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SIERRA Release Notes Version 4.44

SIERRA Development Team

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P.O. Box 5800
Albuquerque, NM 87185

COMPSIM

Abstract

This document contains release information for the Sierra product. These changes are for the 4.44 Sierra release.

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1 4.44.2 addendum

The 4.44.2 release was created in order to address some bugs found in 4.44.1 as well as to provide select ATS-1 Trinity support. The following sections showw the differences between 4.44.1 and 4.44.2.

1.1 ATS-1 Trinity support

Due to difficulties in reliably testing Sierra on the ATS-1 Trinity test platform (Mutrino), the Sierra application development teams decided not to support 4.44.1 on Trinity. A subset of tests was run on Mutrino to ensure code correctness for a subset of Sierra applications so that the following applications are supported in version 4.44.2: Sierra/Aria and Sierra/SM. Other applications will be supported for use on Trinity in future releases.

1.1.1 Aprepro

Some Sierra testing showed issues with use of external Aprepro, i.e., issuing the `aprepro` command as a pre-processing step to a Sierra submission. To circumvent possible issues with external Aprepro, it is recommended that users employ the internal Aprepro capability which is present in most Sierra applications, including Adagio/Presto, Aria, and Fuego.

1.2 Thermal

1.2.1 Enclosure Radiation parallel redistribution

Parallel redistribution was enabled by default for Aria's enclosure radiation solver in 4.44.1 but there were issues where larger models would hang with this option enabled. As a result, parallel redistribution was disabled by default in 4.44.2. As a result, users should remove the following line from the `Enclosure Definition` blocks:

```
Disable Parallel Redistribution
```

Parallel Redistribution will be addressed in future releases.

1.2.2 Known Time Discontinuities

A bug was found and fixed in the `Known Time Discontinuities` feature.

1.3 Solid Mechanics

The code that scales contact bounding box back was reverted to behavior prior to 4.44. This reversion was due to issues noticed in certain models. Though the code behavior is still suspect in 4.44.2 it was deemed appropriate to keep results in alignment with older releases. The development team is working towards a better solution for contact bounding box scaling in the master version of the code.

2 New Capabilities

2.1 New Capabilities for Low Mach

Allow stuck particles to be integrated on the surface. Stuck particles now continue to evolve by heating up/cooling down, evaporating and/or reacting.

Expanded pool evaporation boundary condition to handle mixture-fraction based tabulated approach. Heat flux across the pool surface (therefore, non-adiabatic) is allowed.

Added alternative stabilization procedure: nonlinear stabilization operators.

Added the ability to terminate a simulation based on a user specified wall time limit, which forces an output of restart and results data

2.2 New Capabilities for Structural Dynamics

2.2.1 Improvements to Accuracy of Transient Dynamics

While the Newmark-Beta integrator is provably second order accurate for displacement and velocity, second order accuracy can be lost in acceleration. This is a crucial metric for many of our analysts. Accuracy of the solution was improvied by the following.

1. Providing a post processing algorithm which modifies the output acceleration to obtain second order accuracy.
2. Correcting a long-running issue in establishing initial conditions for structural mechanics. In many cases this requires an additional linear solve at $t = 0$.

2.2.2 Sierra Acoustics MPI Standalone Capability

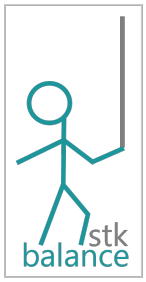
Structural capabilities in Sierra have historically been coupled to a variety of fluids codes through MPI enabled multiple program multiple data (MPMD) methods. Specifi-

cally, Sierra/SD has coupled to Gemini, NEMO, SigmaCFD and Sierra/Aero. This coupling has recently been extended to include coupling of the *acoustics* capability in Sierra/SD to Sierra structural capabilities.

2.2.3 Cluster Pardiso

One essential component of our strategy to perform well on next generation platforms includes use of high performance, threaded sparse direct solvers as part of the domain decomposition linear solve. On platforms where it is supported, we now support utilization of the cluster pardiso solver for both local and coarse grid solves in GDSW. The cluster pardiso solver may also be used as a stand-alone linear solver, providing an industrial strength direct solver for modestly sized problems. This solver has been shown to be quite scalable in both the factor and solve phases of the computation. In addition, it may use less memory than other direct solvers.

2.2.4 Integration with STK balance



The Sierra-ToolKit (STK) team has been working with SD team in STK adoption. In addition, we have observed that significant performance and robustness capabilities may be obtained through a better decompositon of the finite element model. We have worked with the STK team as they developed the STK-balance capability, which improves perfomance and robustness over previous decomposition methods (such as yada). The stk_balance tool runs in parallel on all our production machines. For further information, please contact the STK team directly.

2.2.5 Exploration of Intel/KNL Threaded Solvers

On the newer "Trinity" platform both Intel/Haswell and Intel/Phi chipsets are used. The Intel/Phi, or Knights-Landing (KNL) chipset is significantly different from previous chipsets. Many more compute hardware threads are available, and effective use of this capability requires thread aware software. Figure 1 illustrates the performance of our solvers on this platform. A tradeoff between the number of MPI ranks and the number of threads indicates clear memory and performance gains may be obtained through application of hardware threads.

2.2.6 Coupling to Fluids Analysis through Lighthill Tensor

Customer: Goodyear

Status: Incomplete

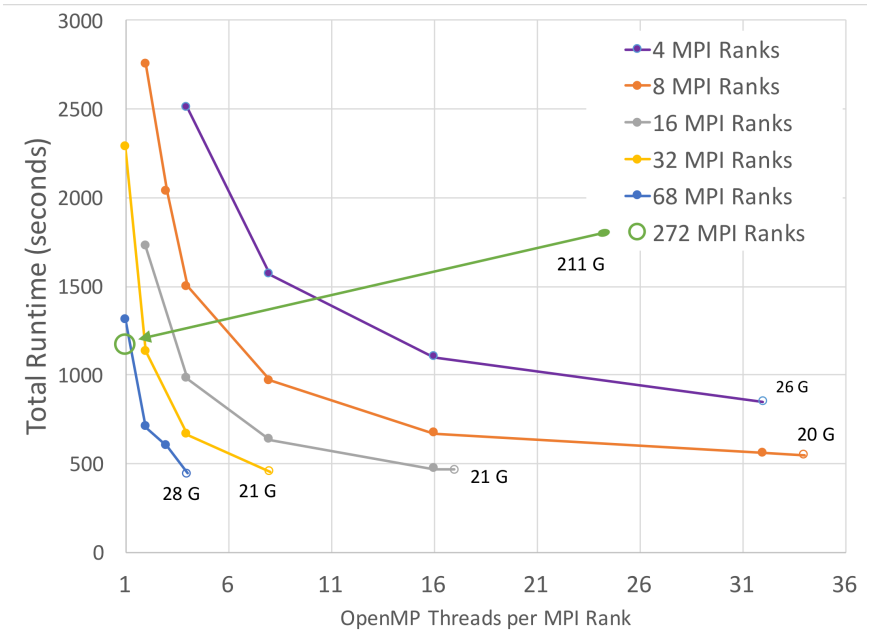


Figure 1: Scaling of Threads on KNL chipset

ETA: Release 4.46

2.2.7 Output of Virtual Nodes and Elements

Virtual nodes and elements are now output as part of the solution. These are entities that were not present in the original topology, but are created as part of the solution process. One example includes infinite elements which are specified on a boundary. Visualization of these elements can help to identify the correctness of the topology. See Figure 2 for an example output.

2.2.8 Modal Force Loading

Purpose: Allow analysts to directly load individual modes for the modaltransient and qmodaltransient solutions.

Customer: ASC. PLATR deliverable.

Status: Complete

User Interface: The user interface is provided as an example in Figure 3. Further details are available in the user's manual.

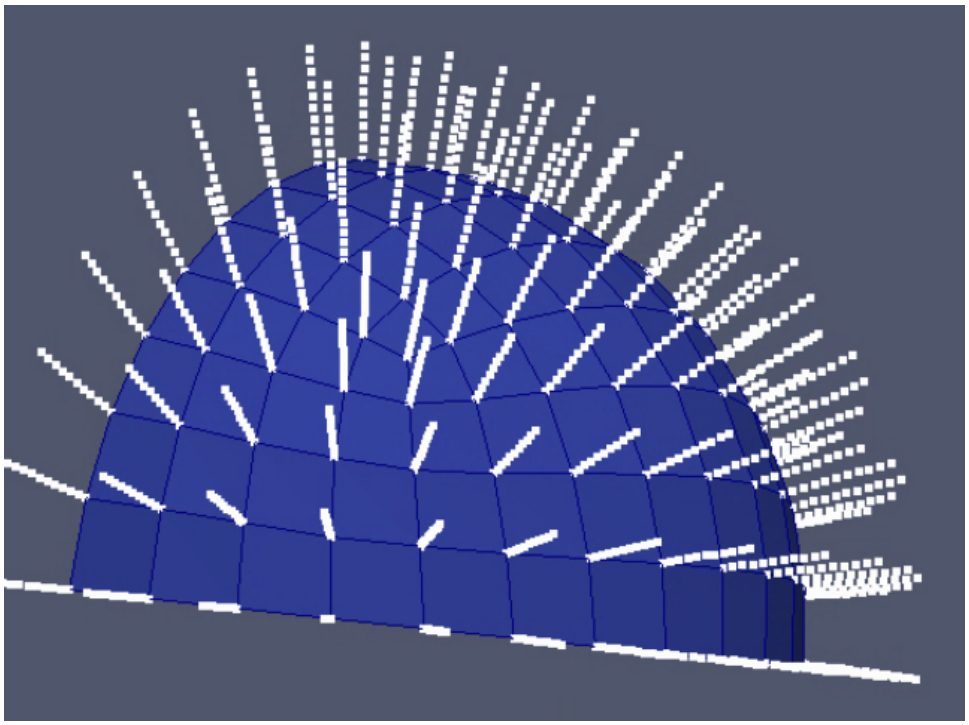


Figure 2: Example Output of Infinite Elements. The acoustic mesh, in blue, is extended using infinite elements, shown as white markers.

```
LOADS
   body
   modalforce
   function 36
END

FUNCTION 36
   type table
     tablename 28
END

TABLE 28
   dimension 2
   size 100 9
   delta 5e-6 1
   origin 5e-6 0
   datafile=Qforce.txt
END
```

Figure 3: Example Modal Force Loading Input

2.2.9 STK Adoption

Use STK as the in-memory database for SD. Gains in compatibility with other Sierra Apps and potential to use STK provided tools (including rebalance).

Customer: ASC

Status: Complete

User Interface: There are no significant changes to the user interface, however see the section on backwards compatibility changes. Overall performance with respect to both memory and solution time is unchanged.

2.2.10 Cavitation

Purpose:Implement a CASE-like non-linear cavitating acoustic element. This supports NAVY analysis of undersea acoustics with cavitation.

Status: Incomplete

ETA: 4.48

2.3 New Capabilities for Solid Mechanics

A new contact friction model `INACTIVE FRICTION MODEL` is now available. This friction model produces no force and can be used to selectively turn off contact for certain interactions or during certain time periods.

A new appendix was added listing other pre and post processing scripts supported by the development team.

The user output coordinate system transformation operation now supports cylindrical coordinate systems. Additionally the documentation of this option has been greatly expanded.

Artificial strains can now access general analytic functions (functions making use of expression variables.) This can be used to define much more general time and space fields for artificial strain.

A new library subroutine was added `aupst_preload_solver`. This subroutine can be used to do a basic predictor corrector iterations in time for unknown preload values. As an example determining the artificial strain required in various bolts to obtain a target clamping force.

A `T AXIS` provided to a beam block now also effects the orientation of the lofted beam contact prism.

The nodal variable `contact_energy` is now available recording work done by contact on a node by node basis.

A new `ABSOLUTE SEARCH TOLERANCE` is available in procedural transfers that allows the user to control the sizes of the search bounding boxes.

The `L2_PROJECTION` transfer is now implemented for use with the `STRONGLY_OBJECTIVE` form of the `SELECTIVE_DEVIATORIC` and `FULLY_INTEGRATED` hex elements. This capability significantly improves remesh/remap use-cases.

A new nonlinear hourglass formulation (`HOURGLASS FORMULATION = HYPERELASTIC`) is available for uniform-gradient hexahedral elements using strongly objective strain incrementation. This hourglass formulation is especially useful when elements are undergoing severe deformation.

The C0 triangular shell element `FORMULATION = C0_TRI_SHELL` is now available for use in an implicit simulation.

Superelements can now be used in a co-rotational form, making them rigid body invariant. Superelements can now be used with a consistent mass matrix. See the capabilities in development manual for details.

It is no longer required to specify `COMPUTE CONTACT VARIABLES = ON` in the input file. Now, the code will determine if a contact variables is being requested for output and compute that variable by default at every output time (unless it is an accumulated contact variable).

Block information involving mass scaling has been added to the log file.

Mass and stiffness damping are now available for use in implicit simulations.

Various improvements to contact have been made.

A bug was fixed in the Tied MPC's so they can now be applied component-by-component.

A bug was fixed in the periodic boundary conditions so they can now be applied component-by-component.

Energy reporting has been improved.

Transfers between an Aria and Sierra/SM coupled simulation have been significantly improved.

Element fields `iplocation`, the integration point locations of the element, and `centroid`, the mass centroid of an element are now available for output with all element types and material models.

Restart write may now be requested on wall clock time.

2.4 New Capabilities for Thermal/Multiphysics

2.4.1 OMD: Multiple Average Pressures

The extract average pressure ideal gas law for density now calculates the average pressure over connected regions and this allows multiple average pressures to be defined for unconnected regions.

2.4.2 Pressurization

Added the option to use a segregated ODE solve for pressurization node coupling.

Allow for use of bulk elements with computed volumes in the pressurization model.

2.4.3 Level Set Burn Front

Added the ability to have multiple burn initiation points on a single block.

2.4.4 Species Naming

Added a check for potentially problematic species names. This includes names like `A`, `B`, `C`, and `GAS` which can conflict with phase names and expressions in unexpected ways (and would generate extremely cryptic error messages). The use of these names will now result in a coherent error messages.

2.4.5 Nonlinear Solution Strategy

Added new line command `Nonlinear Residual Minimum Convergence Rate = 0.9` to enable failing a time step if the residual stalls part way through the Newton solve.

2.4.6 Species induced swelling

Added anisotropic concentration-induced swelling expression. Both the isotropic and new anisotropic species swelling models utilze a `species_expansion_coeff` material property rather than expecting the beta coefficent as an argument.

2.4.7 Wetting edge conditions

Added support for wetting edge conditions which assigns a traction force proportional to the surface tension in the direction of a specified contact angle `theta_s` at the intersection between two sidesets (point in 2D, edge in 3D). `theta_s` is the static angle made between these two sidesets.

2.4.8 Enclosure Radiation

A new viewfactor matrix file format, PNETCDF, has been implemented. This format is machine and parallel decomposition independent. It writes a single viewfactor file from any number of processors that can be subsequently read by any number of processors. We recommend switching to the new format for improved usability, and the existing ASCII and BINARY file formats are being deprecated. We plan to remove them in release 4.46

Radiosity solve MPI scaling performance has been improved for large processor counts. However, at present there is a significant increase in memory usage to enable the improved scaling. Until that implementation limitation can be addressed a line command has been added to allow users who are memory-constrained to disable the change by adding `DISABLE PARALLEL REDISTRIBUTION` to the enclosure definition block.

2.4.9 Mean Beam Length Radiation

Relax restriction of specifying a single surface for the entire enclosure.

2.4.10 Advective Bar

Add optional specification of offset when beginning of entrance does not align with a bar node.

2.4.11 Correlation Library

Enable use of free convection correlation coefficients independent of Reynolds number.

Add diagnostic for missing correlation input parameters.

Allow for use of Gnielinski film gradient correction with correlations 23 and 25.

Allow for use of Gnielinski entrance length correction with correlations 23 and 25.

2.4.12 Embedded Submodel

Prevent use of the model when no temperature is defined on the element block.

Add support for multiple submodels.

2.4.13 Laser Source

Require specification of laser depth direction for Activation Hemisphere source.

For activation sources the required variable `activate` is now a real scalar as opposed to an integer. This allows the variable to more readily be used in an interpolate transfer.

Add default registration of `activate` variable for activation sources which matches the User Global Variable definition. This allows the source to be used without defining a User Global Variable. For restarts the User Global Variable must be used with the `read` option.

2.4.14 Coordinate System

Enable use of coordinate systems with named element blocks.

2.4.15 Boundary Conditions

Enabled use of input file nodeset variable to apply temperature Dirichlet BCs.

2.4.16 Data Probes

Remove cdfem and adaptivity restriction on probes.

Enable use of probes with `Nodal_id` with mesh motion. `Nodal_Location` probes cannot be used with mesh motion.

Add support of vector Field probes.

2.4.17 Transfer

The ability to define element variables on the `Input_Output` region was added. This allows the `Input_Output` region to be used in mapping to grids with overlapping element blocks.

2.4.18 Subroutines

Add support of Fortan subroutines for density, specific heat and scalar thermal conductivity.

2.5 New Capabilities for Coupled Codes

Substantial improvements have been made to transfer of multi-integration point elements between Sierra/SM and Sierra/TF (arpeggio) previously integration point locations could have been scrambled during these transfers.

Super Elements in Sierra/SM now support Craig-Bampton Reduction (CBR) super elements (e.g. as generated by Sierra/SD) undergoing large rotations and translations. A co-rotational formulation allows large rigid body motion with linear distortions, and a consistent mass matrix properly captures dynamic effects (i.e. CBR internal modes).

Saw recognizes the Zapotec input file and syntax and provides content assist.

Zapotec performance has been improved for problems involving significant element death.

There is no longer a limit on the number of processors a Zapotec simulation can be run on.

Zapotec documentation has been updated for the latest version of Zapotec.

2.6 New Capabilities for Verification and Validation Tools

Verification tests of the Zapotec capability were added to nightly test suites, increasing the quality assessment and reliability of the Zapotec product.

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3 Changed Capabilities

3.1 Changes to the User Interface for Structural Dynamics

The following changes affect backwards compatibility of the Sierra/SD product.

3.1.1 Sidesets can no longer be internal to a block

For consistency with other Sierra products, sidesets may only be defined on block boundaries or edges. Previously, defined models with sidesets interior to a block are no longer supported.

Figure 4 illustrates this concept. In this case, a legacy model with a sampling sideset embedded in the lower structure is no longer supported. The model must be split into two blocks as shown.

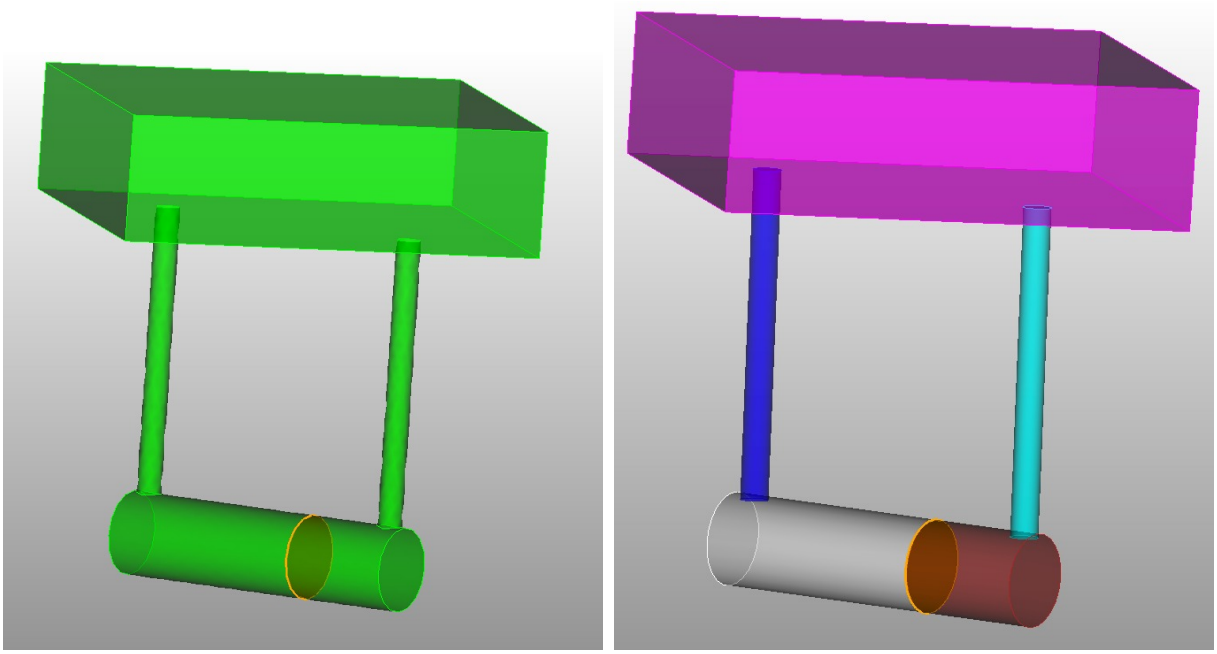

Figure 4: Embedded Block Sidesets. Legacy and Current

3.1.2 Automatically Generated Sideset/Nodeset Fields

The capability for writing data to a sideset is evolving. Often analysts would like data on the nodes of a sideset. While sidesets may have a data field associated each face, and sideset attributes may be associated with the nodes of a surface, there is no standard for writing data to the nodes of a sideset. To enable this, a nodeset may be generated from the nodes of a sideset, and data is written to that nodeset.

3.1.3 "Flushing" of exodus file output

One important performance issue for parallel computing is output of the data to a file. By default, the exodus libraries have used the system buffering capability to reduce the cost of this output. That has the side effect of leaving the data in an unknown state if the analysis aborts buffer the buffers are written (or flushed). As a consequence, the analyst was provided the ability to control the flushing of these buffers with the "flush" parameter. With the STK adoption, the ability to control this buffer has been automated, and the access to this parameter is deprecated.

3.1.4 Parallel output of History and Frequency Files

History and Frequency files provide the ability to output a portion of the model. These are important if analysts wish to sample the response at a few locations over time. Previously, Sierra/SD gathered this data an wrote a single history or frequency file. With completion of the STK adoption, this capability is no longer supported. However, history and frequency files are written in parallel form. A single history file may be generated by use of the "epu" tool. The following example joins the 17 history files through an analysis into a single history file.

```
epu -auto example-out.h.17.00
```

3.1.5 Macroblocks

Macroblocks are no longer supported.

3.1.6 ConMass on Beams

Support for concentrated masses on two noded elements is no longer supported. Please use sphere elements for these masses.

3.1.7 CF FETI

The CF FETI solver is no longer supported.

3.2 Changes to the User Interface for Solid Mechanics

The `MIDPOINT_INCREMENT` strain incrementation option for the selective deviatoric element is deprecated and no longer recognized. The selective deviatoric element will now always use the strongly objective strain incrementation which is more accurate.

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4 Issues Addressed

4.1 Issues Addressed for Structural Dynamics

Table 1 lists issues addressed during this release. Table 2 lists issues still on the backlog.

A major issue was found in the computation of the random vibration von Mises stress. The square of the stress is computed as,

$$\sigma^2 = \sum_{i,j} \sigma_i A_{ij} \sigma_j$$

where σ_i is the natural stress and A is a constant, 6x6 matrix with values,

$$A = \begin{bmatrix} 1 & -\frac{1}{2} & -\frac{1}{2} & 0 & 0 & 0 \\ -\frac{1}{2} & 1 & -\frac{1}{2} & 0 & 0 & 0 \\ -\frac{1}{2} & -\frac{1}{2} & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & \mathbf{3} & 0 & 0 \\ 0 & 0 & 0 & 0 & \mathbf{3} & 0 \\ 0 & 0 & 0 & 0 & 0 & \mathbf{3} \end{bmatrix}$$

Unfortunately, the diagonal terms that should have been coded as "3" were coded as "1". This affects the random vibration estimate for solid elements in shear. Values for shell elements are unaffected, and computation of the acceleration PSD is also unaffected.

4.2 Issues Addressed for Thermal/Multiphysics

4.2.1 Advective Bar

Bug fix for energy equation advection term specific heat coefficient with gases.

4.2.2 Correlation Library

Bug fix for incorrect scaling in Petukov correlation.

Bug fix for incorrect computation of entrance length when using Gnielinski correlations.

4.2.3 Contact

Bug fix for code hanging when no contact enforcement model specified.

id	summary
15650	How is force load distributed to a node set?
15573	constant pressure bc in transient produces incorrect displacements
15596	unexpected acceleration amplification for modal transient
15670	using readnodalset function errors out with 'sideset not found'
15263	direct transient solve iteration issues
15692	invalid quadrature type error from formerly ok energy/thermal field data
15795	yada run in SAW hits time limit
15807	What causes dip in stress plotted from modalfrf analysis?
15057	new material modulus causes old model to now have memory error
15850	Request for input example for orthotropic material
15244	Model seg faults after Cubit mesh export
15908	What DOFs do hexshells have?
15756	Can modalranvib be run from previous eigen solution?
14761	"""no states"" in restart input database for coupled dysmas run"
15915	negative eigen values?
15903	unexpected results from tied contact between solids and shells
15926	NMOUNT is case sensitive
15478	Linear transient case not converging in nonlinear solver?
14841	memusage file is blank
15055	Out-of-memory errors when trying to create superelement
13784	direct transient solution has growing equilibrium error
13339	model runs fine with 4.37.2 but segfaults with 4.37.3 (gap removal issue)
15808	ceigen solve failed
15948	projection_eigen fails if time_step not specified
15900	Craig-Bampton model is grounding
16235	ModalFv not output for sideset-variable loads
16037	gdsw non-convergence in B61 model
16227	What causes "ARPACK: max number of restarts taken" error in 9M-node model?
16324	Can't run yada on red sky
16289	frf eignenvalues reported as modal frequencies?
16096	How is eigenvalue sensitivity info computed?
16190	orthotropic_prop Hex block has no von Mises stress output
16370	How to write output to non-geometry directory?
16290	DirectFRF-MaterialID data file parsing issue
16407	Can results be written out by model parts?
16423	SD-NEMO coupled runs produce no output variables
16342	Error message useless for debugging input
16354	some tied data no longer recognized in post-4.43.5 versions
16124	inverse directfrf to determine material properties not working
15923	Non-zero rotational rigid body modes with tied surfaces
16482	How are von Mises moments calculated in random vibration?
16498	inverse directfrf to determine material properties still not working
16539	How is the 3D orthotropic solid element orientation defined?
16554	eigen results output includes new diagnostics slowing performance
16516	How do I compute shock response spectra?
16529	Request for 3D solid composite example problem
16553	Is this warning about eigen restarts necessary?
16547	Can tied-data fields be named?
16593	Is there a way to have a periodic bc for eigen analysis?
16519	How do superelements affect eigenmodes?

Table 1: Sierra/SD Tickets closed this Release

id	summary	user
14437	conversion of EDEP to thermal strain is not correctly handling the node map	Manktelow
14843	sensitivity block kills simulation with attune output on pecos	Jew
14028	Does TSR load option allow temperature-dependent material properties?	Holzmann
15716	issues with coupled st-acs eigen and modal frf	Schultz
15947	How can CB-reduction be applied to concentric cylinders?	Kuether
16187	What options are available with CBR?	Manktelow
16257	SM-preloaded model with MPCs has issues in SD	Coffin
16375	Can nodal pressure be applied in transient or nodal transient?	Mesh
16430	direct transient OUO model inconsistent proc results with Feti	Robbins
16571	SM-to-SD eigen preloaded analysis segfaults immediately	Manktelow
16499	How can I restart in SD an SM-prestressed structure in an acoustic fluid?	Reynolds
16645	How can I apply spatially-varying displacement BCs without creating nodesets?	Coffin
16649	coupled SD-NEMO history output doesn't get written at specified intervals	Gilbert
16670	fatal errors with RBE3s connected to spring elements	Shields
16653	ignore-gap-inversion set to true causes fatal stkMeshInterface fatal error	

Table 2: Sierra/SD outstanding Issues

4.2.4 Embedded Submodel

Bug fix for model initialization on processors with no embeded element constraints.

4.2.5 Material Properties

Bug fix for activation thermal conductivity not using background conductivity after activation.

Bug fix for sensitivity error in Linear Anisotropic Reference Strain.

4.2.6 Subroutines

Bug fix for case of Fortran element subroutine with no real or integer data.

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5 Known Issues

5.1 Incompatibility Issues for Solid Mechanics

The `MIDPOINT_INCREMENT` strain incrementation option is no longer recognized by the selective deviatoric element. The selective deviatoric element will now always use the strongly objective strain incrementation which is more accurate.

5.2 Incompatibility Issues for Thermal/Multiphysics

5.2.1 Pressurization

Using `Pressure = Pressurization_Model` inside a ChemEq block could cause intermittent errors. This syntax is no longer allowed, and an error message telling you the correct sytnax was added.

5.2.2 Correlation Library

Mark command line `DISABLE GNIELINISKI FILM GRADIENT CORRECTION` for deprecation.

Mark command line `GNIELINISKI FILM GRADIENT EXPONENT` for deprecation.

Mark command line `APPLY GNIELINISKI ENTRANCE LENGTH CORRECTION` for deprecation.

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