Sandia National Laboratories

SAND2024-09025M

Code Release Highlights

Summer 2024

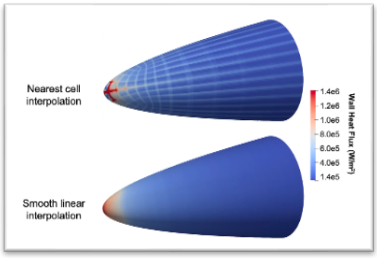
SIERRA 5.20
CUBIT 16.18
SPARC 24.3
SANDIA ANALYSIS WORKBENCH (SAW) 2.13.12

Researching, developing, and deploying state-of-the-art high performance computational engineering simulation codes.

Codes are actively being used for B61, B83, W76, W78, W80, W87, W88, W93, ND Components & Transportation programs. A large fraction of the codes' internal compute cycles supports the Nuclear Weapons Complex: Captive-carry/free-flight aero/acoustic/structural coupled multi-physics for component design, normal/severe mechanical impact scenarios, abnormal thermal structural capabilities, normal/abnormal thermal simulations, aero/aero-structural spin-to-arm, and abnormal mechanical/accidents simulations.

Smooth Transfers in SPARC

Traditionally, SPARC has used a nearest cell strategy for field transfers. This method has been successful when transferring between conformal meshes or from fine-to-coarse meshes; however, a smooth transfer capability using linear interpolation now enables the coarse-to-fine mesh use case. Now, Euler+MEIT simulations can be performed where the MEIT surface mesh is finer than the Euler volume mesh improving the resolution for capturing viscous effects without the added cost associated with a finer Euler mesh. An option for solution limiting enables transfers in the region near shocks. This capability improves the interpolation from a pre-grid tailored mesh to a post-grid tailored mesh leading to faster time-to-convergence. The new method reduces non-physical artifacts present in the previous method.

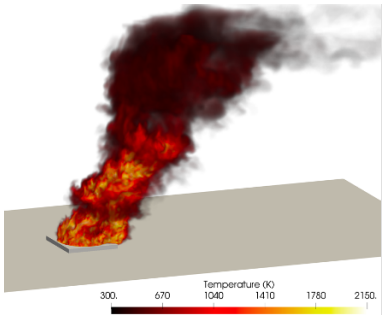


Contours of wall heat flux along SPARC test vehicle solving Euler+MEIT using previous nearest cell transfer strategy and new smooth linear transfer strategy.

GPU Execution for Fuego

The LES flamelet fire simulation capabilities in Fuego have been ported to use Kokkos and provide performant execution on next generation platforms like ATS-2. Large scale pool fire simulations like the one shown below can take weeks to months to provide converged heat flux predictions for abnormal environments. The changes in this release produce node-to-node speedups of up to 10x on ATS-2 vs CTS-1 systems. Preliminary testing on new GPUs, like those on the upcoming HOPS system, has shown substantial speedup over ATS-2, showing that the Kokkos performance portability of the new algorithms can provide continuing benefits as platforms evolve.

These improvements also produced speedups of around 2x on conventional CPU systems and have impacted Fuego use-cases beyond fire simulations, including wall-modeled LES simulations.



Simulation of 5-meter diameter pool fire in crosswind.

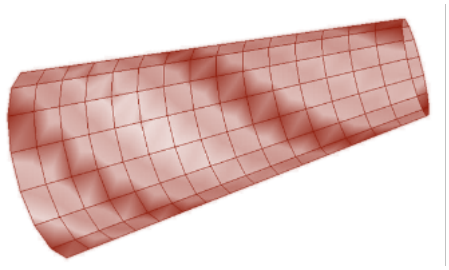
Code Team Office Hours:
- Cubit/Percept: Mondays 3:30-4:30 MT on MS Teams
- Sierra Thermal/Fluid: Tuesdays 10:00-11:00am MT on MS Teams
- Sierra Toolkit: By appointment at stk-ngpteam@sandia.gov
- Sierra DevOps: Tuesdays 10:00-11:00am MT on MS Teams
- Sierra Solid Mechanics: Thursdays 10:45-11:30 MT on MS Teams
- Sierra Structural Dynamics: By appointment to wg-sddev@sandia.gov
- SPARC: Mondays & Thursdays from 9:00 –11:00 MT on MS Teams
- SAW: By appointment at saw-help@sandia.gov
- Post questions or issues at any time on the CompSim Community Channels

Deployment is across the DOE Nuclear Weapons Complex, DoD, and AWE:
Sierra is deployed on 10 different computing platforms (desktop & HPC), supports 400+ internal SNL users and 70+ distinct external licenses.
Cubit is deployed on 3 different architectures (Windows, Mac, Linux), regularly hosts 510 internal users and 1500+ external users.
SAW supports 300+ users and archives over 30 terabytes of analysis data

What's New in Sierra

Structural Dynamics

- Capability: A new capability exists to use multiple input source files for transfer of displacements, temperatures, pressures, and other quantities to Sierra/SD.

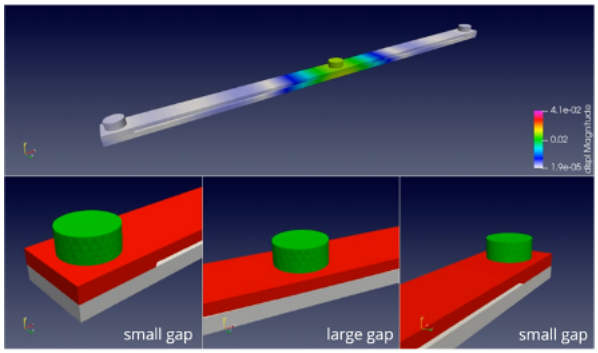


Simultaneous transfer of SPARC and Aria data to Sierra/SD mesh

- Capability: In modal transient analysis, building upon the existing text-based modal displacement and force output, now modal accelerations and velocities are available.
- Usability: Handoff of initial conditions between solutions cases, such from statics to modal transient, is now handled consistently.
- Usability: Geometric stiffness calculations from preload can now be done on a block-by-block basis for greater robustness of preload handoff between Sierra/SM and Sierra/SD.
- Usability: Performance of constraint updating for moving acoustic mesh calculations is significantly improved.
- Bugfix: Transient restarts now work correctly with nonzero start time and multiple time periods.

Solid Mechanics

- Capability: New bolt preload algorithm option in explicit dynamics allows more robust handling of gaps and faster loading to target.
- Usability: New overlap removal option allows it to be disabled for specific contact interactions.
- Capability: Internal moment through a cross section can now be calculated through user output.



Contour plots showing displacement needed to achieve preload.

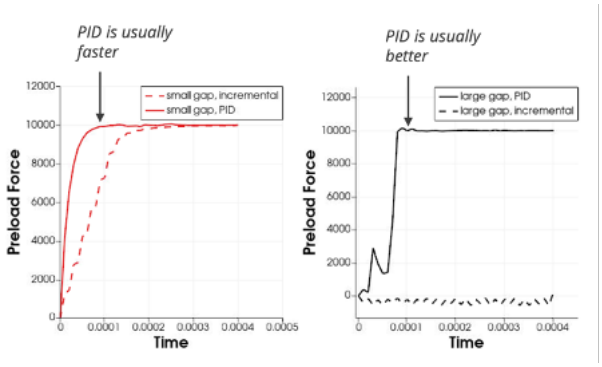
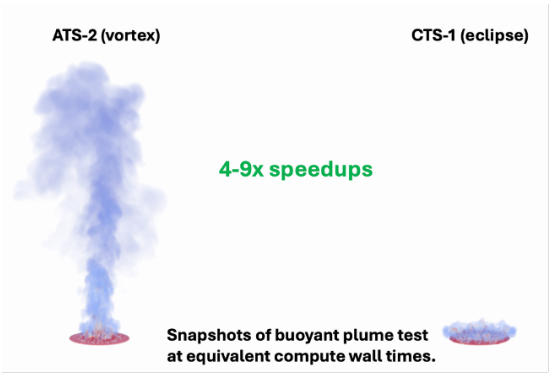


Figure showing faster and more robust convergence of the new PID algorithm compared with the default incremental approach.

Thermal Fluids

- Performance: The thermal fluids team has ported Fuego's baseline large-eddy fire simulation capability to run on GPU-accelerated platforms. Combined with the previous effort to port the participating media thermal radiation capability, users can see 4-10x speedups on ATS-2 (Nvidia V100 GPUs) compared to CTS-1 (Intel Broadwell CPUs).
- Capability: Wall-modeled LES improvements in Fuego focused on adding an exchange-based approach for velocity sampling and a Neumann-based boundary condition for the one-equation kSGS turbulence
- Capability: Support for quad and hex elements in fast marching algorithm for level set redistancing and time of arrival calculations.
- Capability: Support for referencing global variables directly in Aria string functions.
- Capability/Usability: Improved multiphysics linear solver support and documentation for block preconditioning based on Teko.

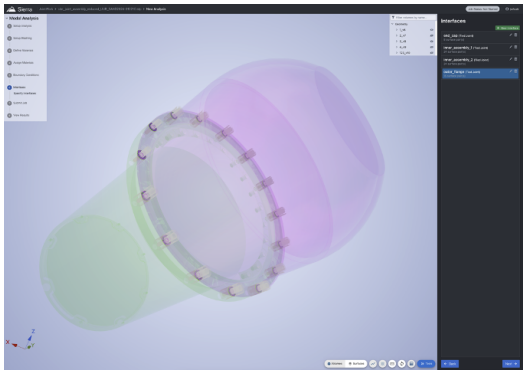
- Usability: New MueLu linear solver presets for thermal problems and fluids problems with high-aspect ratio meshes.
- Capability: Improved convergence detection options for implicit MPMD coupling in aero-thermal problems.



Comparison of Fuego GPU performance on ATS-2 to Fuego CPU performance on CTS-1 for a buoyant plume problem.

Next Generation Simulation (NGS)

- Usability: In the Morph mesher, we now default to a new Krino geometry engine rooted in ACIS facets for both .stp and .sat CAD files. The methodology is increasingly robust and frequently results in meshing times on the order of 10X–100X faster.
- Usability: We are documenting best practices that derive from working groups in structural dynamics and electromagnetics. See https://docs.sierra.sandia.gov/.
- Capability: We released the capability to created conformal meshes with finite-difference sensitivities to CAD parameters for shape optimization within Plato.



New interface for managing an array of bolts comprising a joint in the SD Modal tool. Bolt arrays are idealized via AI/ML and curated for the analyst within the SD Modal tool.

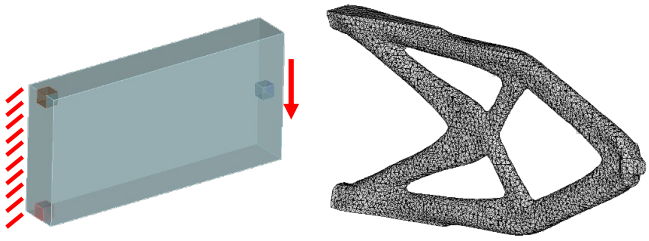
- Capability: Through a DARPA sponsored project, we released an in-core capability for the reconstruction of SPH particles to a tetrahedral representation in Sierra/SM.
- Capability: In collaboration with the G&M team, the SD modal tool now has the capability to create, manage, and visualize bolted structures for structural dynamics. Our goal is to mitigate complexity and provide the user with an ability to quickly probe tied contact, tied joints, and the sensitivity of tied-joint parameters.

SPARC

- Usability: SPARC now has a smooth transfer capability that makes significant improvements when transferring fields between non-matched meshes. Use cases include Euler+MEIT, post-grid tailoring, and volume-to-inflow transfers.
- Usability: Enabled trajectory coupling with the low fidelity aero models.
- Usability: Aerothermal coupling enhancements
    - Improved coupling pattern to increase flexibility of implicit iterative coupling scheme.
    - Implemented coupled time solvers of coupled time solvers, enabling a more flexible N-way coupling and mixed explicit/implicit approaches.

Plato

- Capability: Level-set topology optimization using Krino to enable multi-physics design topology design problems with more precise interface definitions.



Problem setup (left) and optimized result (right) for standard bracket design problem using level sets in Plato.

FuSED

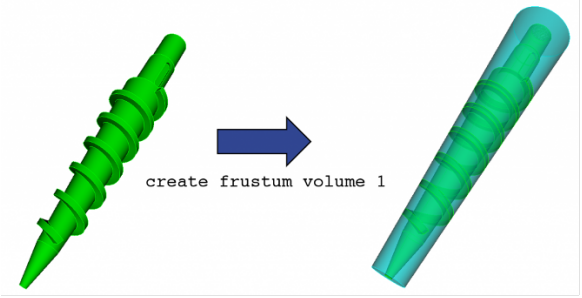
- Capability: Optimal Experimental Design (OED) tool now supports Mean-Squared Error (MSE) and Mean-

Squared Prediction Error (MSPE) objective functions for sensor placement optimization.

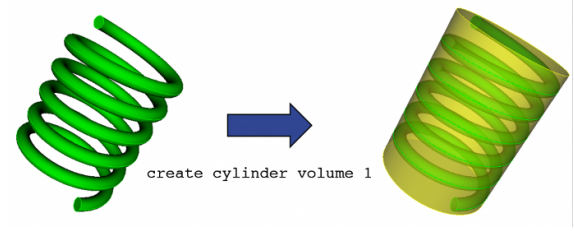
- Capability: OED tool now supports source placement optimization for MIMO testing.
- Usability: Sierra/SD inverse methods for material identification now automatically apply design variable scaling and bound constraints for improved optimization performance.
- Usability: Progress towards beta release of Support Vector Machine (SVM) decision surface tool:
  - Input deck and improved user experience
  - Parallelization of post-processing for constructing confidence intervals

Cubit

- Capability: Ability to create a frustum that tightly fits an input volume. The axis of the frustum is automatically computed, and in complicated cases, users can guide the creation by supplying the optional axis parameter.
- Capability: A previous command to create a cylinder that tightly bounds an input volume has been made more general. The previous version required the input volume to contain cylindrical or circular features to guide the cylinder creation, which is no longer required. Additionally, an optional axis parameter has been added to guide the cylinder creation in the event an incorrect axis is computed.



Ability to create frustum that tightly fits an input volume.

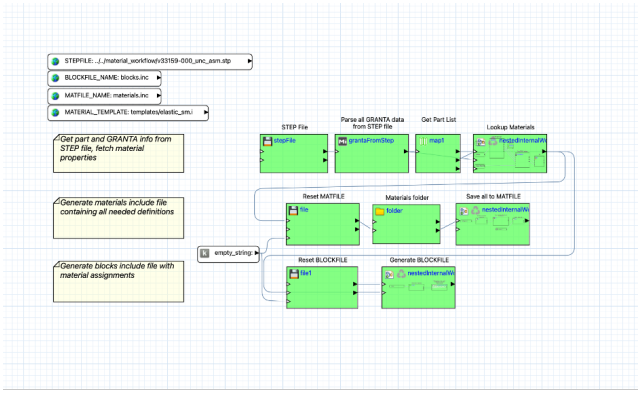


Command to create cylinder that tightly bounds an input volume.

- Usability: It is now possible to use the lower bound interval setting to ensure a minimum number of elements along a curve when triangle meshing. Previously, this setting was only effective when doing quadrilateral meshing.
- Usability: When adding a node to be respected for tet meshing, it is now possible to specify a size with that node. When given a size, the resulting tets surrounding that node will have a size matching the user supplied size. This feature may be useful when the user wants refinement at certain locations within a tet mesh.

SAW and NGW

- Capability: Next-Gen Workflow integration for the GRANTA material database allows just-in-time updates of material data used in simulations
- Capability: New REST components for Next-Gen Workflow let you easily integrate automated calls to web services APIs into your workflows
- Capability: Next-Gen Workflow now supports exchange of Python class instances between components
- Usability: New local job cleanup tools enhance your ability to manage a large portfolio of HPC simulation runs
- Usability: Improved error reporting for Sierra node in Next-Gen Workflow helps you quickly diagnose simulation failures



A Next-Gen Workflow that fully automates the process of building a Sierra input deck from a template by using material assignments embedded in CAD and the GRANTA material database.

On the Horizon

(SD) A full featured Sierra capability for numerically consistent handoff of energy deposition from RAMSES/ITS to Sierra/SD or Sierra/SM is under development.
(SD) Sierra/SD is reworking output syntax for greater flexibility of outputting multiple files, solution case specific outputs, discrete time steps, and other long requested features.
(SM) Certain GPU-capable explicit analysis capabilities will be deployed
(SM) Ordered bolt preloading: will allow users have multiple bolt preload blocks and load them in sequence.
(SM) In-core remeshing prototype for large deformation analysis.
(TF) GPU port for ablation models.
(SPARC) More accurate and robust simulations at all Mach numbers using tetrahedral meshes
(NGS) We continue to extend Emend for in-core operations on mesh-based geometries. Increments will include a facet-based representation with edge detection and increased smoothness. In the next release, we will collaborate with Sierra/SM to perform in-core mesh adaptivity on 10-node tetrahedral elements with refinement, coarsening, and smoothing.
(NGS) In a push to include Morph within Cubit, Morph now exports Cubit m2g files that associate geometric entities with the discretization. Both the G&M and the NGS(D) teams are working towards integration.
(NGS) UX research for TF workflows has provided insight into the utility of web-based interfaces to reduce complexity and decrease cycle time for thermal analysts. A broader survey was recently conducted to provide increased insight in the spaces of discretization and visualization. Those findings will be release with recommendations for new, needed applications.
(NGS) We will release the SD Modal tool on the SCN in 5.22.
(FuSED) Beta release: Support Vector Machine (SVM) for constructing decision surfaces.
(FuSED) Robust OED method that can account for uncertainty in FEM models.
(FuSED) Reduced basis (RB) methods for accelerating Sierra/SD calculations for optimization and multi-frequency RB for broadband frequency sweeps.
(FuSED) Inverse contact area extraction with spot welds in SD models.
(FuSED) OED tool support for multi-type, multi-budget sensor placement optimization.
(Cubit) Improved smoothing implementations with surface node smoothing.
(Cubit) Advanced geometry healing options
(NGW) A new template wizard for Next-Gen Workflow will make it easier than ever to get started automating engineering tasks.

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