Advanced Simulation and Computing

Los Alamos NATIONAL LABORATORY

News and Operational Highlights

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MATERIAL INTERFACE RECONSTRUCTION

Multi-plane moment-of-fluid interface reconstruction in 3D

One objective of LANL's Advanced Simulation and Computing Integrated Codes NUMIC project is to provide an efficient, accurate, and robust interface reconstruction algorithm that is applicable to general 3D meshes for an arbitrary number of materials in the computational mesh cell. When simulating the flow of multiple materials, their shape must be accurately captured over a discrete computational mesh. Then, simulation data can be used to approximate the intersection of the region occupied by material with each mesh element—the per-cell fragments of material (FOM)—while conserving the volume of each FOM. This is called material interface reconstruction, and it is employed by all LANL Lagrangian Applications (LAP), Eulerian Applications (EAP), and Safety Applications (SAP) production codes.

To improve the algorithm, we developed a moment-of-fluid (MOF) method for interface reconstruction of the FOM in each mesh element through reference only to the element's geometric moments. To do so, the FOM in each cell is represented as the convex intersection of the cell and multiple half-spaces, selected to minimize the least-squares error between computed moments of the approximated material shape and provided reference moments.

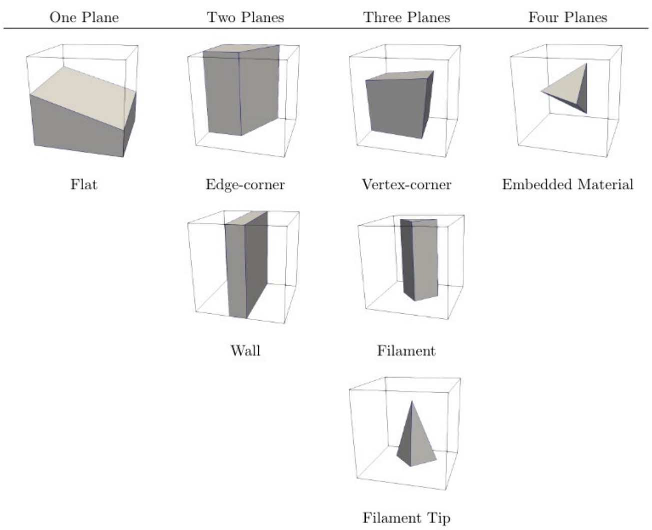

Figure 1 The 3D MOF method exactly reproduces several important and complex features defined by up to four half-spaces, such as corners, filaments, filament tips, and embedded material in the cell.

This optimization problem is highly nonlinear and nonconvex, making the numerical result very sensitive to the initial guess. To create an effective initial guess in each cell, we constructed an ellipsoid from zero to second order reference moments such that its shape corresponds to that of the FOM. Within this ellipsoid, we inscribe a polyhedron and initialize the minimization problem with the half-spaces defined by each of its faces. The inscribed polyhedron has at minimum four faces, and using up to third order moments permits optimization over up to 20 unknown values. We therefore defined MOF methods that use four, five, or six half-spaces, correspondingly initialized with the faces of a single inscribed tetrahedron, triangular prism, or hexahedron. Using this approach, the non-linear least-squares solver reliably converges to a near-global minimum from a single initial guess.

Importantly, this newly developed 3D MOF method exactly reproduces important and complex features, such as corners, filaments, filament tips, and embedded material in the cell - Figure 1. We demonstrated the robustness and accuracy of the method with both single-cell and multi-cell examples for several different geometries, e.g. see reconstruction of ellipsoid - Figure 2. This improved method of material interface reconstruction supports the accuracy of the simulations LANL uses for mission applications.

For more information contact **Jimmy Fung** (fung@lanl.gov), IC Program Manager. We acknowledge the work of Mikhail Shashkov and Jacob Spainhour.

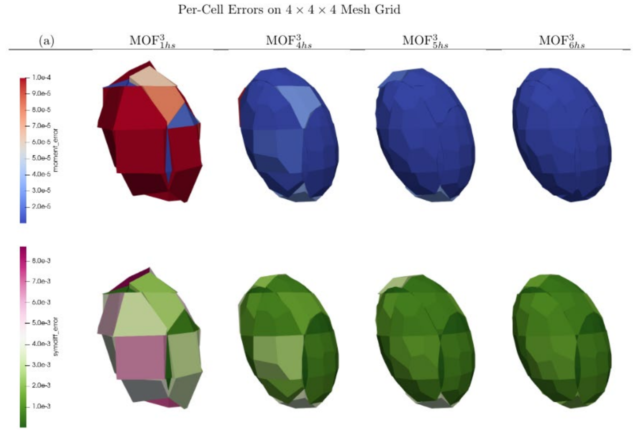

Figure 2 Interface reconstruction for the ellipse on a 4 × 4 4 mesh grid using different numbers of half-spaces and corresponding errors.

EXPERIMENTAL DATA INTO MODERN WORKFLOWS

NSDSConnect: A toolkit to integrate organized experimental data into LANL's Common Modeling Framework

The LANL weapons-modeling community has long desired a computational infrastructure that enables a modeler to set up and run a problem, compare the computational output to pedigreed experimental data, and then archive that model and its comparison to experimental data. However, until now, simulation workflows could not connect to a centralized database that curates, labels, and shares experimental data in a tractable method. Over the past several years, two separate frameworks were built independently: the Common Modeling Framework (CMF) was developed by our design community to provide the simulation workflow needed; and the National Security Data Solution (NSDS) has come online as the LANL weapons data–management tool that will eventually provide access to decades worth of experimental data. A recent FY24 Level 2 Milestone solved the tractability of experimental data in simulation workflows by connecting CMF's simulation workflows with NSDS experimental data, a watershed moment.

NSDSConnect, a tool that provides a straightforward methodology to access and query NSDS experimental data that was collected and curated for the LANL Weapons program, was released for this milestone. The tool can also retrieve metadata from the NSDS data records within a simulation workflow and included it in the pedigree. Now, it's possible to share CMF problem setups that automate the comparison of computational outputs with experimental data. A proof-of-concept workflow, based on using high explosive (HE) data for simulation validation, shows how a user can compare experimental and simulation data (Figure 1). This workflow provided feedback on the accuracy of HE material models and paves the way for CMF users to interact directly with experimental data through NSDS.

The NSDSConnect milestone will provide for a much stronger and easier-to-use integrated computational methodology that directly connects simulations to the experimental data used to validate those simulations. This is an integral part of the Verification and Validation (V&V) program and part of modernizing the V&V workflows that give LANL confidence in its simulation capabilities.

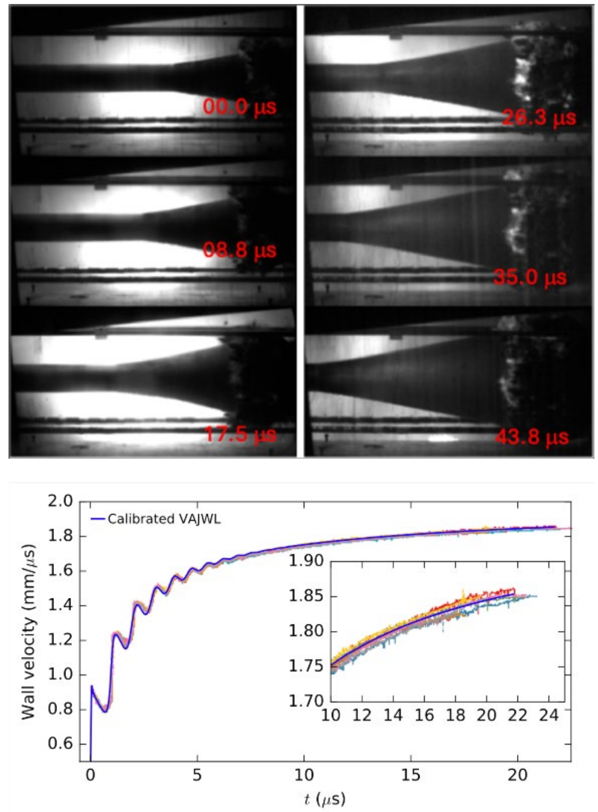

Figure 1 NSDSConnect allows CMF users to directly access data such as this detonating PBX 9502 cylinder expansion test (S.I. Jackson, Intl. Det. Symp., 2014). In the proof-of-concept shown here, the wall velocity data can be used to automatically diagnose the accuracy of a calibrated Jones-Wilkins-Lee model (C. Chiquete et al., APS-SCCM, 2023).

For more information, contact **Gowri Srinivasan** (gowri@lanl.gov), V&V Program Manager. We acknowledge the work of Jasper Thrussell, Carlos Chiquete, Mike Ham, and Common Modeling Framework co-project-leads Chris Biwer and Leslie Sherrill.

ARTIFICIAL INTELLIGENCE BREAKTHROUGH

LANL Leverages Cutting-Edge AI Technology to Support ASC Code

Artificial intelligence (AI) experts at Los Alamos National Laboratory (LANL) have successfully restructured and tokenized an AI-ready data set from Lawrence Livermore National Laboratory to finetune a large language model (LLM) with 70 billion parameters. Researchers used SambaNova's advanced AI hardware to take on the job. This high-performance hardware, located onsite at LANL (Figure 1), is part of a strategic partnership with SambaNova, an AI solutions provider. The collaboration explores using LLMs to translate computer codes between programming languages to improve maintainability and assure long-term software sustainability for the national security mission of the National Nuclear Security Agency laboratories. Support for advancing ASC integrated codes is critical to the Stockpile Stewardship Program.

Figure 1 ASC program's AI testbed, called Jarvis, where SambaNova equipment is hosted.

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