Code Release Highlights

Fall 2024

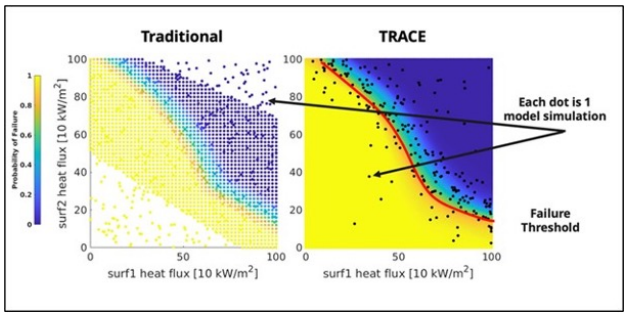
SIERRA 5.22
CUBIT 17.02
SPARC 25.1
SANDIA ANALYSIS WORKBENCH (SAW) 2.13.17

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.

TRACE Machine Learning Tool Enables Calculation of Performance Envelopes

The FuSED team is excited to deliver TRACE, a machine learning classification tool that efficiently locates decision boundaries (e.g., between safe/unsafe zones) for Nuclear Deterrence (ND) applications. TRACE reduces the number of model evaluations required to accurately locate decision boundaries in high-dimensional spaces, thereby enhancing computational efficiency and accelerating qualification timelines. This enables current and future ND analysts the ability to explore a broader range of previously unexplorable parameter spaces, which increases coverage of uncertain simulation conditions.

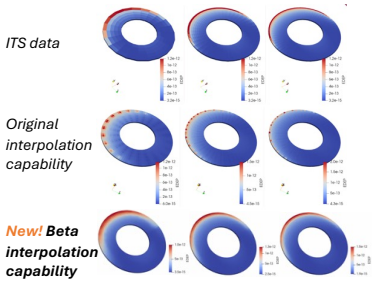


(Left) Many ND workflows involve a brute force parameter search to locate the decision boundary with a computationally expensive grid of evaluation points. (Right) TRACE intelligently samples the parameter space to find the desired threshold using the minimal number of model evaluations.

Its2Sierra

To support more credible handoff analyses between the RAMSES code ITS and Sierra Mechanics, the Sierra/SD team is excited to deliver a new and improved version of Its2Sierra. After many years of no development, Sierra/SD has implemented feature requests and expanded testing and verification. Its2Sierra now preserves mesh metadata and QA information on both input (ITS) and output (Sierra) Exodus databases and allows for conservation of total energy transferred between ITS subzones and Sierra mesh elements.

Also, all-new beta capabilities are available in Its2Sierra including an improved, smooth interpolation method to transfer energy data to Sierra elements in difficult mesh geometries, a parallel execution mode to support large Sierra mesh databases, and geometry transformation and scaling to accommodate dissimilar ITS and Sierra domains. The Its2Sierra user documentation is updated and included in the Sierra 5.22 release package.



Enhancements to Its2Sierra interpolation to support accurate energy deposition mapping.

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

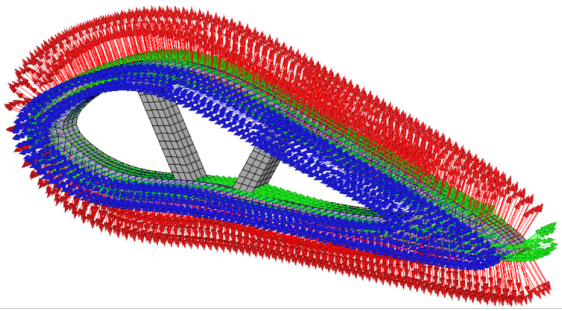
What's New in Sierra

FuSED

- Capability: TRACE (TRACE Rapidly Acquires Contour Envelopes) has been released as a beta capability for finding decision boundaries in high-dimensional parameter spaces.
- Capability: InverseSD supports interface identification through the inverse solution of distributed stiffness in spot weld elements in SD.
- Capability: The OED app now supports multi-sensor, multi-budget optimization of sensor placement.
- Capability: InverseAria now supports multiple design variable types, e.g. cases where it is desired to invert for flux and conductivity simultaneously.
- Usability: In InverseSD, the MAC objective function for matching mode shapes and frequencies of SD models to test data has been improved with increased robustness of mode-matching and several bug fixes.
- Usability: InverseAria supports L2 regularization to mitigate effects of non-unique solutions for thermal inverse problems.

Structural Dynamics

- Capability: Frequency band damping is the most exciting new feature in Sierra/SD, allowing users to specify uniform damping over a frequency range of interest at a reduced cost compared to modal damping.
- Capability: The Its2Sierra tool is now supported for transferring energy data between ITS and Sierra Exodus meshes. It preserves mesh input/output database information and features an expanded set of tests to verify behavior. Its2Sierra has all-new beta capabilities as well: smoother and more accurate interpolation of energy to SD elements, scaling and transformation of ITS/Sierra meshes for robust transfers, and parallel execution to handle large mesh databases.
- Capability: Sierra/SD now supports element-wise coordinate system definitions for anisotropic material properties.
- Capability: Several modifications have been made to transfer and function definitions to support reading data from specific times or steps on input mesh files.
- Capability: Basic support for element variables as analytic function output has been added.
- Capability: Superelements now accommodate parameters that incorporate mildly nonlinear behavior on fixed interface modes (or "internal" degrees of freedom), including cubic spring/damper, Iwan, and Riwan formulations.
- Usability: An estimate of the simulation runtime to completion is now output to the SD result file for direct and modal transient analyses.
- Usability: New scripts to help identify duplicate input sections have been added to SD's suite of auxiliary tools, including "sortSections" and "uniqSections," intended for use in tandem with the existing "extractSections" tool.
- Usability: Several improvements and fixes have been made to the default behavior of loads that modify stiffness, such as gyroscopic or follower loads.
- Usability: Fuzzy name matching is now supported and the default for suggested syntax when an input deck typo or error is encountered, and the "error detail" parameter also now allows the user to control error output levels.
- Bugfix: Long block names of greater than 30 characters are now supported. Previously, long block names with names identical up to the first 30 characters may have introduced model bugs.
- Bugfix: History output with coordinate transformations previously introduced potential bugs into SD calculations by unintentionally modifying the SD model's underlying coordinates; this bug has been fixed.
- Bugfix: Incorrect handling of RBAR attributes, specifically "CID_FLAG_DEPEND," has been fixed in version 5.22.



New element-wise coordinate system support for composite modeling in Sierra/SD.

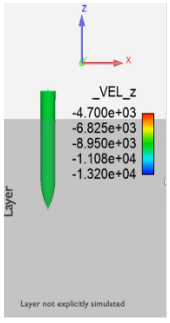
Thermal Fluids

- Capability: Productionized wall-modeled LES capabilities in Fuego.
- Capability: CVFEM wedge & pyramid element support.
- Capability: GPU support for ablation models.
- Usability: Automatic support for 64-bit mesh global IDs in output.
- Usability: Simplified user input syntax for Teko block preconditioners and enabled use of preset solvers as solvers for diagonal sub-blocks.
- Bugfix: Resolved issues with energy conservation in heat of ablation models.
- Performance: Improved DD-ILU preconditioner performance on GPUs.

"Credibility assessment for wall-modeled LES that includes fire-engulfed objects in crosswind", Standford Proc. CTSRP (2024)

Solid Mechanics

- Capability: Transitioned to an in-house cavity expansion capability for penetrator modeling from a third-party library to being fully implemented in Sierra/SM which allows for further performance improvements and extensions. Added new functionality to support 4-noded and composite 10-noded tetrahedral elements.



In-house cavity expansion capability for penetrator modeling.

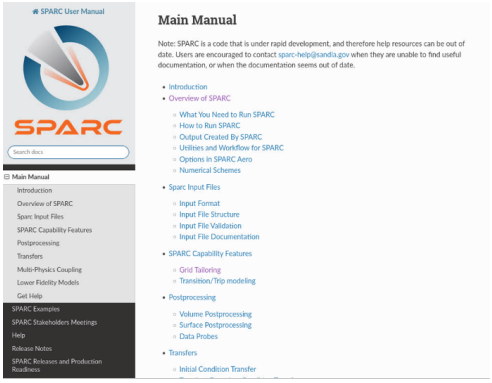
- Capability: Implemented a new capability for multi-stage preloads, allowing users to apply preloads in a specific sequence or order, improving control over complex simulations.

Now, Sierra/SM users can apply preloads in specified order.

- Usability: SM subroutines can be replaced with plug-ins to enable re-use and avoid creating new SM executables.
- Capability: The 10-node composite tetrahedral stabilization algorithm is now more accurate across remeshing/adaptivity events.

SPARC

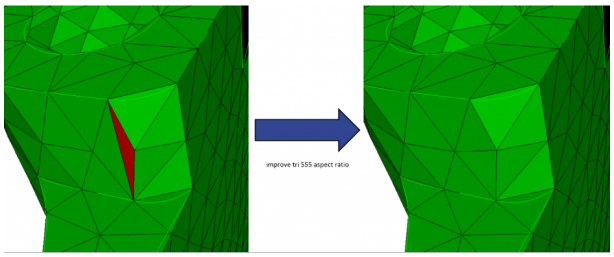
- Usability: Improvements to the unstructured finite volume discretization now show equivalence to the structured finite volume discretization when applied to the same mesh.
- Usability: A new SPARC/TAOS interface leverages Python-based user functions, which improves user flexibility and robustness on HPC systems.
- Capability: Roughness models have been implemented for heat flux, shear stress, and transition augmentation for the RANS and MEIT aero models.
- Usability: A new Sphinx-based SPARC user manual can now be opened directly from the run environment, providing easier access to user documentation.



A new Sphinx-based SPARC user manual.

Geometry and Meshing

- Capability: The primary triangle and tetrahedral mesher in Cubit® has been updated to MeshGems 2.15. This upgrade comes with more robustness, better quality elements, and improved capabilities.
- Usability: The normalized inradius metric now returns negative values for inverted elements. Though not common, robustness is gained by checking for inversion.
- Usability: The 'remove overconstrained tet' command now takes volume ids, automatically finding overconstrained tets and removing them. A 'preview' option has also been added to show which tets will be removed.
- Capability: The new 'improve tri' command collapses and swaps mesh edges to improve mesh quality of triangle elements. The operation that results in better quality is used.

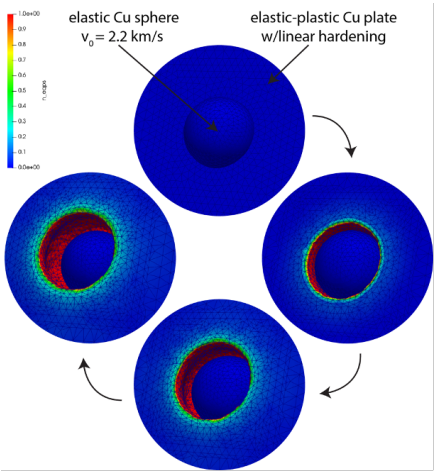


New 'improve tri' command to collapse and swap mesh edges to improve mesh quality.

- Usability: The ACIS geometry kernel has been upgraded to ACIS 2023.1. This upgrade comes with improved geometry healing.
- Usability: You may include a tolerance parameter for equality operators rather than write a lengthier selection with inequalities. e.g. select volume with volume = 5 tolerance 1e-3 rather than select volume with volume > {5 - 1e-3} and with volume < {5 + 1e-3}
- Usability: To assist in finding syntax errors in Python scripts, the cmd() and parse_cubit_list() functions in the cubit module now raise exceptions for syntax errors. This can reduce the amount of time debugging and tracking down programming mistakes in scripts.
- Capability: A new Python function find_overlapping_curves returns sets of overlapping curve ids, given a list of curve ids.

NGS(D)

- Usability: Improved performance of the in-core particle mesher in Sierra/SM. In some cases, we decreased the computational time for mesh generation by 100X.
- Usability: The SD Modal tool now supports both the ACIS and the SGM geometry engines with an ability to import both .step and .sat files for rapid analysis.
- Capability: The Emend toolkit has been extended to faceted geometries which include support for tri6 surfaces via four tri3 facets. The executable wrapping the Emend toolkit, improve_mesh, has been employed for file-based remeshing with localized plastic strains exceeding 6.
- User Experience: Conducted and analyzed interviews with the TF and the EM community regarding cavities for radiation. Constructed backlog for future, prototyping efforts.

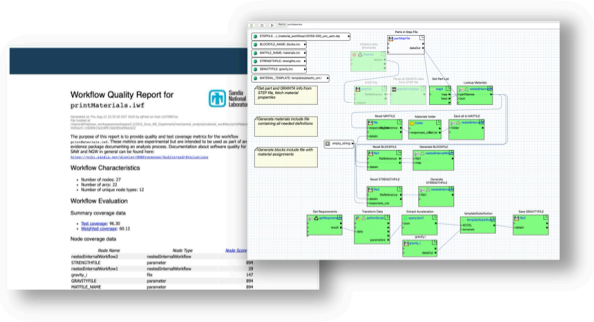


An illustration of robustness in Sierra/SM employing the composite tetrahedral element with new methods for mapping VEM stabilization and the Emend toolkit for mesh adaptivity in a file-based workflow via SierraRemesh.py with roughly 80 remeshing steps.

SAW/NGS

Capability: The Feature Coverage Tool for Workflow (FCTW) generates test coverage reports for user-authored workflows, providing valuable credibility evidence for high-consequence analysis results. (See possible figure on the next page)

Capability: A new workflow wizard and a template library representing many common tasks let you create a workflow from known working examples
Usability: Next-Gen Workflow nodes now have "required" properties, helping users to quickly understand how to use them correctly.
Usability: The Dakota integration for NGW has many usability improvements, including convenient management of Dakota install locations and clear, detailed error reporting.



Feature Coverage Tool for Workflow (FCTW) generates test coverage reports for user-authored workflows.

On the Horizon

(FuSED/OED) Improved support for multi-physics types (pressure sensors combined with accelerometers, EM probes, etc). Release of gradient-based optimization and greedy algorithms for OED with robustness to model uncertainty. Performance improvements to OED for frequency domain problems.
(FuSED/InverseSD) Inverse formulation with SD models to better match measured Shock-Response Spectra (SRS) from mechanical tests.
(FuSED/InverseAria): Adaptive time-stepping and support for enclosure radiation.
(FuSED) Full release of TRACE
(Sierra/SD) Reworking output syntax for greater flexibility of outputting multiple files, solution case specific outputs, discrete timesteps, 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 in Sierra/SD are planned for an upcoming release.
(Sierra/TF) AMD GPU Support
(Sierra/TF) Two-way aero-thermal coupling improvements
(Sierra/SM) Hops platform support
(Sierra/SM) Training for preload simulations
(Sierra/SM) Porting more capability to run on GPU platforms
(SPARC) More accurate and robust simulations at all Mach numbers using tetrahedral meshes
(SPARC) Embedded error prediction for adaptivity
(GMTK) Improved smoothing implementations with surface node smoothing
(GMTK) Propagation of Granta material properties
(NGS) New algorithms for improved cutting which result in better geometric resolution and improved element quality. This work will also entail the differentiation between collapsing a material and a void in the construction of watertight internal cavities.
(NGS) In an effort to rapidly discretize cavities for EM and TF applications, we are prototyping web-based methods for concurrently visualizing the geometry and the mesh in Blueprint JS.
(NGS) Our embedded work on the SCN coupled with UX research for both electromagnetics and radiation is yielding new workflows via the Morph mesher. We will document these new workflows via best practices at https://docs.sierra.sandia.gov/.
(NGS) New methods for employing AI for fastener identification and joint reduction via a web-based interface, the SD Modal tool.
(NGS) We will release the SD Modal tool on the SCN in 5.24.
(SAW/NGW) An overhaul of SAW's Sierra Editor will bring improved performance, accuracy, and usability to this important tool.
(SAW/NGW) New production RAMSES components for Next-Gen Workflow

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