Code Release Highlights

Fall 2025

SIERRA 5.26
CUBIT 17.06
SPARC 26.1
SANDIA ANALYSIS WORKBENCH (SAW) 2.14.5

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.

Support for ATS-4 El Capitan

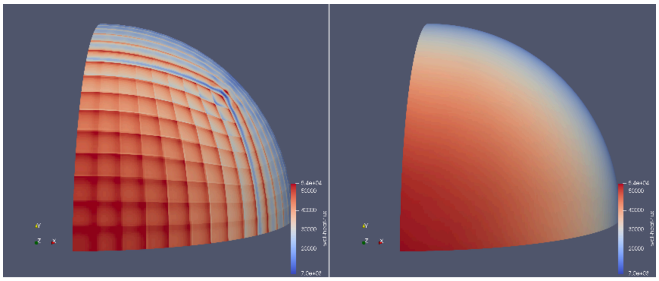
Sierra 5.26 is the first release with official support for the LLNL ATS-4 El Capitan platform. ATS-4 uses a new Accelerated Processing Unit (APU) architecture that combines CPU and GPU, allowing them to share memory. Performance is on par with Hops, Cascade, and Citra but with a smaller memory footprint thanks to the APU architecture. ATS-4 is expected to take the place of ATS-2 as the primary platform for Sierra Structural Dynamics analysis, and the Sierra group has worked across product teams to release 5.26 on ATS-4.

	CPU only *(Intel Cascade Lake)*	CPU only *(Intel Sapphire Rapids)*	ATS-2 GPU *(Nvidia V100)*	Hops GPU *(Nvidia H100)*	ATS-4 GPU *(AMD MI300A)*
HPC nodes	23	20	40	20	20
CPU cores	800	800	960	480	480
GPUs	--	--	160	80	80
Linear solve time	~54 hours *(est., DNF)*	42.5 hours	0.6 hours	0.5 hours	0.3 hours
Total runtime	**~59 hours** *(est., DNF)*	**46.5 hours**	**2.5 hours!**	**2.3 hours!**	**1.9 hours!**

Example CPU and GPU performance on a parking garage model: eigen solution, 18M dof, 5K modes.

Reentry Environment Improvements

Sierra/TF team has made several notable improvements to the robustness and usability of reentry simulations coupled with SPARC. First, data probes in Aria have been improved to provide more flexibility in handling when the data probe leaves the mesh, which is often the case in ablation problems. Instead of an error or clipping to the nearest surface, users can choose to set the probe to a NaN or large value when it leaves the mesh to help with post-processing. Second, Aria now supports coupling 2D axisymmetric models with 3D SPARC models for reentry ablation problems. This greatly simplifies the meshing process for the Aria domain while also simplifying problem setup and improving computational cost and stability. Lastly, the SPARC/Aria coupling transfer now includes a B-Spline smoothing algorithm that maintains symmetry planes and works in both 2D and 3D Aria problems. This capability significantly improves the simulation robustness when there is a large mesh size mismatch between SPARC and Aria and allows ablation simulations to progress farther in time. See figure below for details.



Heat flux using linear interpolation (left) and B-Splines (right)

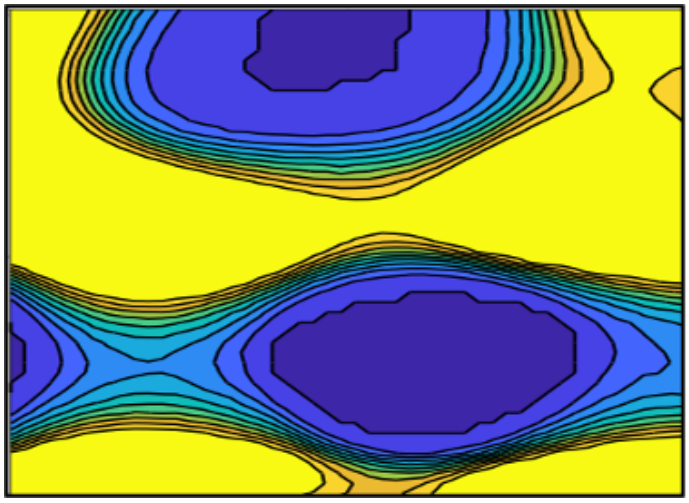
Code Team Office Hours:
- Cubit/Percept: Mondays 3:30-4:30 MT on MS Teams
- Sierra Thermal/Fluid: Tuesdays 10:00-11:00am MT on MS Teams
- Sierra Toolkit: By appointment at stk-ngpteam@sandia.gov
- Sierra DevOps: Tuesdays 10:00-11:00am MT on MS Teams
- Sierra Solid Mechanics: Thursdays 10:45-11:30 MT 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

FuSED

- Capability: Full release of TRACE in 5.26 (TRACE Rapidly Acquires Contour Estimates) with automatic hyperparameter tuning using multi-dimensional bi-section to choose the best settings for the user at each training iteration.
- Capability: Budget constraints can now be enforced with gradient-based optimization in OED (Optimal Experimental Design); robust formulation for handling sensor drop-out/loss-of-data
- Capability: New features in InverseAria include support for sensors with arbitrary spatial locations and support for adaptive time-stepping.
- Usability: Eigen 'MAC' objected is no longer supported in InverseSD; similar functionality can be achieved with the 'Matching' objective with a scalar. Changes improved code robustness and usability
- Usability: Improvements in TRACE include improved output options and refactor of input deck, more frequent and more informative messages to users, and use of 'duck typing' to allow users more flexibility in defining their models.
- Usability: Improvements in OED include input option xml checker, expanded output information (objective function, sensors), and training example on team wiki page for electromagnetic sensor placement optimization.
- Bug Fixes: Added saving of initial training data along with printouts for user debugging in TRACE.



Probability contours from executing a post-processing step in TRACE. Instead of calculating the probability at every point, improvements in TRACE permit significant speedup by finding a set of user-specified contours directly.

Structural Dynamics

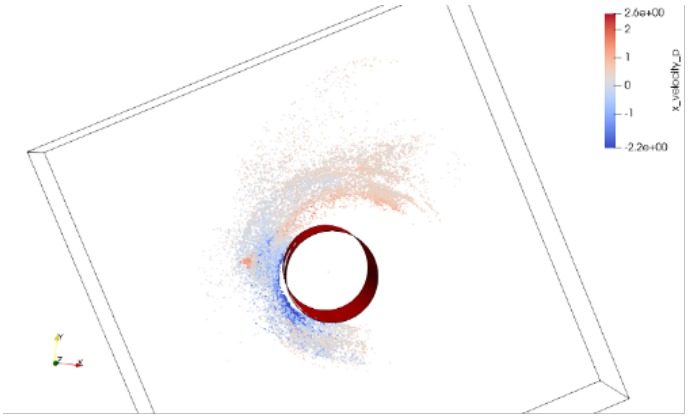
- Capability: ATS-4 El Capitan is supported in the 5.26 release of Sierra/SD. Performance is expected to be on par with Hops, Cascade, and Citra but with a smaller memory footprint thanks to the APU architecture with shared GPU/CPU memory.
- Capability: Craig-Bampton Reductions (CBRs) received several fixes and improvements for 5.26. These include an "all" option for specifying "nmodes" and the addition of an "untilfreq" option.
- Capability: Residual vectors are now supported in eigen and CBR solution cases. In addition, pressure and force boundary conditions can be used to form residual vectors.
- Capability: The "modalfrf" solution case works with viscoelastic materials through "viscofreq" that is now enabled with "sa_eigen".
- Capability: Springs support more general function-based definitions of stiffness parameters.
- Capability: SD's transfer capabilities support non-matching and misaligned meshes.
- Usability: Restarts have improved guardrails to help prevent simple input mistakes. Many input sections are checked to prevent changes, with some exceptions that are allowed to be added or ignored.
- Usability: SM/SD shared contact is more flexible through new "cutoff variable" specification, either per-interaction or for "interaction defaults".
- Usability: A new helper script is available to convert between SD and SM viscoelastic material input syntax.
- Usability: Omitted blocks are fully supported with restart, with additional testing and guardrails added.
- Usability: Results files include more information about omitted blocks.
- Bug Fix: The interaction between coordinate systems, angular velocity, and acceleration loads is fixed.
- Bug Fix: A fix for rare problems using a specific boundary condition removed double counting on parallel boundaries.

Thermal Fluids

- Capability: Enclosure viewfactor calculation is an expensive operation in Aria that used to be triggered by any mesh modification anywhere in the problem. Now users can choose to only update viewfactors if the enclosure geometry changed, enabling using mesh adaptivity and runtime mesh improve tools in

other parts of the domain without incurring a large penalty from viewfactor calculations.

- Capability: Particle simulations in Fuego now support mesh motion, allowing simulations of sprays impinging on rotating parts. This capability allows modeling of plasma spray deposition processes and other moving deposition problems.



Visualization: inertial particles sprayed at a rotating cylinder

- Capability: Our participating media radiation solver (PMR) now supports using the multigrid preconditioner from Trilinos (MueLu) providing substantial improvements in scaling to large problems.
- Capability: Both Fuego and Aria now support user utility plugins, and documentation on using these has been added to the respective user manuals. This capability lets advanced users test out complex model development, including using AI/ML to evaluate properties, source terms, or other equation terms.
- Capability: When coupling Fuego and PMR on identical meshes, there is a new “Copy Transfer” option for copying data directly without interpolation. This substantially improves memory use, enabling running large problems on GPU platforms like hops.
- Capability: Numerous performance and robustness improvements to the Teko Multiphysics solver are included in this release, including better GPU performance and better heuristics for adaptive block preconditioner selection.
- Bug Fix: Several bugs in the rotated BC causing simulations to fail or hang were resolved. These bugs were affecting both thin-wedge ablation cases and CDFEM flow problems, causing simulations to either diverge or hit a parallel hang and stop progressing.

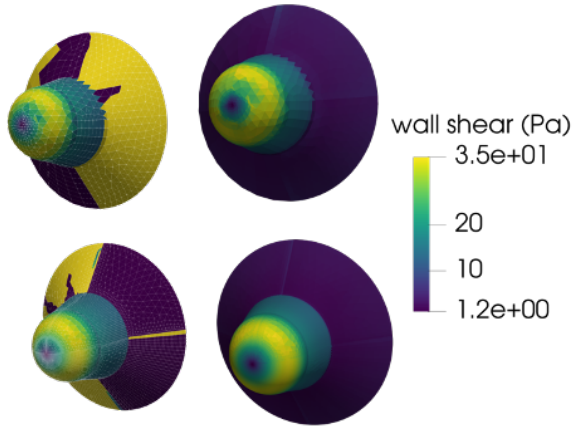
Solid Mechanics

- Usability: New commands and syntax updates to enhance simulation workflows and flexibility. Key additions include the TRANSFER EVERY <N> STEPS command in VARIABLE INTERPOLATION for precise control over interpolation frequency and the COMPUTE NODAL ... SURFACE NORMAL command in USER OUTPUT for surface normal calculations at nodal points. The COMPUTE AT ... command in SENSOR blocks enables frequency specification for advanced monitoring, while the FILTER command in VARIABLE INTERPOLATION provides new options for data filtering. These updates streamline workflows and offer greater flexibility in defining simulation parameters.
- Usability: Default changes and usability improvements make simulations more accurate and easier to set up. The volume-averaged Jacobian is now the default for Total Lagrange (TL) elements, enhancing stability and accuracy.
- Usability: Additional enhancements improve robustness, documentation, and training resources for users. Integration-point field calculations in USER OUTPUT have been made more robust. HTML documentation now includes updated training materials, preload training slides and the Shock Addendum User’s Guide. Robustness improvements were made for implicit contact and overlap removal, while guardrails were added to catch zero-mass nodes in dynamic simulations.

SPARC

- Capability: Improvements to the lower fidelity boundary layer model formulation
    - Enabled fast two-way coupled axisymmetric aero/ablation simulations that include more complex physics such as expanded transition modeling and significant shape change.
    - Robustness improvements have enabled sharp geometry changes that previously led to solver failures.
- Capability: Introduced framework for incorporating atmosphere modeling via EarthGRAM to better support the random vibration workflow.
- Capability: Improved trajectory simulations by 1) enabling trajectory continuation for faster simulation times for steady-state RANS and 2) implementing a shock detection algorithm that increases robustness.

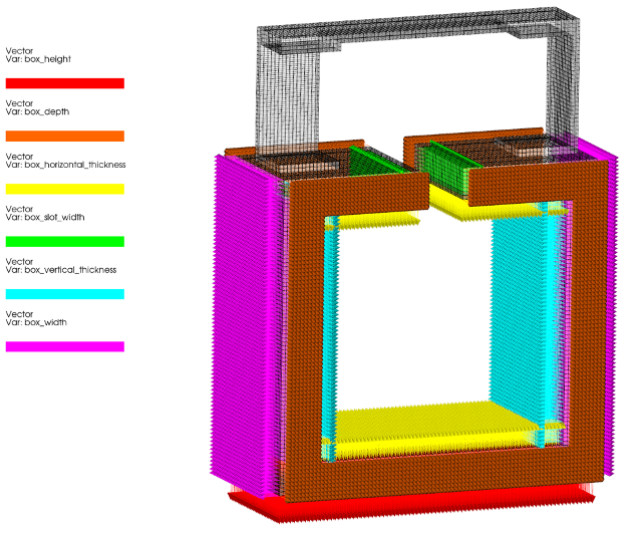
- Usability: Fixed a corner case transfer bug that improves coupled aero/ablation simulations.



Hypersonic stress test asserts robustness of lower fidelity boundary layer model with automated smoothing in handling large compressions on coarse (upper) and fine (lower) meshes of multiple element types. Left: previous solution. Right: new solution.

PLATO

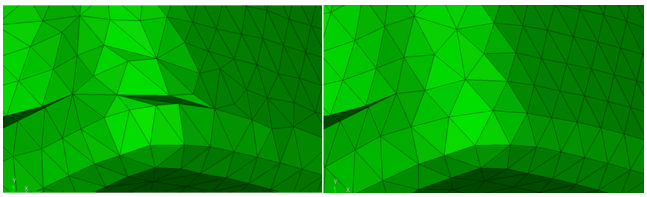
- Capability: Shape optimization in Plato using parametrized Cubit journal files, illustrated below on the BARC model. In the past, shape optimization with Plato required Engineering SketchPad, a third-party library with its own user interface. Now, such problems can be solved natively with Cubit.



Colored arrows emanating from surface indicate finite-difference mesh sensitivity to CAD parameters in Cubit journal file, allowing us to apply the chain rule to the physics codes to do gradient-based optimization of CAD parameters.

Geometry and Meshing

- Usability: Meshing improvements including increased robustness of triangle and tet meshing, increased accuracy and precision when computing mesh quality metrics, new mesh quality metrics for higher order elements, and new skew control option for curve skinning

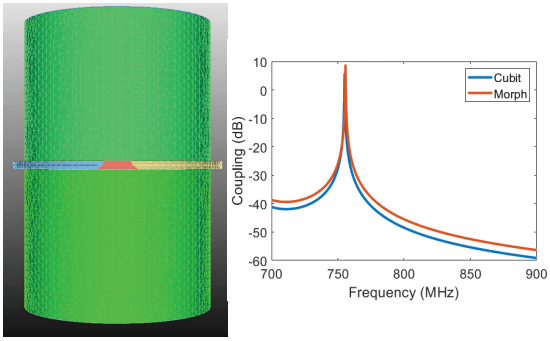


Left: Tet meshing defect previously occurring on composite surfaces. Right: New corrected tet meshing result on the same composite surfaces.

- Capability: New cohesive element generation for crack propagation and cohesive interfaces
- Usability: Multiple user interface improvements including dark mode support, making PNG default for shortcut when saving image file of graphics view, and journal editor enhancements.
- Capability: New IO capabilities including new support for additional ABAQUS cards when importing files, new 64 bit ID support in Exodus files, and new input deck creation for electromagnetic models.
- Usability: Other miscellaneous improvements like new set error on/off for filtering messages, an updated Python 3.12 version included in distribution, and improved documentation for Python API
- Usability: More robust cavity selection

AMD

- Usability: To enable the capture of thin-walled structures with anisotropic discretizations, Morph now accepts a local geometry deviation factor for mesh-based defeaturing. This enables one to invoke mesh-based defeaturing for the complex geometries and still capture local, thin features.
- Capability: A new capability for generating watertight discretizations from discontinuous surfaces is now available in the Morph mesher (see figure below). Termed surface collection volumes, one can generate



A watertight discretization via newly implemented surface collection volumes in the Morph mesher and the predicted electromagnetic coupling in Gemma for the current (Morph) and prior (Cubit) discretization.

either a watertight volume or surface discretization without tedious geometry repair.

- Capability: A viz component for HPC computing was delivered as a standalone or embedded capability. Websight.sandia.gov enables the rapid development of purpose-driven tools to support design iteration.
- User Experience: Developed user-journey maps for both structural dynamics and electromagnetics to illustrate pain points and develop a backlog for 10X increases in cycle time.

SAW/NGW

- Capability: Next-Generation Workflow (NGW) now automatically generates a machine-readable pedigree for results, increasing the transparency and reliability of solutions. Captured in an industry-standard format, it not only provides essential context regarding the quality, trustworthiness, and history of each data element, but also facilitates effective recall of historical results and will be useful for processing via AI.
- Usability: Next-Gen Workflow now supports a plain-text format, based on YAML, for specifying workflows.

NGW now automatically generates a machine-readable pedigree for results

Workflows can now be managed like other software-engineering artifacts using a traditional text-based toolchain. Furthermore, YAML workflows will be amenable to both parsing and generation by large language models (LLMs).

On the Horizon

(FuSED/InverseSD) Productionizaton and improved interface identification; exodus output/restart
(FuSED/InverseAria) support for enclosure radiation
(FuSED/OED) sensor placement that is robust to drop-out/loss-of-data with fixed locations
(FuSED/TRACE) Reinforcement learning to leverage models of varying fidelity. Transfer learning to leverage legacy data when moving between similar systems or models.
(Sierra/SD) Deliver RVToolkit as a production tool across Sierra release platforms.
(Sierra/SD) Usability enhancements to the CBRs or superelement capability are planned for an upcoming release.
(Sierra/SD) Expanded support for thermal effects across element types.
(Sierra/TF) Adaptive meshing of aeroshells
(Sierra/SM) GPU Uniform Gradient Hexahedron option for production use
(Sierra/SM) User output performance improvements
(SPARC) Automated mesh adaptivity
(SPARC) Integrated input file editor
(G&M) Evaluation of hex dominant mesher for solid mechanics applications
(G&M) Fast primitive creation in the Combinatorial Geometry Modeling Tool (CG Tool)
(Plato) New and improved stress-constrained mass minimization capability.
(AMD) Initiated efforts to support anisotropic mesh adaptivity for hypersonics in SPARC. We are generalizing the Emend Toolkit to move beyond a scalar size fields and accept a metric tensor for local refinement on idealized CAD geometries.
(SAW/NGW) Tools for generating workflows automatically from an English description using a large language model (LLM.)

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