SAND2024-03092O

Sandia National Laboratories

Code Release Highlights

Spring 2024

SIERRA 5.18
CUBIT 16.16
SPARC 24.2
SANDIA ANALYSIS WORKBENCH (SAW) 2.13.13

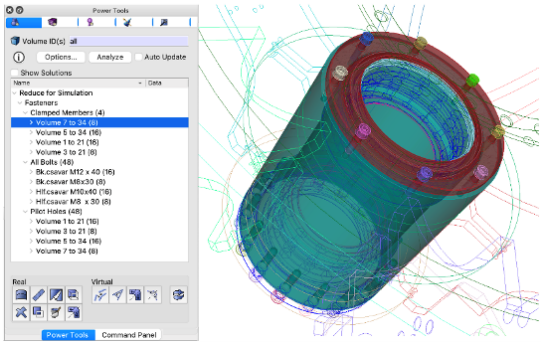
Researching, developing, and deploying state-of-the-art high performance computational engineering simulation codes.

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.

Reduce for Simulation in Cubit

The Geometry Power Tool now includes a Reduce for Simulation feature which introduces a collection of ML-driven diagnostics within the Reduce for Simulation category, designed to streamline geometry for simulation. In addition, a new fasteners category adds three bolt categorization methods:

- Clamped Members: Groups bolts by the members they fasten.
- All Bolts: Categorizes bolts by name, derived from step or ACIS file definitions.
- Pilot Holes: Lists concentric hole pairs for potential fastener application, irrespective of existing fasteners.

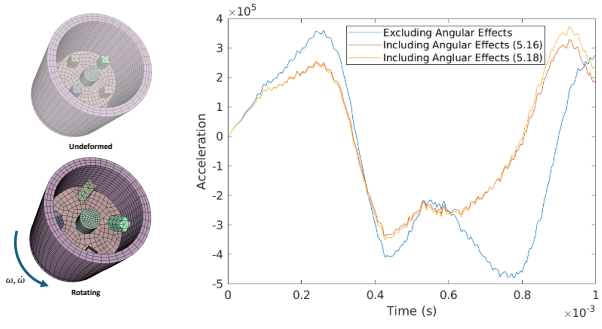


New Fasteners diagnostic shows clamped members with their associated bolts.

Angular Acceleration in Sierra/SD

Sierra/SD typically operates in a linear, small-deformation regime of structural analysis. Thus, rather than introducing large rotational motion about a structure's axis, analysts may instead incorporate the structural effects of angular acceleration and velocity through a clever combination of effective stiffness, damping, and loading changes.

Historically, SD analyses have been restricted to a constant rotational velocity. Incorporating accelerations comes with added complexity, including breaking the natural symmetry of the structural stiffness matrix. Nevertheless, building upon the theory that underpins Sierra/SD, developers were able to quickly deliver a new capability to consider structural deformation due to both rotational velocity and acceleration.



SD exemplar model (left) and sample acceleration response (right). The plot compares response without angular effects (5.16) and with angular effects (5.18).

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

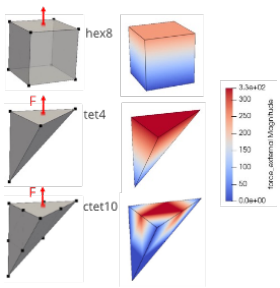
What's New in Sierra

Structural Dynamics

- Capability: New "omit blocks" feature supersedes dead blocks. Omitting blocks is preferred over dead blocks for more predictable analysis behavior, especially in contact.
- Capability: L^2 projection of element stress fields to nodes has been moved from beta to production. Use this feature for smooth, accurate visualization of high-order element fields.
- Capability: New "extractSection" script to aid in removing duplicate input blocks from large collections of included model component input files.
- Usability: Better handling of user output variable names in frequency, history, and outputs.
- Usability: Sideset history output now includes elements attached to sidesets for ease of visualization. *Note:* history database file size may increase significantly for models with many sidesets in history output.
- Usability: In multicase analysis, both modal and direct transient cases now consistently include initial conditions from preceding cases by default (previously ignored in modal).
- Usability: "mass = block" now includes block names in the mass properties table printed to the SD result file.
- Usability: Improvements to stress handoff with thermal stresses

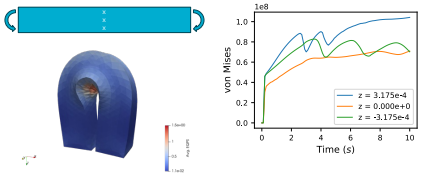
Solid Mechanics

- Performance: Optimizations and library upgrades have improved performance for simulations with heavy I/O, having large numbers of element blocks, or substantial amounts of element death.
- Capability: Spot welds on composite Tet10 faces are supported.



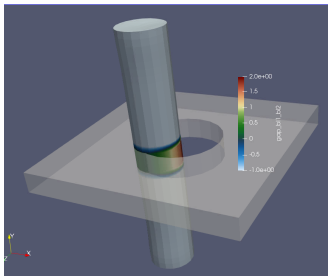
Force spread for spot weld at center of face.

- Capability: Contact can be restricted to spherical subdomains, improving performance in many scenarios.
- Capability: Composite Tet10 elements are now able to interpolate fields for user output.



Von Mises stress extrapolated to nodes and then interpolated at specific points with user output.

- Capability: In Zapotec runs the pressure applied to a structure from CTH loads can now be output.
- Usability: Gap calculation capabilities are improved to capture a wider range of desired use cases.

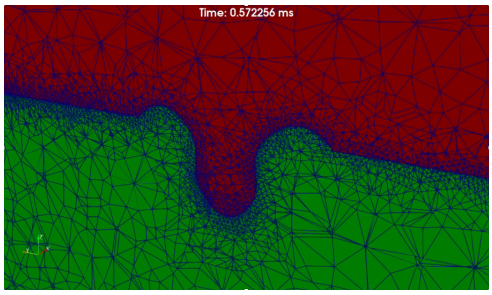


Nodal max normal gap result.

Usability: New SIERRA203: Sierra/SM Implicit Training provides a comprehensive introduction to implicit analysis using Sierra/SM. Technical topics include the multi-level solver, implicit contact and dynamics, and troubleshooting strategies.

Thermal Fluids

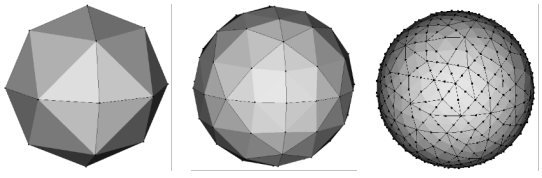
- Capability: Improved support for dynamic mesh adaptivity in Aria enabling faster turnaround times and lower computing resource requirements for many problems.
- Usability: Fuego manuals converted to easier to use web documentation.



Example of Aria's dynamic mesh adaptivity for resolving the solid-gas interface in a keyhole laser welding simulation.

Next Generation Simulation (NGS)

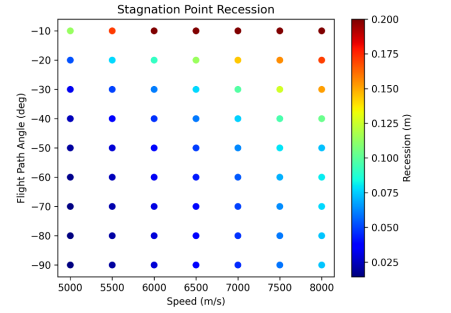
- Usability: Incrementing capabilities for resolution and hinge detection for structural dynamics. Implemented the ability for the user to maintain two elements through the thickness for thin-walled structures. Increased the robustness of faceted representations when the radius of curvature is on the order of the element size. We also now include a “clean-up” option that both detects and removes hinges in structures that result from mesh-based defeaturing.
- Usability: The web-based SD modal tool now includes a “Download Movie” feature that enables the automatic capture/download of both stills (.png) and the animation (.mp4) of the selected mode and orientation.
- Capability: Improved slot modeling for electro-magnetics with the addition of separate blocks adjacent to external slots. Collaborating with G&M to increase the scope of slot creation via ML in Cubit.
- Capability: Implemented a geometry layer in Emend for respecting geometry during refinement and coarsening. Includes the projection of mid-edge nodes for higher-order tetrahedral elements.



Subsequent refinement of a sphere using Emend. Coarsening and refinement now respect a geometric representation for the placement of both edge and mid-edge nodes.

SPARC

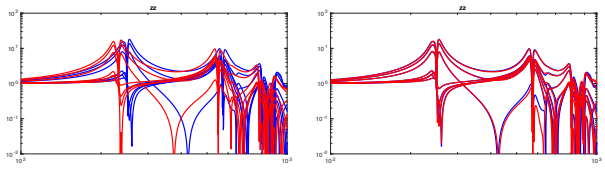
- Usability: Productionized the the momentum and energy integral technique (MEIT) boundary layer model when coupled to inviscid Euler or Modified Newtonian Aerodynamics (MNA) simulations for reduced-fidelity, faster-turnaround aerodynamic heating and drag predictions.
- Usability: SPARC now natively supports
  - Automation for setting up many trajectories.
  - Automation for setting up SPARC/Aria coupled analyses with any aero fidelity.
  - Running simulations concurrently on a single HPC allocation. For example, users can run 100 four-rank Euler+MEIT simulations on an allocation with 48 available ranks.



Total recession is shown for a map of different reentry flight path angle and speed for a notional vehicle with straight-line trajectories using MNA coupled with the MEIT to compute aerodynamic heating and Sierra/Aria to compute recession due to vehicle ablation.

Plato

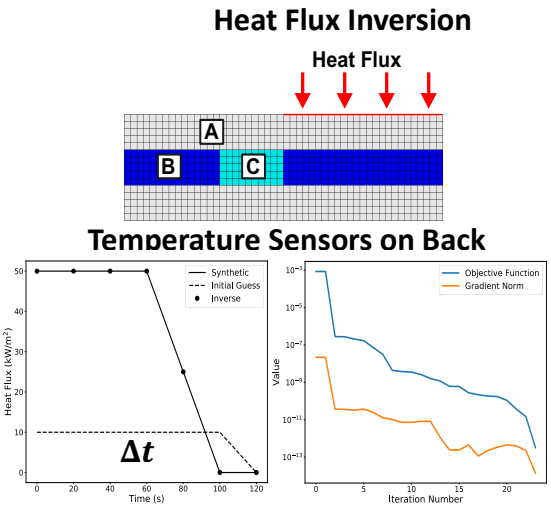
- Capability: Shell thickness optimization with Sierra/SD.
- Bug Fix: Plato Analyze now using correct mass matrix integration rule for Tet4 elements.



Before (left) and after (right) optimization of shell thicknesses for dynamics matching.

FuSED

- Capability: Inverse Aria Beta Release: The Inverse Aria tool has been made available in the Sierra module as a beta feature. Inverse Aria solves thermal inverse problems for boundary heat fluxes, thermal conductivities, and thermal contact resistances. The beta capability can solve some non-linear problems with temperature-dependent material properties and boundary radiation. Current capabilities do not support reactions, species transport, and enclosure radiation, but these features are targets for future development.



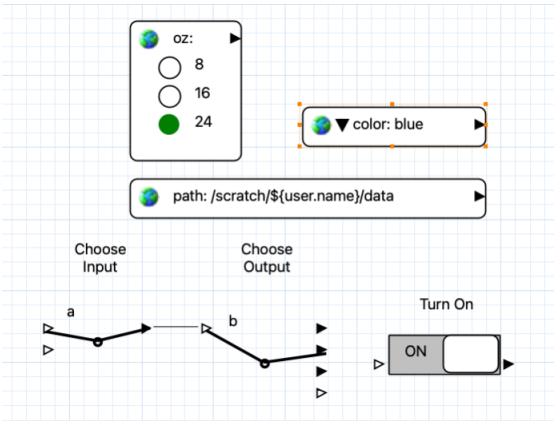
InverseAria workflow for heat flux inversion in thermal testing.

Cubit

- Capability: Element blocks, nodesets, and sidesets created from mesh (not geometry) are now copied when owning geometry is copied if the block/nodeset/sideset settings are active for copying. Previously, only boundary conditions containing geometry were propagated during a copy.
- Capability: When using the tetmesh respect capability to insert locations into a tet mesh, the given nodes are now consumed and used by the resulting tets. This also means the specified nodes are no longer duplicated. Using the original nodes is useful for being able to query tets related to the given nodes.

SAW and NGW

- Usability: A new reporting framework in Next-Gen Workflow understands other CompSim tools and provides detailed error information to help the user debug workflows and quickly understand and recover from failures
- Usability: Interactive controls in Next-Gen Workflow, including radio buttons, dropdown menus, and switches, let you create intuitive, easy to use workflows
- Capability: Next-Gen Workflow will now strip “smart quotes” and other non-ASCII characters from input decks preventing a common source of error.
- Usability: New “Favorites” and “Recently Used” folders in the NGW palette help you build workflows faster by keeping your most important components at your fingertips.
- Capability: New Job Status filtering tools help you manage a large portfolio of HPC jobs easily.
- Capability: Next-Gen Workflow now supports hierarchical maps and exchange of complex JSON data structures between components.



Using Next-Gen Workflow, you can build interactive tools that include a variety of graphical controls including radio buttons, dropdown menus, and switches.

On the Horizon

(SD) Support for multiple history, frequency, and Exodus output files in SD.
(SD) Band-limited damping capability for finer control over damping behavior in direct analysis in SD.
(TF) Significant progress towards GPU support in Fuego with anticipated production release in 5.20.
(SM) Prototype coupling of SIERRA/SM and SABLE for future blast/crash simulations is being evaluated for accuracy and robustness, with a capability demonstration to follow.
(SM) Ability to do in-core remeshing in Sierra/SM is being investigated, with further development work planned for FY2024.
(SM) Significant progress on GPU acceleration is being targeted for FY2024 developments.
(NGS) In collaboration with the G&M team, the SD modal tool will soon release capabilities to create, manage, and visualize bolted structures for structural dynamics.
(NGS) Through a DARPA sponsored project, we will release an initial capability for the in-core reconstruction of SPH particles to a tetrahedral representation in Sierra/SM.
(NGS) UX research for thermal fluid workflows will provide insight into the utility of web-based interfaces to reduce complexity and decrease cycle time for normal thermal environments.
(SPARC) More accurate and robust simulations at all Mach numbers using tetrahedral meshes.
(SPARC) Smooth, higher-accuracy transfers between physics models.
(SPARC) M-to-N restart capability.
(Plato) Level-set topology optimization using Krino.
(FuSED) Support Vector Machine (SVM) for estimating decision boundaries.
(FuSED) Robust OED method that can account for uncertainty in FEM models.
(FuSED) Reduced basis methods for accelerating structural dynamics calculation.
(FuSED) Inverse contact area extraction with spot welds in SD models.
(DevOps) Upgrade production compiler to LLVM-based Intel 2023.1 with MPI options of OpenMPI 4.1.6 and IntelMPI 2021.5 or newer.
(NGW) integration for the GRANTA material database will allow just-in-time updates of material data used in simulations .

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