Advanced Simulation and Computing

Los Alamos NATIONAL LABORATORY

News and Operational Highlights

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3D MESHING TOOLS & MODERN MODELING WORKFLOWS

Crosslink integration into the Common Modeling Framework for improving the setup and reproducibility of 3D simulations

The National Nuclear Security Administration (NNSA) relies on advanced computational modeling and simulation capabilities to maintain the safety, security, and effectiveness of the nuclear deterrent without nuclear testing. These capabilities are critical for understanding complex physical phenomena, assessing the performance of nuclear weapons systems, and supporting stockpile stewardship activities. The Common Modeling Framework (CMF) at Los Alamos National Laboratory (LANL) plays a crucial role in this mission by providing computational infrastructure that enables modelers to set up, run, and analyze simulations; compare results to experimental data; and archive workflows for future studies. CMF's ability to accurately model complex 3D geometries and effects is particularly important for reproducing real-world scenarios and enhancing the fidelity of nuclear-weapons simulations.

However, meeting the national security need for advanced 3D-modeling capabilities presents significant challenges. CMF's most widely used geometry and meshing tool, Ingen, was primarily designed for 2D simulations, and requires 2D-to-3D transformations and additional scripting to build 3D simulations. This approach limits the efficiency and accuracy of 3D modeling efforts, potentially impacting the quality and reliability of some 3D simulation results. Furthermore, the increasing complexity of modern weapons systems and the demand for higher-fidelity simulations require more intuitive and scalable tools to create and manipulate 3D geometries and meshes. These challenges necessitate developing new tools and workflows that can handle the complexities of 3D modeling while maintaining the reproducibility and customization capabilities that are essential for rigorous scientific analysis.

To address these challenges and advance the state of the art in 3D modeling for national security applications, LANL's ASC/IC PUMA project has developed Crosslink, a block topology-based meshing tool. Crosslink provides a more intuitive approach to building block-structured meshes in 3D, offers a graphical user interface for enhanced usability, includes some specific meshing

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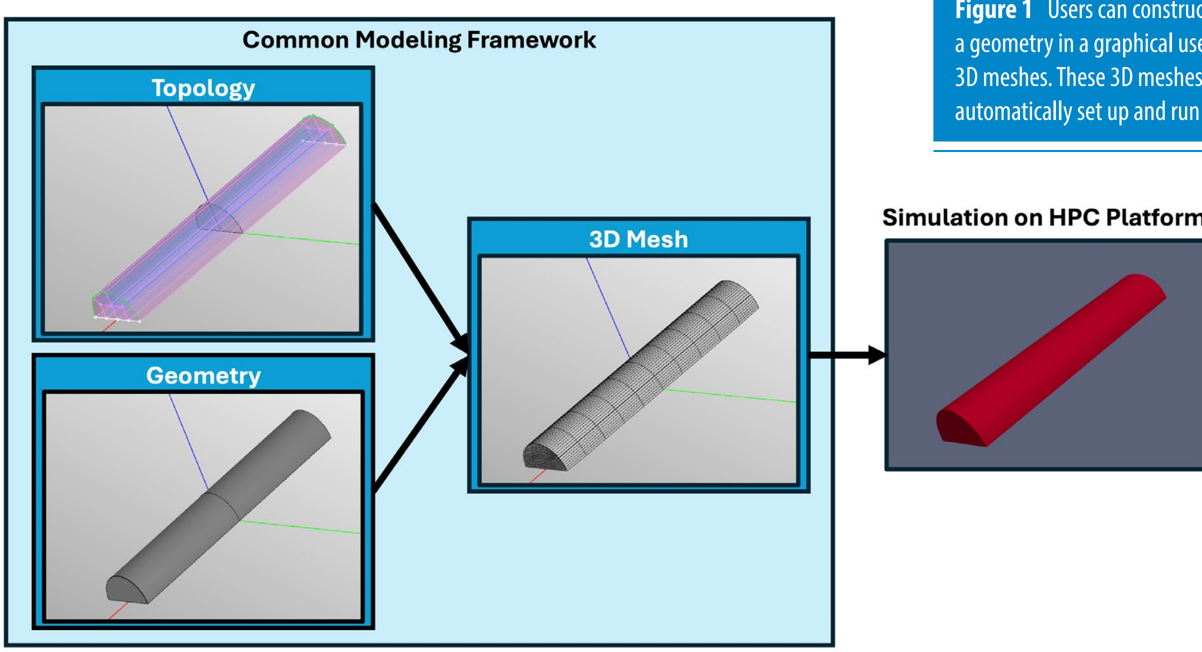

Figure 1 Users can construct a block topology of a geometry in a graphical user interface to create 3D meshes. These 3D meshes produced by CMF are automatically set up and run on LANL's HPC platforms.

features for LANL multi-physics simulations, and is intended to scale to larger problems on NNSA's advanced computing platforms. Crosslink was recently integrated into CMF workflows, a significant step forward in enabling modelers to design simulations directly in 3D space, accelerating the setup of 3D Lagrangian simulations within CMF. This integration allows users to load pedigreed geometries, build block topologies, and automatically generate high-quality meshes for simulations. By streamlining the 3D modeling process and improving the efficiency of workflow execution on high-performance computing systems, these advancements contribute to the modernization of verification and validation capabilities, ultimately enhancing confidence in the simulation tools used for critical national security assessments.

For more information, contact **Gowri Srinivasan** (gowri@lanl.gov), V&V Program Manager. We acknowledge the work of Gabe Rockefeller, Quincy Wofford, Grace Longo, Rao Garimella, Dylan Gatlin, Lily Latimer, and Common Modelling Framework co-project leads Christopher M. Biwer and Leslie Sherrill.

LOCAL WAVENUMBER MODEL

A spectral model for turbulent mixing layers

Imploding high-energy-density (HED) experiments, such as inertial confinement fusion (ICF) capsules, experience mixing at material interfaces because of a variety of canonical fluid instabilities, primarily acceleration-driven Rayleigh-Taylor (RT) and shock-driven Richtmyer-Meshkov (RM) instabilities. To design HED experiments, rapid, high-throughput simulations are needed. These simulations require an approach to modeling mix in lower dimensions or scenarios where instabilities are not directly resolvable.

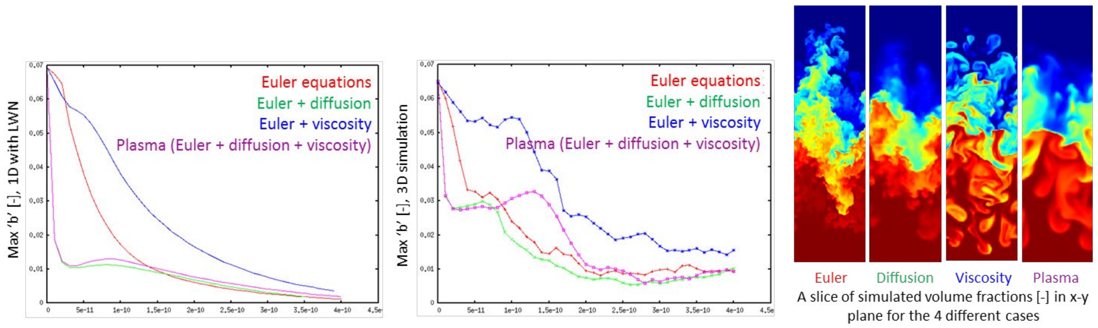

Figure 1 Decay of *'b'* (density-specific volume covariance) in simulations using LWN (left) and in 3D simulations with no turbulence modeling (center, right). All simulations used xRAGE. The simulations are run either with the inviscid Euler equations (red), with only diffusion (green), with only viscosity (blue), or with both (purple). LWN captures the qualitative trends shown in the 3D simulations regarding the effects of viscosity and diffusivity.

Los Alamos National Laboratory (LANL) is developing the Local WaveNumber (LWN) model, a new model for turbulent mixing instabilities. Unlike previous turbulence models in use at the Lab, which track total mean turbulent kinetic energy, LWN models the full turbulent kinetic energy spectrum, i.e., the distribution of turbulent kinetic energy across a range of different eddy sizes. This approach increases model complexity and computational cost, but evolving the turbulent spectrum provides many benefits, such as being able to relax the assumption of high Reynolds number equilibrium between large and small eddies. The finite Reynolds number construction of LWN allows it to be coupled to models for plasma viscosity and diffusivity, as illustrated in Figure 1, which is relevant in applications like ICF where plasmas can become very hot and viscous. LWN can also capture initial condition sensitivity in problems such as decaying homogenous isotropic turbulence (Figure 2), which depend on the shape of the initial spectrum.

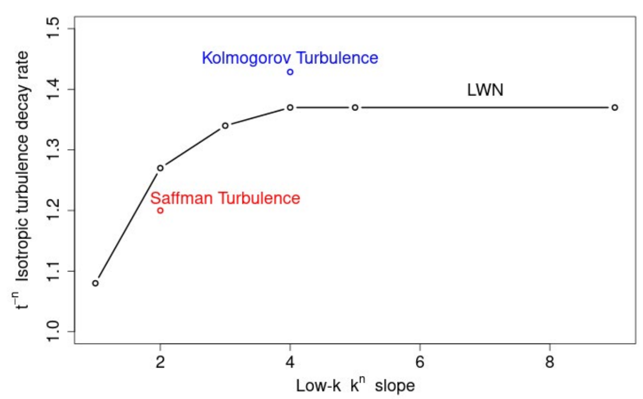

Figure 2 Late-time exponential decay rate of homogenous isotropic turbulence. Red and blue points are theoretical results for different initial conditions. Lower values on the x-axis represent initial conditions with more energy at long wavelengths.

HED experiments encompass many complex problems that involve interactions between multiple physical processes. Further development of the Laboratory's mix models will continue to improve their predicative capabilities to address this wide range of experiments.

For more information, contact **DJ Luscher** (djl@lanl.gov), PEM Program Manager. We acknowledge the technical contributions of N. Braun, R. Gore, D. Livescu, J. Velechovsky, J. A. Sáenz, and several other collaborators, with support from the ASC PEM Mix and Burn project.

MOLECULAR THEORY CAPABILITY

LANL-PEM-Atomic implements universal descriptions of molecular photoionization

Photoionization of atomic ions, the process through which atoms in bound states absorb radiation by losing electrons, is a vital part of describing radiative transfer in mission-relevant dynamics. The photoionization of molecules dominates radiative transfer of ultraviolet (UV) and extreme UV (EUV) radiation in colder atmospheres (temperature < 30,000 degrees Kelvin). Consequently, air, which is quite transparent to our eyes (i.e., in the visible frequency regime) is remarkably opaque to radiation in much of the UV and EUV frequency regimes. This opacity makes air and other gas systems quite efficient at absorbing UV and EUV radiation, which heats the gas until ionization makes it transparent. This effect is important in describing a host of relevant phenomena, ranging from charge separation in high-altitude nuclear events and the dynamics of a nuclear fireball to the electrostatic discharges (sparks) that complicate weapons disassembly at Pantex.

The Los Alamos National Laboratory (LANL) ASC-PEM-Atomic team is developing a unique "universal" molecular theory capability. In contrast to academic efforts in the field, which often focus on low-energy methods of increasing sophistication that tend to become species-specific, the Atomic team took a different approach: By applying physics approximations, the team developed across-the-board descriptions that can be applied to all molecular species. In the multiple-species sense, the resulting descriptions are universal.

Recent work to test these approximations shows that configuration-averaged distorted wave (CADW) and pseudo-independent-atom (PIA) methods, both applied in the fixed-nuclei approximation (with some corrections), give surprisingly good results. Figure 1 shows the total photoionization cross-section of the ground state oxygen molecule (O_2).

These results point the way to further improvements of the air-opacity tables, a first version of which the team completed last year. In a cross-laboratory collaboration with the SNL-EMPIRE code team, the new photoionization cross-sections will be implemented in their code.

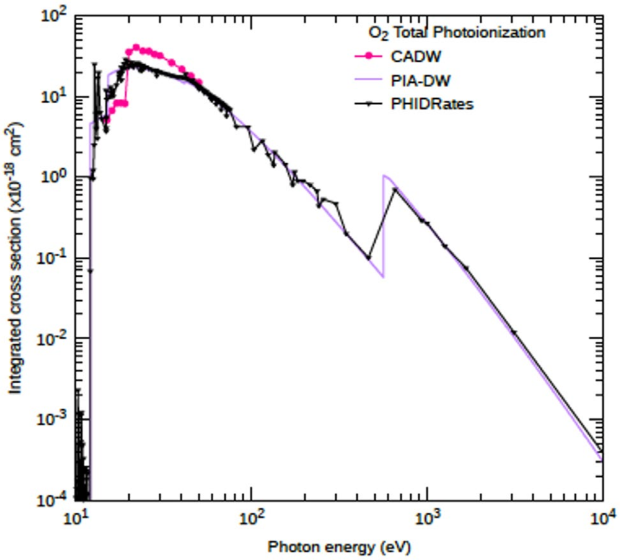

Figure 1 The total cross-section for the photoionization of the oxygen molecule, O2, as calculated in the configuration-averaged distorted wave approximation (CADW) and in the pseudo-independent-atom distorted wave approximation (PIA-DW). The results are compared to experimental data (PHIDRates).

For more information, contact **DJ Luscher** (djl@lanl.gov), PEM Program Manager. We acknowledge the work of Mark Zammit, James Colgan, and Chris Fontes.