SANDIA REPORT

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Sierra Release Notes Version 4.52

Sierra Development Team

Prepared by
Sandia National Laboratories
Albuquerque, New Mexico 87185
Livermore, California 94550

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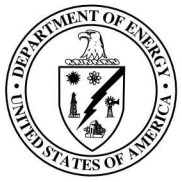

ABSTRACT

This document contains release information for the Sierra product. These changes are for the 4.52 release.

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1. NEW CAPABILITIES

1.1. New Capabilities for User Support

In addition to emailing sierra-help@sandia.gov and cubit-help@sandia.gov when you need help, you can now create your own requests at and of the customer portal by going to any of the following URLs (redirect to the same location):

https://compsim-help.sandia.gov
https://sierra-help.sandia.gov
https://cubit-help.sandia.gov

Before submitting your request you can search the Knowledge Base that the CompSim Help team has created to solve your issues more quickly. Submission via the customer portal also ensures that the team has the necessary information they need to categorize and solve your problems more quickly.

1.2. New Capabilities for Low Mach

Support for mesh motion driven by global variables

Added implicit under-relaxation option per equation system

Added options for specifying upwinding and under-relaxation as functions of time in the input file

Added sponge layer for open BCs

Added new entrainment options for open BCs with better stability

Added wider stencil option for mixture fraction property evaluation

Added mixture fraction ignition blending to help with startup

1.3. New Capabilities for Structural Dynamics

Several improvements have been made to viscoelastic material input. Temperatures for time-temperature-shift can now be given in the `block` input. This is the preferred method with `t_current` specified in the material being deprecated. A new `t_g` parameter is available to control the form of the shift function above or below the glassy transition temperature. Several guardrails were added to the prony term input such as checking for negative relaxation times.

Support for Perfectly Matched Layers (PML), an absorbing boundary condition for an unbounded acoustic mesh, was added. PML currently only work for directfrf solutions and acoustic elements. They can be applied to an exterior sideset of an acoustic mesh, much

like infinite elements. For large problems, PML show a substantial performance improvement compared to Infinite Elements.

Modal Effective Mass is now output immediately after modal participation factor for the mpf solution case.

It is now possible to read in a time variant temperature in transient analysis. See documentation for the `nUpdateTemperature` and `nUpdateDynamicMatrices` keywords for details.

Shells are now supported with dash contact, including "doubly wetted" shells with acoustic elements on both sides.

Improvements were made to thermal strain and temperature dependant material properties. Temperatures can now be read in from a transient input mesh, and the thermal loads and material properties can be updated periodically throughout the simulation.

A new SM/SD handoff capability is available.

The fatigue capability was updated to handle both Narrowband and Wirsching damage output, as well as to handle stress range fatigue material properties. Numerous clarifications were made in the documentation.

Element volume can now be output by requesting volume in the outputs block.

Contact in the deformed configuration.

For problems with thermal strain, output stress is now thermal stress, with âĂIJstrainâĂİ unchanged, `elastic_strain` and `thermal_strain` added.

New training material is available under the training folder of the Sierra release documentation.

1.3.1. Performance and robustness improvements

Exodus mesh part names can now be directly referenced in the input file. This includes block names, sideset names, and nodeset names.

Performance improvements were added for the modal transient load ID by reducing matrix vector operations to only those of the load points. Additionally, the estimated forces is output at each iteration and can be used to restart an inverse run.

Usage guidelines were added for running with threads, and the deafult solver was changed on some thread enabled platforms to fully utilize the processors available for the quickest solution.

A block preconditioner solver was added to reduce memory requirements for extremely large constraints.

Additional documentation and verification are provided for acoustic point sources.

A SAND Report is available demonstrating parallel scalability of **Sierra/SD** up to 1 billion degrees of freedom.[?]

The serial dry run `-check-syntax` option was added to allow a serial execution to check the syntax of an input file before submitting to an HPC queue.

The memory impact of storing large number of eigenvectors was reduced, including a new option to store eigenvectors outside of core memory and on physical disks.

1.4. New Capabilities for Solid Mechanics

Multi-Point Constraints now support higher-order tetrahedral element topologies such as the 10-noded composite tet.

The composite tetrahedral element supports viscous damping.

Users may now control the amount of Sierra log file output from element death.

The user output `EXTRAPOLATE` command supports specifying different projection types via the `EXTRAPOLATE PROJECTION TYPE` command.

1.5. New Capabilities for Thermal/Multiphysics

Enabled use of hydrostatic source on mesh equation with porous flow system.

Enabled `MESH_DEFORMING` porosity evaluation on a surface.

Enabled post process mass and volume with multiple equation systems.

Enabled use of DOF phase temperature.

Enabled query access to the associated Data Block name.

Enabled use of RuntimeWarning from within the subroutine.

Added conical energy source model.

Added activation parallelepiped energy source model.

Added model for relative magnetic permeability.

Added equation for magnetic flux intensity scalar potential and enable output of the associated magnetic field.

Several core algorithms and a limited subset of material models now support running on Nvidia GPUs.

Users interested in running on GPU systems are encouraged to contact sierra-help to get in touch with the development team and determine what additional work is needed to use your model on the GPU.

Aria now has support for string functions to define scalar, vector, and tensor expressions. - Examples:

```
viscosity = scalar_string_function f = "1e-3*exp(TEMPERATURE/1000)"
BC for velocity on block_1 = vector_string_function f_x = "2*y" \$
    f_y = "200*sin(t)"
Intrinsic Permeability = tensor_string_function_symmetric f_xx = "1e-12*x" \$
    f_yy = "1e-13*Solid_Phase_Porosity^2" f_xy = "0"
```

Currently only scalars can be used as arguments in the string functions. As shown in the examples, (x,y,z,t) can be used as arguments as well as any expression name registered from your input deck. These work for new style BC and ICs, as well as for material model definitions. These can replace many of the specialized models in Aria as well as encore functions. More complete documentation can be found in the 4.52 Aria Manual.

1.6. New Capabilities for Sierra Tools

In 4.52, the Sierra DevOps Team implemented native builds of Trilinos (using the CMake-based Tribits), an important step towards continuous integration with Sierra. This implementation also included expanded bake options, as well as a new utility to enable users to untar packages and build with CMake.

For the internal user and developer communities, the `assign` utility was modified to assign tests (using the Google Repo version management tool) across Sierra Computational Simulation repositories.

1. Made the tests repository a Google Repo-based repository with a Plato sub-repository
2. Modified assign to collect tests from the Google Repo-based tests repository
3. Added capability for users to untar and use CMake
4. Added a CMake version checker and an option to add a CMake executable
5. Added Trilinos software to packaging and builds
6. Modified GCC version check to now check for version 7.2.0
7. Upgraded Message Passing Interface from IntelMPI-5.1 to IntelMPI-2018.4

2. CHANGED CAPABILITIES

2.1. Changes to the User Interface for Low Mach

Added more strict checks on field states in transfer to prevent unintended behavior.

Simplified input deck syntax for selecting Tpetra solvers.

Friendly users are encouraged to try switching existing input decks to the new solvers and inform sierra-help of any issues. We anticipate beginning the deprecation process for the non-Tpetra solvers with release 4.54.

2.1.1. Bug Fixes

Fixed bug preventing Favre averaging of vector fields.

2.2. Changes to the User Interface for Structural Dynamics

Units were corrected for buckling mode frequency output, from rad/s to Hz. Previously the frequency was reported to be exactly the same as the eigenvalue.

Support was added for Superelements used in conjunction with dash contact.

A more aggressive parser and spellchecker was implemented to aggressively catch inconsistencies in input files, including warning when an input file references a mesh part that does not exist.

A bug was fixed to allow the inclusion of preload terms in eigen sensitivity analyses.

2.2.1. Deprecated Features

The explicit transient dynamics solutions case was deprecated.

The `transfer` solution option has been deprecated in favor of `receive_sierra_data`.

Many navy specific loads were deprecated, including ShockWave and GenBub. These capabiltiies are encompased by the genera functions Undexshockwave and multicyclebubble.

Yada is deprecated as the recommended decomposition tool. We strongly recommend using stk_balance instead.

A large number of features were transitioned from production to beta. While these features are still available in this release, the **Sierra/SD** team should be contacted if their support is required long term.

The deprecated `receive_sierra_data` solution case option `read_from_file`, and the Tied-Joint option `Shear distribution` have been removed. Those keywords did nothing in previous versions.

The Tied-Joint options `interaction` and `transverse=friction` have been removed. They were both previously documented as unsupported.

The "syntax_checking" parameter has changed from 0/1/2 to ignore/warn/abort for clarity and to match the existing parameter syntax of "RequireMatchedBlocks", which has a similar effect on the code.

2.3. Changes to the User Interface for Thermal/Multiphysics

Add deprecation warning for view factor smoothing on partial enclosures.

Add warning for potential view factor errors.

Add deprecation warning for Phase Change Specific Heat. Usage should be transitioned to Melting heat source model.

Deprecated the legacy ChemEQ solver. Using it will result in a warning in this release (4.52), and an error in the next release (4.54). Use the `ODE Solver = X` command to use a solver from the newer set.

Simplified input deck syntax for selecting Tpetra solvers.

Friendly users are encouraged to try switching existing input decks to the new solvers and inform sierra-help of any issues. We anticipate beginning the deprecation process for the non-Tpetra solvers with release 4.54

2.4. Changes to the User Interface for Sierra Tools

In the 4.52 release cycle, Team DevOps upgraded both the gcc development compiler and the intelmpi library (i.e., gcc-7.2.x, intelmpi-2018.4), together with all of the necessary adjustments.

1. Modified setup script to handle different MPI types
2. Modified GCC version check to now check for version 7.2.0
3. Corrected C++11 settings
4. Added capability for users to untar and use CMake
5. Changed MPI version error to a warning (from an error)
6. Added a CMake version checker and an option to add a CMake executable
7. User subroutines will only work if CMake is utilized in the Trilinos builds

3. ISSUES ADDRESSED

3.1. Issues Addressed for Low Mach

Stability improvements to Non-Conformal interface

Fixed bug preventing Favre averaging of vector fields

3.2. Issues Addressed for Solid Mechanics

The Dash interface material capability has been fixed for the Tvergaard Hutchinson and Thouless Parmigiani surface models.

Spot welds now evaluate weld failure only at the converged state of an implicit analysis load step rather than at each nonlinear iteration.

Some parallel issues in extrapolating variables on a block-by-block basis were addressed.

Corrected initialization of data filtering with restart and results output.

3.3. Issues Addressed for Thermal/Multiphysics

Construction of Calore, legacy, and new style const BCs use the same code path for more consistent results. Users should not require any changes to their input decks.

Dirichlet BCs now warn on duplicate BC application and the last parsed BC gets applied. Previous behavior could result in additive contributions for Dirichlet BCs.

Renamed `Water_1` material component to `Water1` to eliminate subindex mangling for that material component. In general, it is recommended to use `Material_Phases` to do porous flow and not the material components. Please Contact the development team for more details.

Bug fix for parsing of Encore function absorption coefficient model.

Improved support for aria input files in SAW model builder.

Improved support for next generation Tpetra solver stack.

3.4. Issues Addressed for Sierra Tools

In the 4.52 release cycle, the Sierra DevOps Team addressed bugs (e.g., MPI handling, correct and complete passing of build system options) in the Sierra setup software stack to ensure efficent and correct configuring, building and installation of Sierra.

The DevOps Team also developed use case-driven patches for user subroutines and user plugins for Cray XC40 and Linux desktop platforms.

1. Modified setup script to handle different MPI types
2. Changed MPI version error to a warning (from an error)
3. Improvements made to Cray MPI handling in packages
4. Corrected C++11 settings

4. KNOWN ISSUES

4.1. Incompatibility Issues for Solid Mechanics

The Fortissimo product is no longer supported.

Volume repulsion (undocumented feature) is deprecated and scheduled for removal on or after the 4.54 release.

The `ENHANCED_STRAIN` element formulation is deprecated and scheduled for removal on or after the 4.54 release.

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