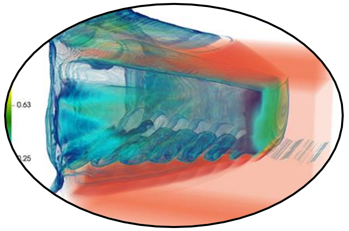
Introduction and History of Hydro at Labs – then and now



Overview of hydro algorithms at the Labs and current challenges



Application highlights from the NNSA Labs



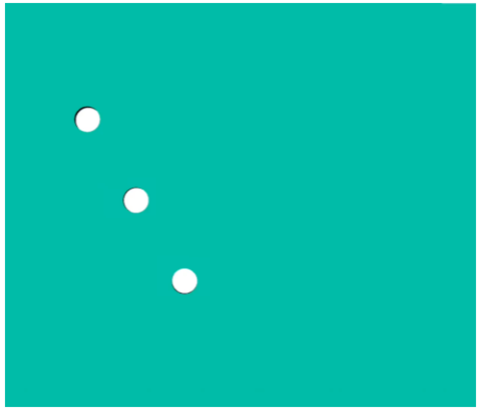
Caveats/Foreword

- This talk is **not a comprehensive review of computational fluid dynamics methods** or history; even as it pertains to the NNSA Labs.
  - It's a narrow view into the Labs' challenges, experiences, and applications with hydrodynamics simulations.
- The speaker makes **no claim of being an expert in all the methods/applications that will be discussed.**
  - I've worked on many hydro codes at LLNL but please excuse incompleteness, lack of rigor, or poor context in this talk. This talk draws from the expertise and content of many folks from the NNSA Labs.

The goal of this talk is to give you a view into the NNSA Labs' experience with computational hydro and our present and future challenges and applications.

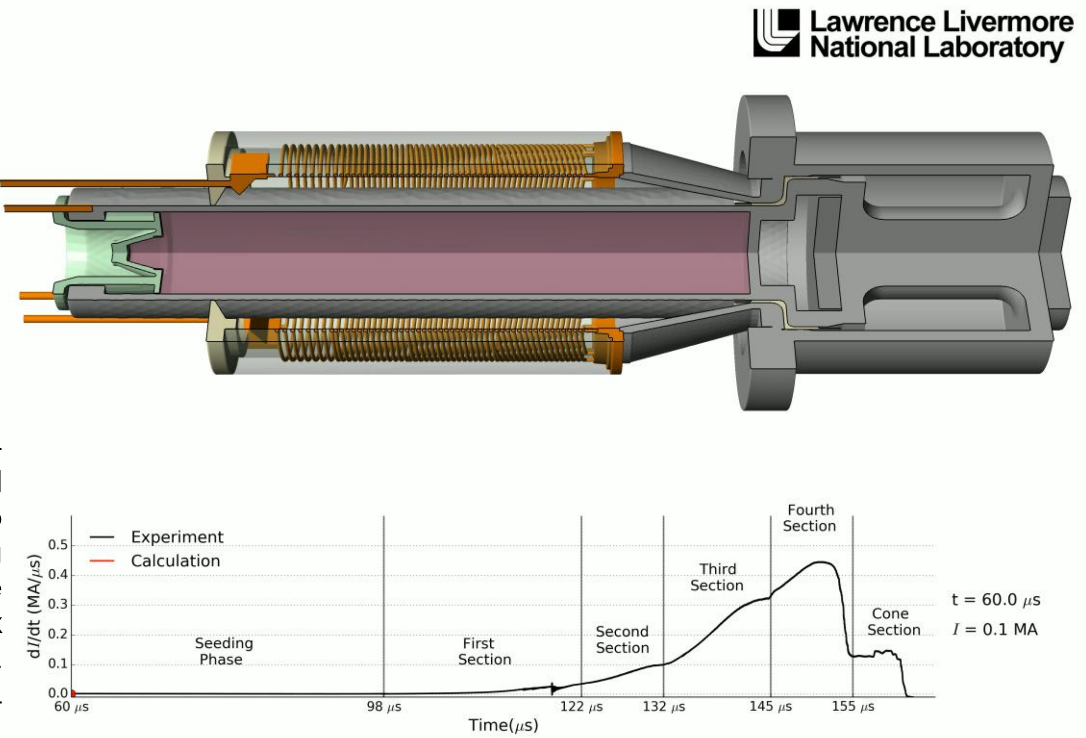
Hydrodynamics = conservation of mass, momentum, and energy

- For NNSA Labs, the term “hydrodynamics” or “hydro” can take on a few meanings.
  - Computational fluid dynamics (CFD) of the Euler equations and/or the compressible Navier-Stokes (NS) equations.
  - General continuum dynamics problems using NS equations but with strength, damage, fracture, melt, etc. models.
  - Modeling a shock driven experiment with no reacting elements.
    - *You hit anything hard enough, it’ll behave like a fluid…*



Left: Simulation of 3 cylinders at super-sonic speeds showing shock turbulence interations. LLNL

Right: Three-dimensional hydro simulation of a high-explosive drive flux compressor. LLNL



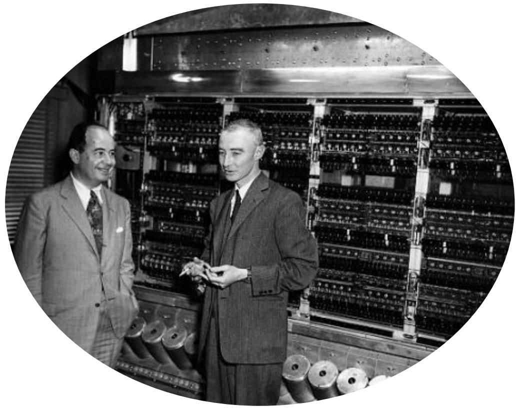
NNSA Laboratories began solving “hydro” in 1942

1942
Los Alamos, NM

Simple shock wave calculations were performed by “computers” which were typically the spouses of Lab physicists.

1945
Los Alamos, NM

John Von Neumann develops programming model for ENIAC computer.



MANIAC
N. Metropolis

IBM machines were configured to solve for converging shocks; E. Teller and S. Ulam solved simplified equations and used EOS approximations

1944
Los Alamos, NM

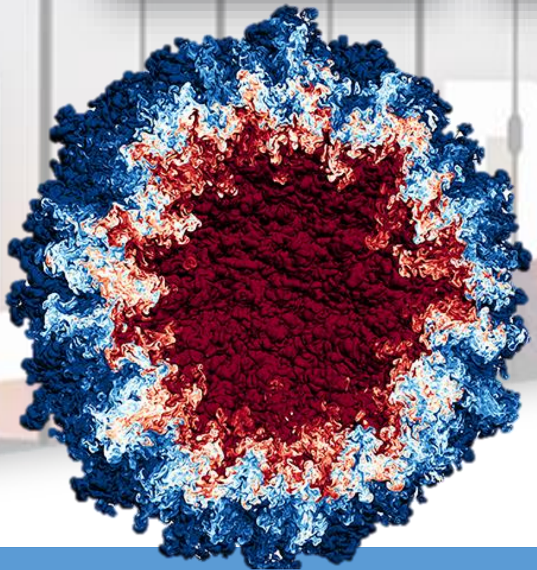
Von Neumann publishes seminal paper on artificial viscosity for shock capturing with Richtmyer.

1950
Los Alamos, NM

References
- https://www.osti.gov/opennet/manhattan-project-history/Science/ParticleAccelerators/computer.html
- https://ahf.nuclearmuseum.org/ahf/history/computing-and-manhattan-project/
- https://discover.lanl.gov/publications/national-security-science/2020-winter/computing-on-the-mesa/
- “Equation of State: Manhattan Project Developments and Beyond”, Scott Crockett, Franz J. Freibert, LA-UR-21-20443 (2021)

State of the art hydro calculations today benefit from world class computing resources

- Computing power has grown by a factor of 4^{15}!
  - (500 FLOPS, ENIAC -> 2 EXAFLOPS, El Capitan)
  - Same ratio as the weight of a pebble to El Capitan!
- Large scale 3D calculations are now part of the design process
  - The once "hero" calculations are now part of ensembles and uncertainty quantification (UQ) suites.
- Challenge of having multi-disciplinary (MD) teams; methods development, performance portability, and multi-physics modeling
  - We need staff trained and experienced on MD teams.
  - Our codes must make advances on all fronts to stay viable and relevant



Left: 100B zone spherical mixing layer calculation was run on Sierra to help understand the physics of mixing in ICF capsules at LLNL.

Exascale computing presents great opportunities but significant challenges for hydro.

An overview of hydro algorithms at NNSA Labs

Lagrangian, Eulerian and everything in between

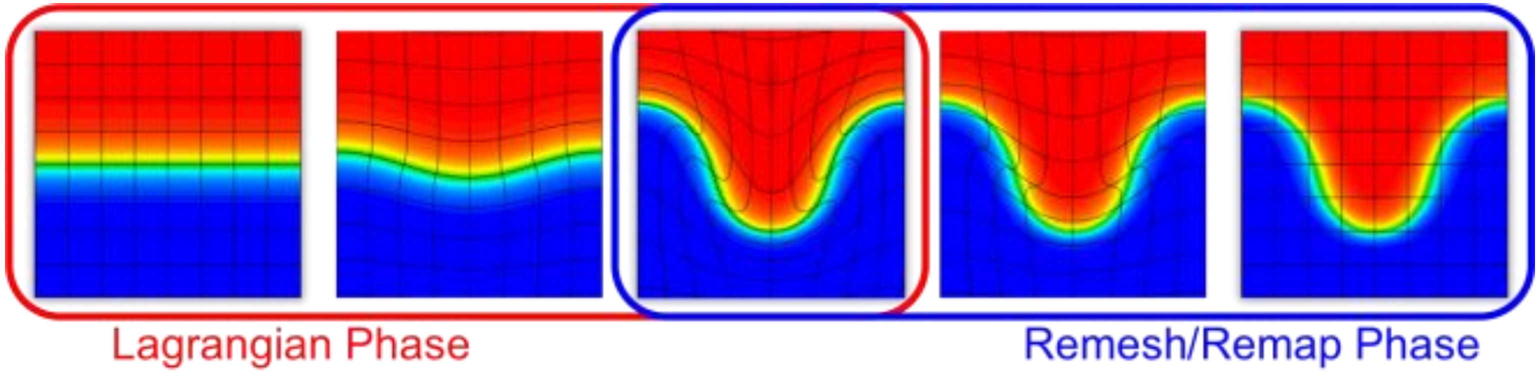
- Many of the NNSA laboratory hydro codes are considered ALE (Arbitrary Lagrangian-Eulerian)
  - What we call ALE is typically a Lagrange step + Remesh/Remap (L+R)
  - Remap can be purely geometric or advection based
  - Capturing the evolution of material interfaces and vortical motion challenge the robustness of our codes.
- Eulerian (direct or L+R) codes also provide solutions on simple regular grids

$$\frac{D\rho}{Dt} = -\rho\nabla\cdot\mathbf{u}$$

$$\frac{D\mathbf{u}}{Dt} = -\frac{\nabla p}{\rho} + \mathbf{g}$$

$$\frac{De}{Dt} = -\frac{p}{\rho}\nabla\cdot\mathbf{u}$$

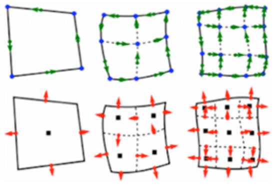
The Euler equations expressed using the material derivative, assume the mesh moves with the fluid.

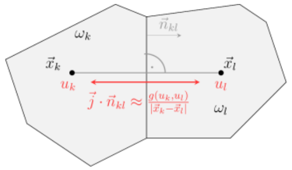


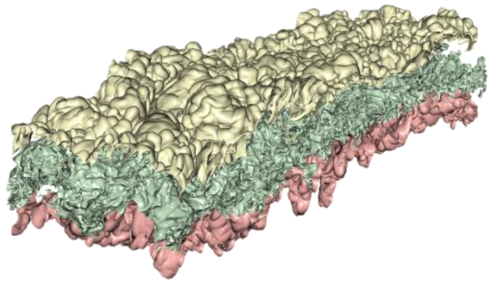
ALE hydrodynamics presents the challenge of remap.

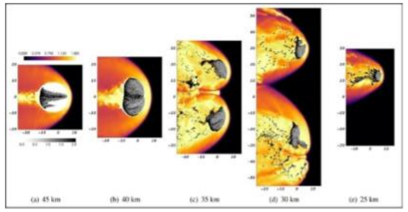
Numerical methods for hydrodynamics

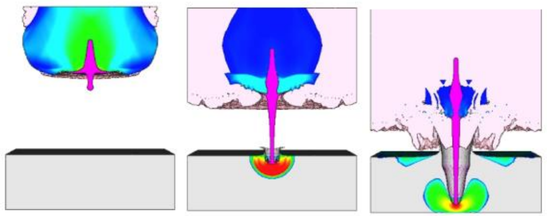
- Discretization methods:
  - 2nd order Finite-volume; TVD, Godunov, FCT, etc.
  - Finite difference; pseudo-spectral
  - Finite-element; arbitrary order; Virtual Element Method
  - Space-time, Discontinuous Galerkin
  - Smooth particle hydrodynamics (SPH); Material Point Methods (MPM)
- Mesh types:
  - Block structured, unstructured, adaptive mesh refinement (AMR) particle based, hybrid, space-time, etc.
- Time integration
  - Explicit schemes; 2nd order predictor-corrector method, 1st order operator splitting in multi-physics problems, higher-order RK schemes
  - Implicit methods, IMEX (Implicit-Explicit) multi-rate time integration

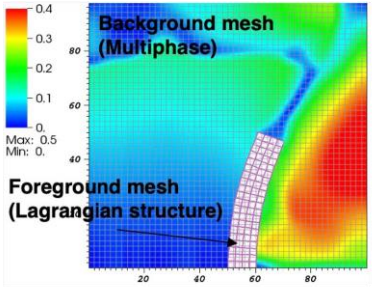








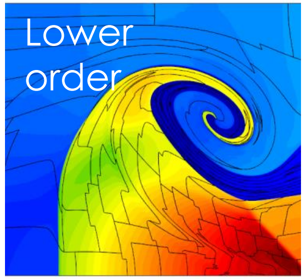




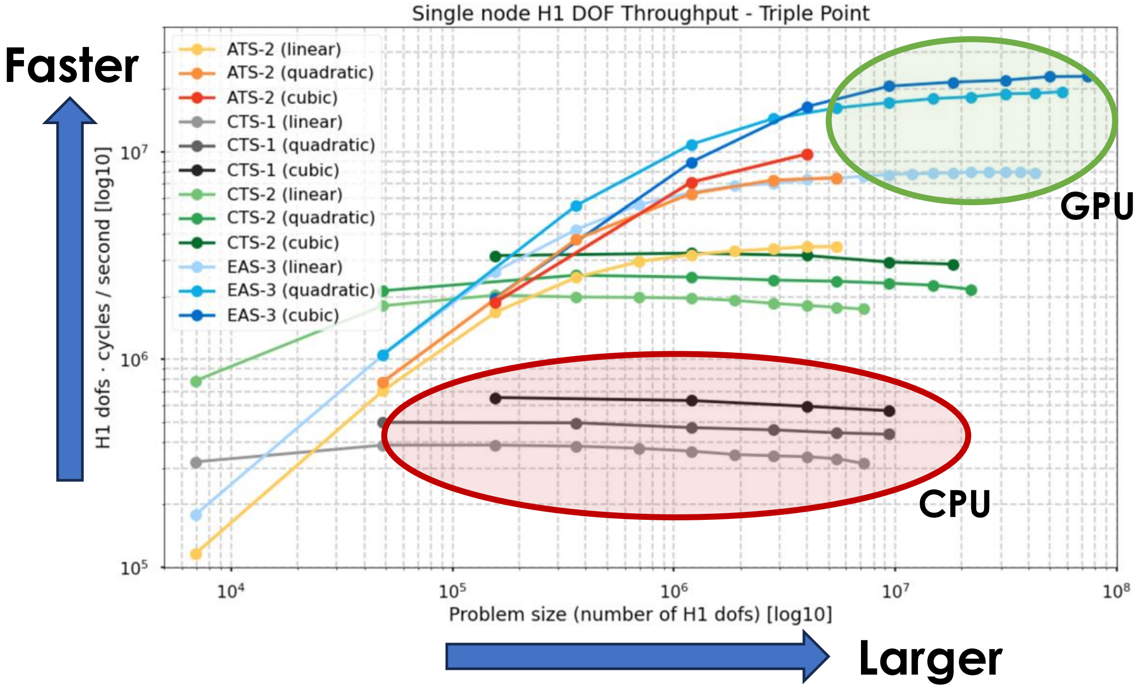
NNSA Labs' programs support a diverse portfolio of numerical methods for hydro suited for different applications.

High-order vs. low-order

- Higher-order accuracy methods (O(h^3) and higher) can offer <u>superior *error:cost* ratios</u> over lower-order schemes.
- Higher-order schemes with larger FLOP/memory requirements can offer additional advantages on heterogeneous architectures.
- Lower-order schemes offer added robustness, simplicity, and institutional knowledge and support.



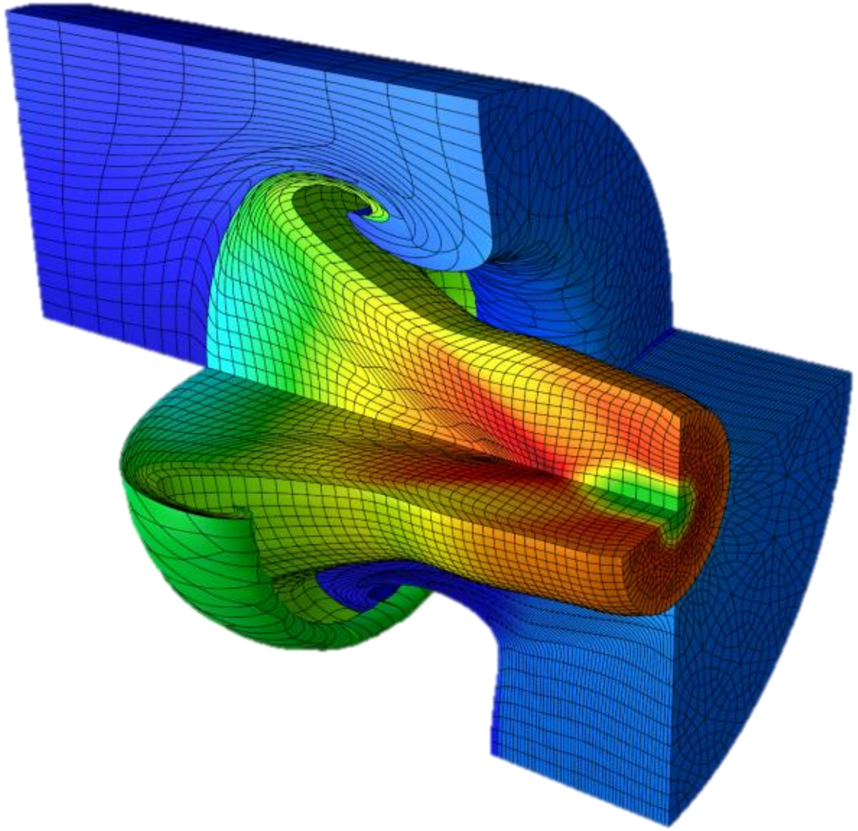
Computational throughput



The answer is nuanced and both approaches will remain in NNSA Labs' programs & codes.

Multi-material models and interfaces

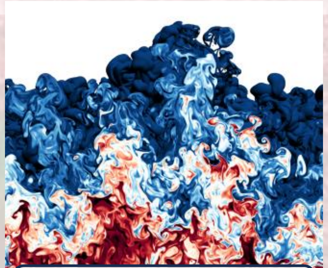
- Interfaces:
  - The volume of fluid method is used by many of our ALE codes.
  - The diffuse interface approximation (DIA) is also used.
  - Others; Lag, particle based, mesh adaptive, etc.
- Materials: Continua with dependent constitutive properties close the system; equation of state, material diffusivities, strength, etc
  - NNSA Labs also extensively use tabular databases; e.g. an EOS that gives P,T = F(rho,E) for each material.
  - Multi-material closure problem, N-materials; most of our codes solve:
    - P/T equillibrium between materials (4 equation model)
    - Independent thermodynamics state for each material (6 equation model)
    - Independent hydrodynamic state for each material (7 equation model)



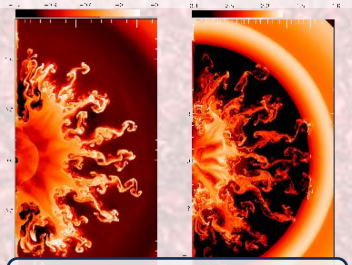
Multi-material schemes and EOS closure models must be robust and general.

Turbulence modeling and hydrodynamic instabilities

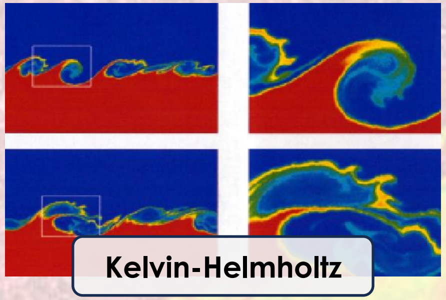
- NNSA codes perform DNS, LES, and RANS calculations on a range or problems.
  - Industry has largely motivated turbulence research in aerodynamic, wall bounded flow.
  - NNSA Labs are also concerned with interfacial instabilities and the resulting turbulence:
    - Rayleigh-Taylor (RT), Ritchmyer-Meshkov (RM), Kelvin-Helmholtz (KH), etc
- DNS & LES & experiments inform our RANS and reduced order modeling methodologies for turbulence in multi-physics applications.



Rayleigh-Taylor



Ritchmyer-Meshkov

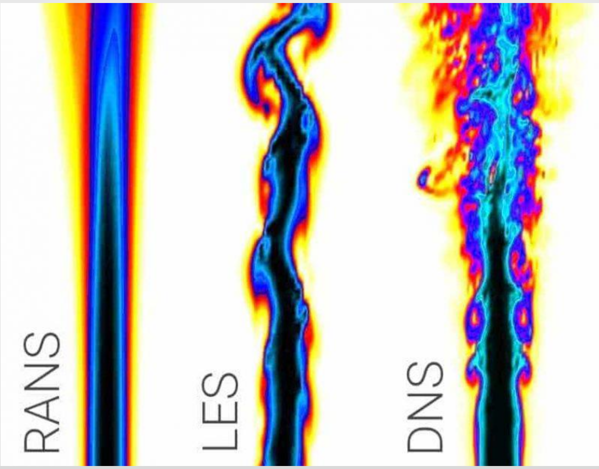


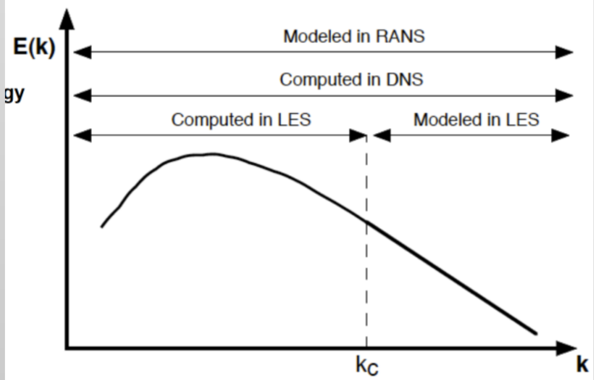
Kelvin-Helmholtz

Reynolds-Averaged Navier-Stokes

Large Eddy Simulation

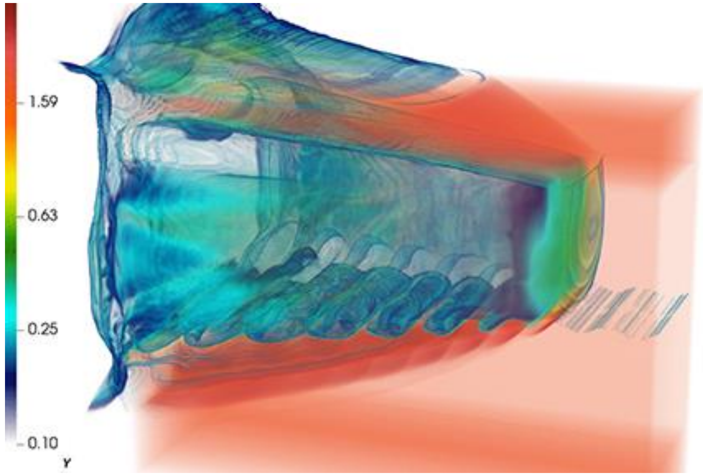
Direct Numerical Simulation



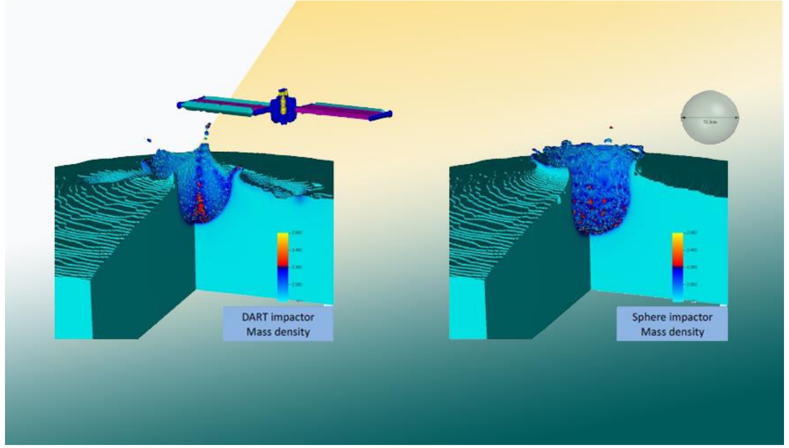


DNS/LES are not practical for all applications, so we rely on physics informed lower fidelity models.

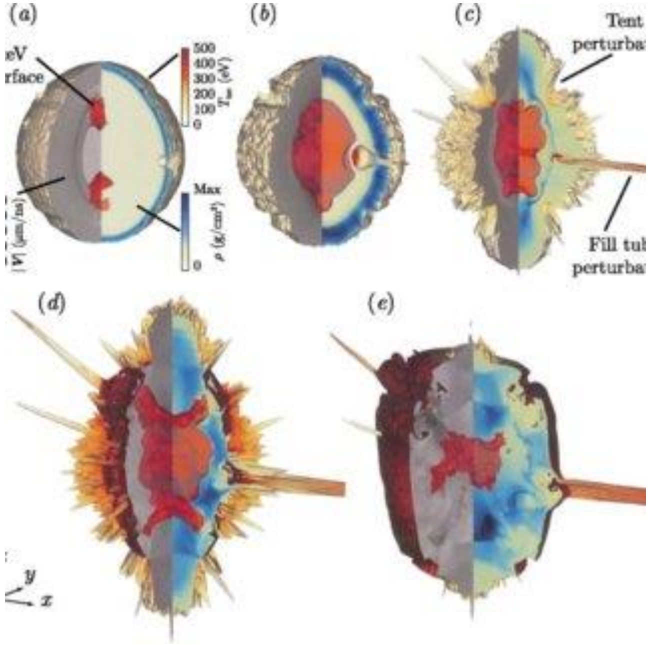
A few examples of NNSA hydro applications (1)



Radiation-driven Kelvin–Helmholtz instability experiment. LLNL

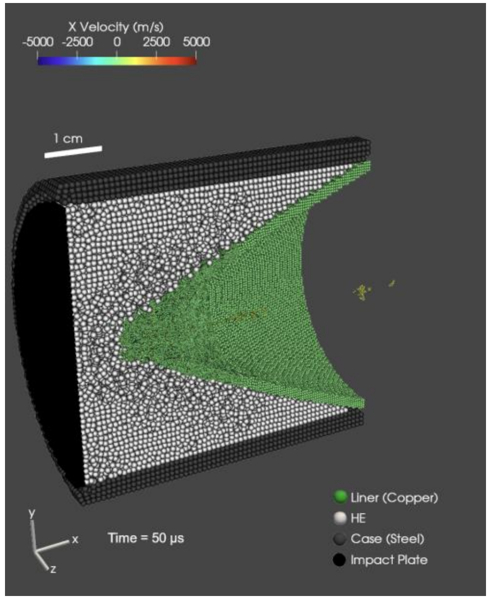


Simulations of NASA's DART spacecraft, which will crash into asteroid Dimorphos in fall 2022, show the differences between modeling the full spacecraft geometry and a spherical approximation of the spacecraft. LLNL

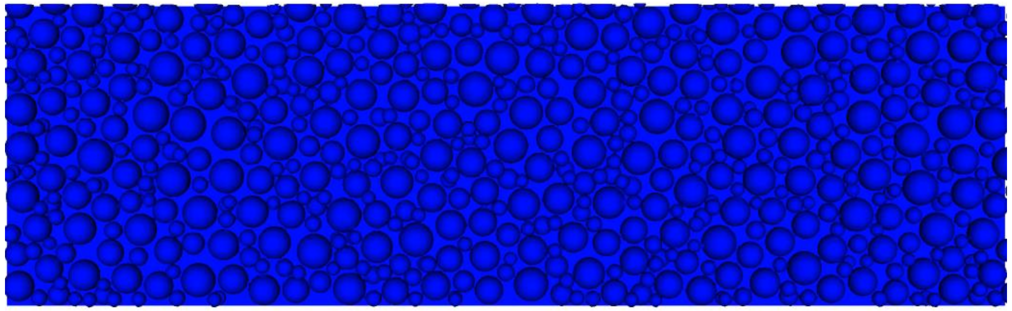


ICF implosion calculation time history and rendering of the fuel ablator interface at bang time (22.83 ns) from a 3-D simulation of NIF shot N120321. LLNL

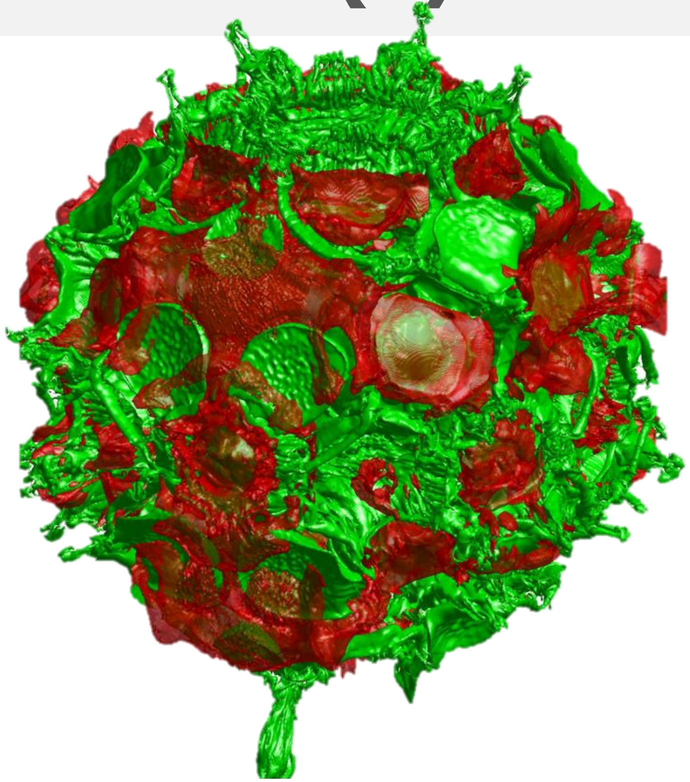
A few examples of NNSA hydro applications (2)



A shaped charge problem using the duel domain material point (DDMP) method, showcasing a particle methods interacting with a mesh-based fluid model. LANL



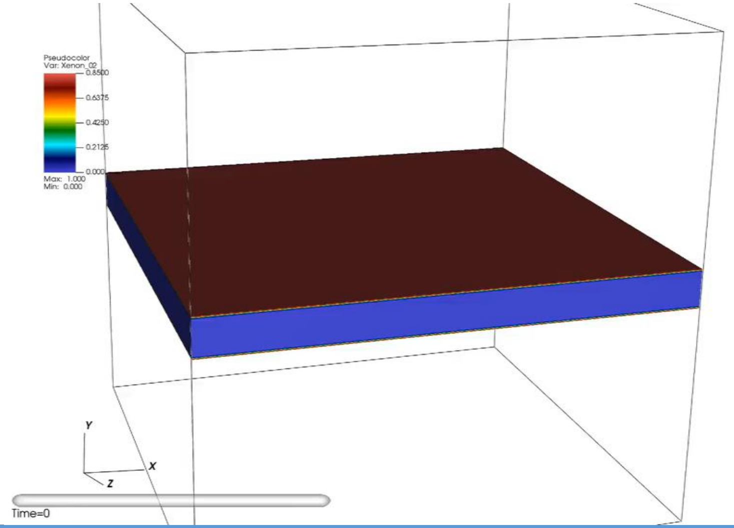
Simulation of laser powder bed melting showing melt pool instabilities and spatter that can degrade build quality. LLNL



Simulation of a layered NIF ICF implosion showing shock interactions with porous material in a MARBLE experiment. LANL

Conclusions

- Hydrodynamics calculations continue to be critical to the NNSA Labs' missions and applications.
- Advancing computer resources and multi-physics codes will <u>require a workforce with multi-disciplinary experience on heterogeneous architectures.</u>
- Continued development of <u>hydro algorithms</u> is vital especially in areas of:
  - Multi-material closure models and interface treatment
  - ALE strategies, including consistent and conservative remap
  - High-order methods development
  - Turbulence modeling
  - Advanced/novel algorithms



Partnerships with NNSA Labs and Academia through PSAAP will continue to support hydro algorithms development.

Disclaimer