Code Release Highlights

Spring 2025

SIERRA 5.24
CUBIT 17.04
SPARC 25.2
SANDIA ANALYSIS WORKBENCH (SAW) 2.14.1

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 Hopper GPU platforms

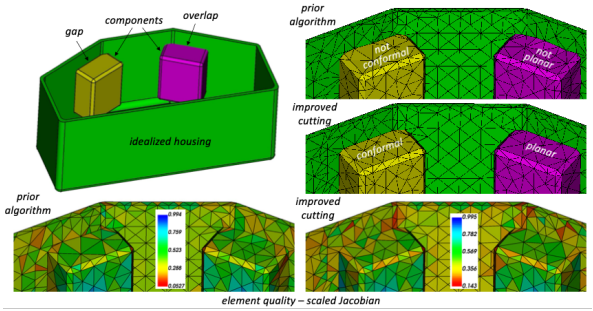
The Sierra 5.24 release is the first release with official support for Nvidia "Hopper" GPU acceleration. These newer chips bring a huge improvement in computational throughput and memory capacity for large simulation models over the previous "Volta" architecture, the backbone of Sierra Structural Dynamics workhorse platform ATS-2 (Sierra) at LLNL. After diligent work troubleshooting issues in the Sierra codebase to support building and running efficiently and credibly on these novel GPUs, the Sierra teams delivered on both "Hops" (SRN) and "Cascade" (SCN) platforms.

	Cascade	ATS-2	Stout	Cayenne
compute nodes	15	25	18*	56*
processors	300	500	1000	1000
GPUs	60	100	0	0
total wall time (hr)	**2.36**	**3.17**	**25.30***	**51.10***

Sierra/SD performance across GPU-accelerated and conventional platforms for an eigen solution with 6 million elements and ~30 million degrees of freedom. *Analysis timed out, estimated time to completion.

Discretizing ND assemblies

The Morph tetmesher is a background tetmesher that has been developed to facilitate the rapid discretization of the complex assemblies inherent in ND design without requiring the geometry to first be cleaned of imperfections. While the underlying CAD geometry is "cut" from the background tetmesh, Morph has the opportunity to remedy erroneous gaps and overlaps in the CAD description via a geometric tolerance and a relative priority. Prior algorithms did not project lower priority CAD curves and vertices onto nearby higher priority surfaces. Algorithmic improvements result in cleaner and more consistent meshes at the interfaces between assembly components. Testing a suite of ND components and systems illustrated a broad improvement across physics and 1000's of meshed volumes having up to 10X increase in element quality.



An assembly demonstrating improvements in the Morph tetmesher during the "cutting" of a CAD geometry containing both erroneous gaps and overlaps. Improved algorithms result in conformal/planar discretizations and improved element quality with 3x increase in the scaled Jacobian.

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

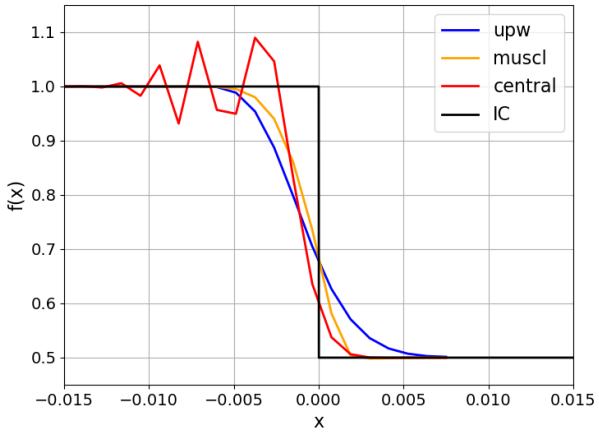
- Capability: TRACE (Trace Rapidly Acquires Contour Envelopes) improved post-processing enables more rapid construction of decision surfaces with uncertain model parameters.
- Capability: A new objective function enables model parameter estimation (stiffness, damping) to match SRS (Shock-Response Spectra) objective function in InverseSD.
- Capability: Improved Optimal Experimental Design (OED) code enhances runtime performance of gradient-based optimization algorithm for multi-observation (e.g. frequency domain) problems.
- Capability: InverseAria now supports hyper-reduction for adjoint solves when coupling with Pressio.
- Usability: Training examples for using TRACE with Sierra/SM and Aria and video of quick-start tutorial added to team wiki page.
- Bug Fix: Allow consistent output between ROL and design variable output files for inverse methods.

Structural Dynamics

- Capability: More accurate and robust support, and improved examples and documentation, for pre-loaded beams and shells when handing off from Sierra/SM.
- Capability: New five- and thirteen-node pyramid elements to allow transitioning between hexahedral and tetrahedral meshes.
- Capability: Support for user-defined element field output, including in analytic functions.
- Usability: Omitted blocks are now fully compatible with Dash contact (begin contact definition). Block definitions for omitted blocks are also no longer required in the input file.
- Usability: The "convertUnits" utility now supports shifting model coordinates by a vector value; previously only a scalar value was allowed.
- Usability: Blocks defined in the input file but not present in the exodus file will issue a fatal error by default. For information on working around this change in behavior, consult the documentation.
- Bug Fix: Addressed significant slowdowns in transient problems with many reads from the exodus file in "exodusread" functions.
- Bug Fix: A bug was addressed in the "sa_eigen" option in "qevp" for coupled structure-acoustics problems, which manifested in incorrect response at zero frequency in frequency response functions.

Thermal Fluids

- Capability: The mesh motion governing equations used in ablation modeling have new stabilization options (MUSCL) that can eliminate oscillations seen in conserved quantities in prior approaches.



Stabilization comparison for advection of sharp material profiles in deforming ablator, showing elimination of oscillations with new stabilized options.

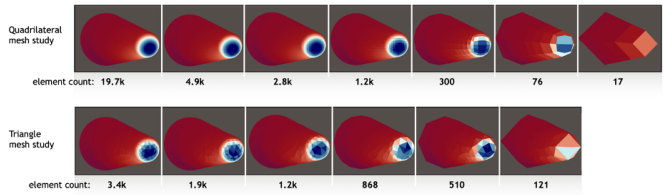
- Capability: Users running CHEMEQ models that transition to a simplified burn front model when reactions accelerate can now specify custom criteria for that transition other than temperature including reaction rates and other physics-based indicators.
- Usability: Added a new "teko_multiphysics" preset solver that can automatically set up a Teko sub-block preconditioning strategy based on your problem physics without user tuning. This solver approach adapts to the problem difficulty and can provide substantial improvements in linear solve time while greatly simplifying solver complexity for end-users.
- Bug Fix: Fixed a bug where ray tracing heat fluxes would "leak" through double-sided shell elements to the back face.
- Performance: The 5.24 release integrated a new version of Trilinos which provided substantial (2-3x) speedups in MueLu solve times on ATS-2.

Solid Mechanics

- Capability: A new Cohesive Surface Element (CSE) is available and compatible with 10-node composite tetrahedral elements. This element further enhances tetrahedral mesh-based workflows that enable faster turnaround times and robust, accurate simulations of complex geometries and large deformations. Cohesive surface elements are used to better predict failure mechanisms, such as surface separation and fracture energetics, and improve fidelity when modeling material interface behavior, such as delamination in composite materials and debonding of adhesives.
- Capability: The Total Lagrange Hexahedron and the 10-noded Composite Tetrahedral element now support energy-dependent equation of state material models. These models are essential for predicting material response in high-pressure, high-temperature, or high-energy environments. Expanding to these new element types allows for greater flexibility, ease of use and higher fidelity responses.
- Usability: User Material (UMAT) definitions are now supported through user subroutines and plugins. This new capability allows users to define and integrate custom material models into their simulations, offering greater flexibility for material behavior characterization.

SPARC

- Usability: Several Improvements to the lower fidelity MEIT method were made including:
    - Core robustness improvements have been developed through extensive torture tests
    - Improved accuracy for stagnation regions
    - Expansion of transition modeling capabilities
    - User-facing enhancements including optional inputs and improved error messages

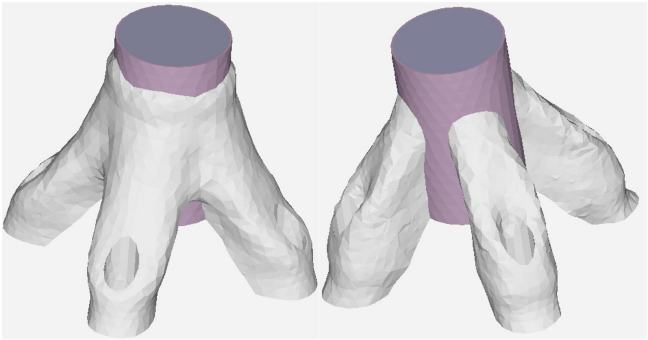


Mesh resolution study on an arbitrary sphere-cone highlights significant robustness improvements for both quadrilateral and triangle meshes.

- Usability: Robustness improvements have been made for aero/ablation axisymmetric problems.
- Capability: The many-species reacting gas model has been enabled on the GPU.

PLATO

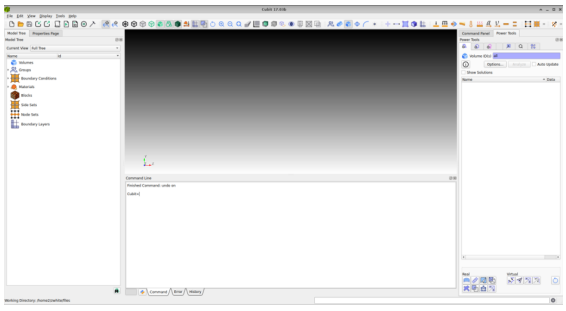
- Capability: Shock Response Spectra (SRS) objective function in FuSED available in Plato for topology optimization problems.



Compliance-minimization solution (left) and SRS-optimized result (right) for cylinder with vertical shock indicates ability of SRS objective to reduce SRS beyond what the compliance objective achieves.

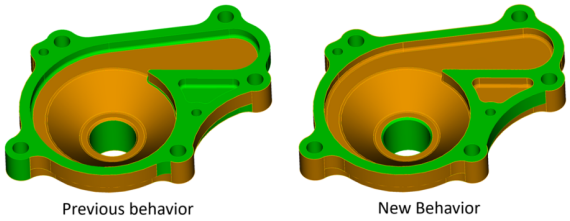
Geometry and Meshing

- Usability: Enhanced recognition of bolt features and improved patch reductions.
- Usability: New default parameter in 'simplify' command simplifies larger patches and better aligns with customer expectations.
- Usability: Improved accuracy while selecting entities in graphics window in perspective mode.
- Capability: Better support for modern desktops with user interface upgraded to Qt6.



Cubit Desktop GUI with new Scalable Vector Graphics (SVG) Icons

- Usability: Low resolution icons replaced by vector icons, so they will stay sharp at any resolution.
- Usability: Cubit now avoids inverting tiny wedge elements during import.
- Capability: Improved support for python virtual environments.
- Usability: Improved stability by removing ability for groups to include other groups in a circular fashion.



Left: Previous default behavior of the "simplify" command excluded many surfaces that could be included in the simplified composite. Right: The new behavior uses the previous "local_normals" parameter as default behavior which results in composites more aligned with user expectations.

NGS(D)

- Usability: Enable users to group multiple volumes into a single block in the Morph mesher.
- Capability: New “cutting” algorithms in the Morph mesher result in higher quality and more consistent meshes at the interfaces between assembly components. See first page highlights for more information.
- Capability: SD Modal tool now operable on the SCN.
- User Experience: Conducted and analyzed interviews with the radiation community to understand current and future needs to build a backlog for the one-dimensional stack-up capability for rapid design assessment.

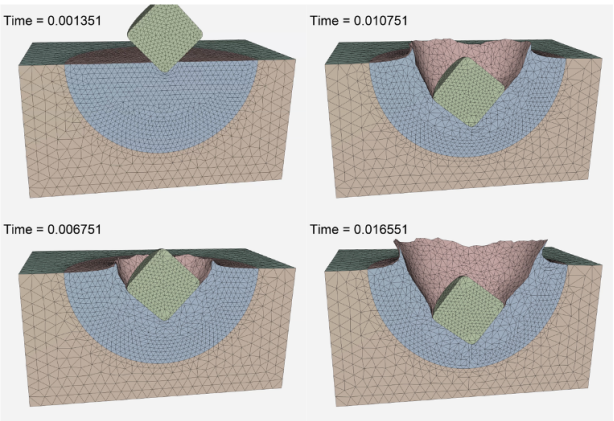
SAW/NGW

Capability: SAW Online now provides access to SAW Simulation Data Management via a convenient Web interface on the Sandia Restricted network (SRN). Analysts and stakeholders now have easy access to over a decade's worth of ND simulation data, effectively dismantling barriers between analysts and their customers.
Usability: Next-Gen Workflow now includes significant improvements to graphical layout, easing workflow construction and improving communication by providing a clearer view of analysis processes automatically.

On the Horizon

(FuSED/OED) Improved support for multi-physics types (pressure sensors combined with accelerometers, EM probes, etc)
(FuSED/InverseAria) Adaptive time-stepping, support for enclosure radiation
(FuSED/TRACE) Full release
(Sierra/SD) Reworked output syntax for greater flexibility of outputting multiple files, solution case specific outputs, discrete time steps, and other frequently requested output features.
(Sierra/SD) Support for the ATS-4 “El Capitan” GPU-accelerated platform at LLNL is planned for the next Sierra release.
(Sierra/SD) Usability enhancements to the Craig-Bampton reduction or superelement capability are planned for an upcoming release.
(Sierra/TF) Support for 2D Aria / 3D SPARC ablation MPMD coupled problems to enable faster turnaround simulations and simplified problem setup
(Sierra/TF) Support for mesh motion with particles in Fuego for plasma spray deposition problems
(Sierra/SM) ATS-4 Platform Support
(Sierra/SM) Mixed mesh usability improvements
(SPARC) Embedded error prediction for adaptivity
(SPARC) Improved NaN handling
(Plato) New and improved stress-constrained mass minimization capability
(GMTK) Support for CSE and degenerate hex elements
(GMTK) Support for Granta material IDs in STEP files
(NGS) A one-dimensional stack stack-up capability has been developed for the radiation community for rapid assessment. Given an input geometry (.stp, .sat), a host of rays, and a length scale for defeaturing, construct_1d_stackups generates a yaml file for each ray indicating the relative thickness of volume intersections. This capability is currently in user testing and will be released in 5.26. Future work will incorporate targeted, exponential size fields in one-dimensional Exodus discretizations.
(NGS) To rapidly discretize cavities for EM and TF applications, the team is exploring rapid methods for surface selection and a new capability in Morph to accept a set of discontinuous surfaces and yield a watertight discretization. This effort leverages the winding number for both “cutting” and in/out and can fill large gaps in the selected surfaces. With targeted smoothing, this capability has the potential to yield significant gains for the EM/TF community to reduce cycle time.

(NGS) Developing strategies for mesh adaptivity with a focus on large deformation contact problems pervasive in manufacturing and abnormal environments. This advancement hinges on the Emend toolkit for the incremental mesh improvement of tetrahedral elements to honor evolving contact surfaces. Below figure illustrates the new methodology currently being hardened for production and release in 5.26.



The impact of a metallic can traveling 200 m/s into sand. Rather than employ element death, the NGS team leverages new methods in the Emend toolkit to honor the contact surface via refinement and mesh improvement (swaps, collapses) that preserve geometry.

(NGS) New methods for employing AI for fastener identification and joint reduction via a web-based interface, the SD Modal tool
(SAW/NGW) Full NGW access to Model-Based Systems Engineering data, including requirements
(SAW/NGW) Online deployment to the SCN
(SAW/NGW) Supported libraries for writing Next-Gen Workflow in Python or YAML

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