Preparation of Codes for Trinity

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Trinity

- Cray XC40
- Total of about 19000 nodes
  - About half are Intel Haswell with 2 processors per node and 16 cores per processor running at 2.3 GHz and 128 GB memory per node
  - About half are 60+ core Intel Knights Landing processors
- About 42 PetaFlops peak

Intel and Cray Center of Excellence

- Focus on SIERRA applications
  - SIERRA/Solid Mechanics (SM)
  - SIERRA/Aerodynamics
  - SIERRA/Structural Dynamics (SD)
- SIERRA is a large C++ framework
  - provides framework for several codes
  - Includes several Third Party Libraries
  - Contains common C++ classes and methods
  - Common infrastructure for parallel codes

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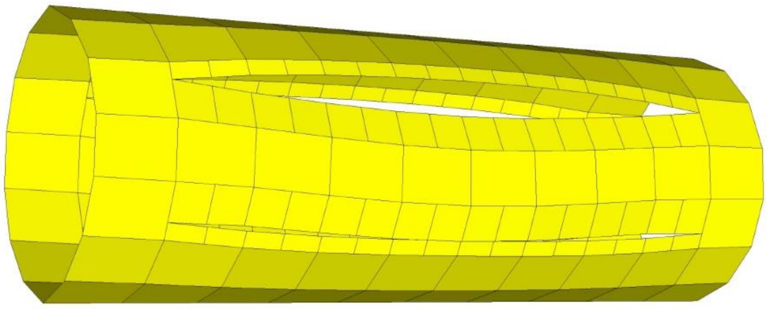
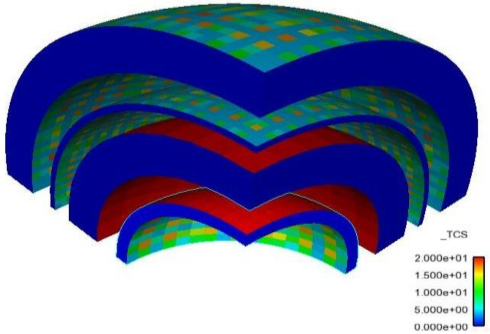
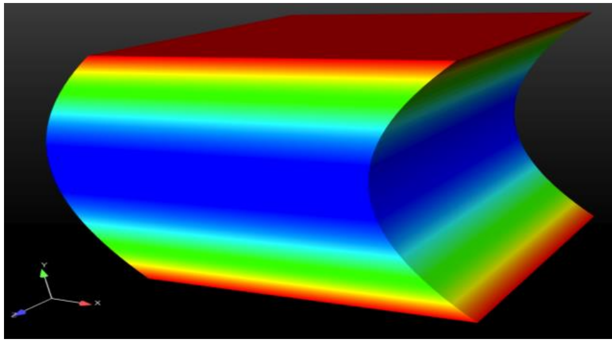
SIERRA/SM (Solid Mechanics)





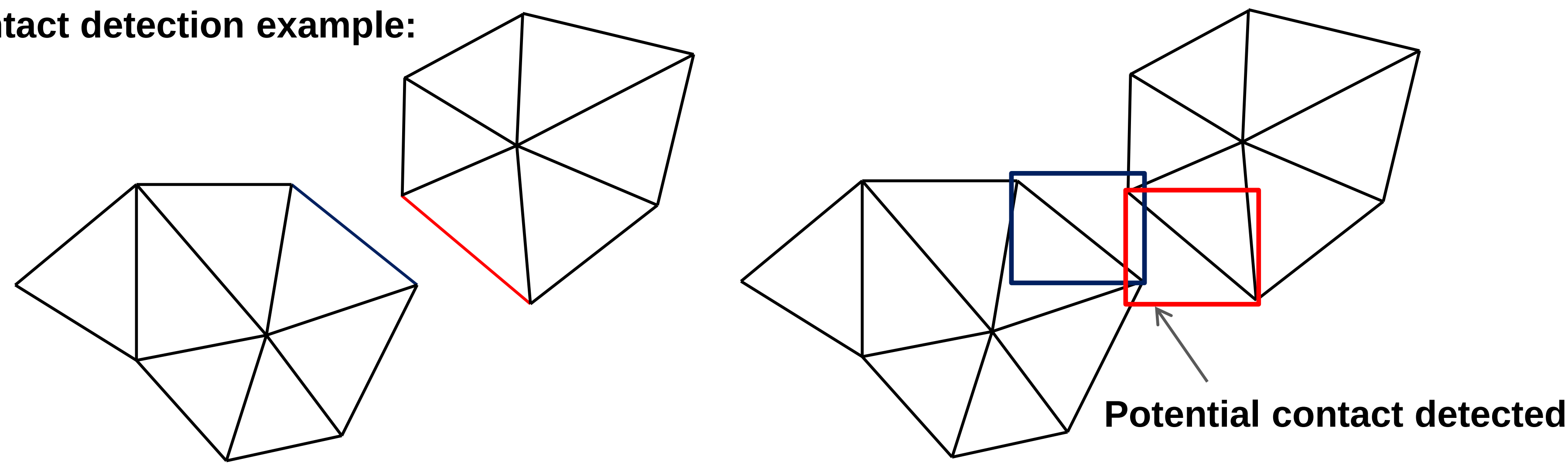


- **A general purpose massively parallel nonlinear solid mechanics finite element code for explicit transient dynamics, implicit transient dynamics and quasi-statics analysis.**
- **Built upon extensive material, element, contact and solver libraries for analyzing challenging nonlinear mechanics problems for normal, abnormal, and hostile environments.**
- **Similar to LSDyna or Abaqus commercial software systems.**

SIERRA/SM Bottlenecks

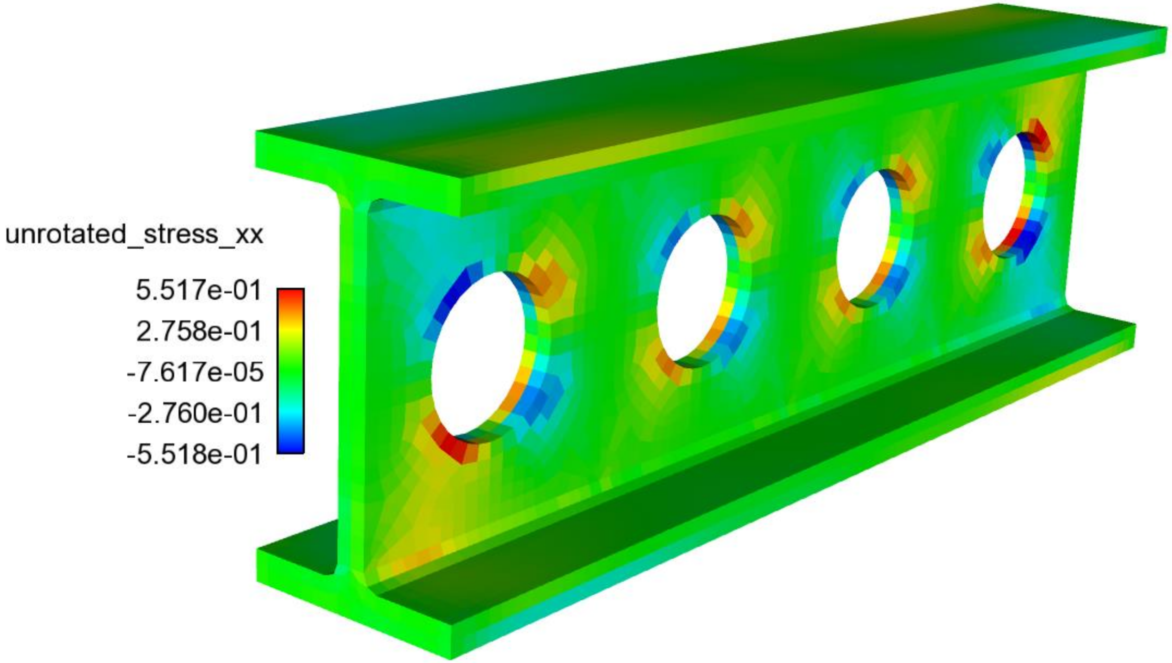
Application:	**Explicit dynamics with contact**	**Implicit with FETI pre-conditioner**	**Explicit dynamics w/o contact**
Hot spot:	Parallel **proximity search** and enforcing contact constraints	Serial **sparse direct solve**: matrix factorization and forward/backward solves	Assembling nonlinear **element residuals** and computing material response

Contact detection example:



I-Beam Problem (Quasi-Static)

-provided by Joe Bishop



<u>Mesh</u>:

- 3 Different mesh refinements: 8,576, 68,608, and 548,864 elements
- Mean Quadrature and SD hex elements

<u>Unique Features:</u>

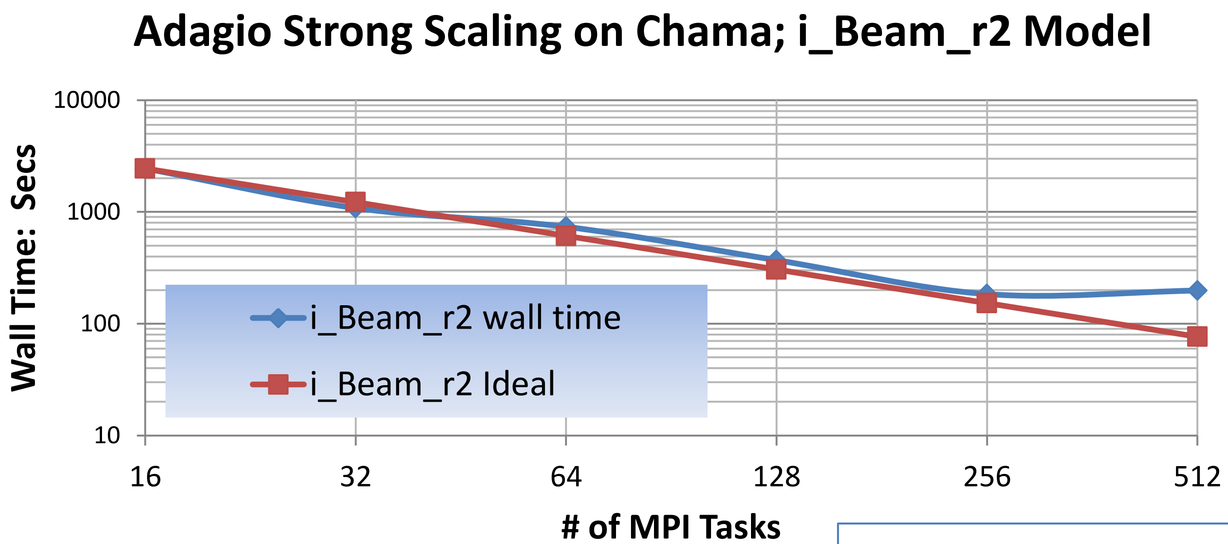
- Crystal Plasticity material model
- Problem does not converge when mesh is refined

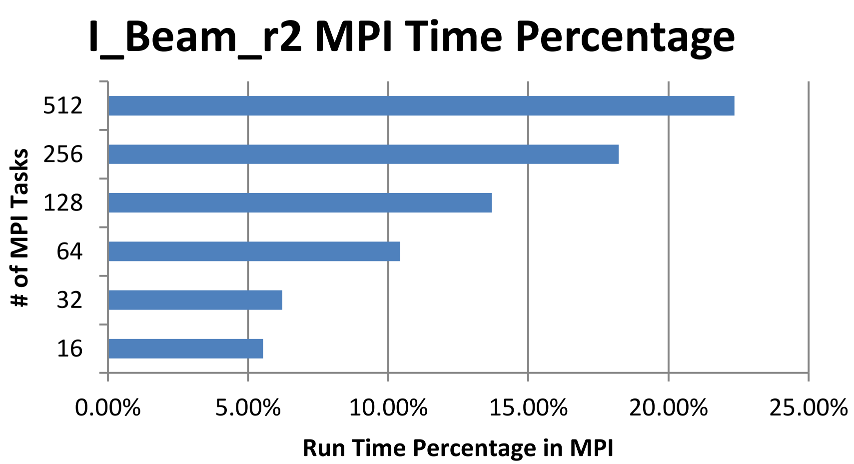
Preconditioning with linear solver

- The preconditioning step dominates the cost (>90%).
- Occurs one per time step
- Accomplished with a Jacobian matrix which requires an iterative linear solver algorithm to provide M^{-1}
- Iterative linear solve done with the FETI (Finite Element Tearing & Interconnecting) domain decomposition algorithm
- FETI requires a local solve, coarse solve, and a preconditioner solve (similar to most domain decomposition algorithms)
- Extensively uses sparse direct solvers

QS Model Strong Scaling on Chama and MPI overhead with scale

(nodes= 619,581, elements=548,864)





@--- Aggregate Time (top twenty, descending, milliseconds) ----------------

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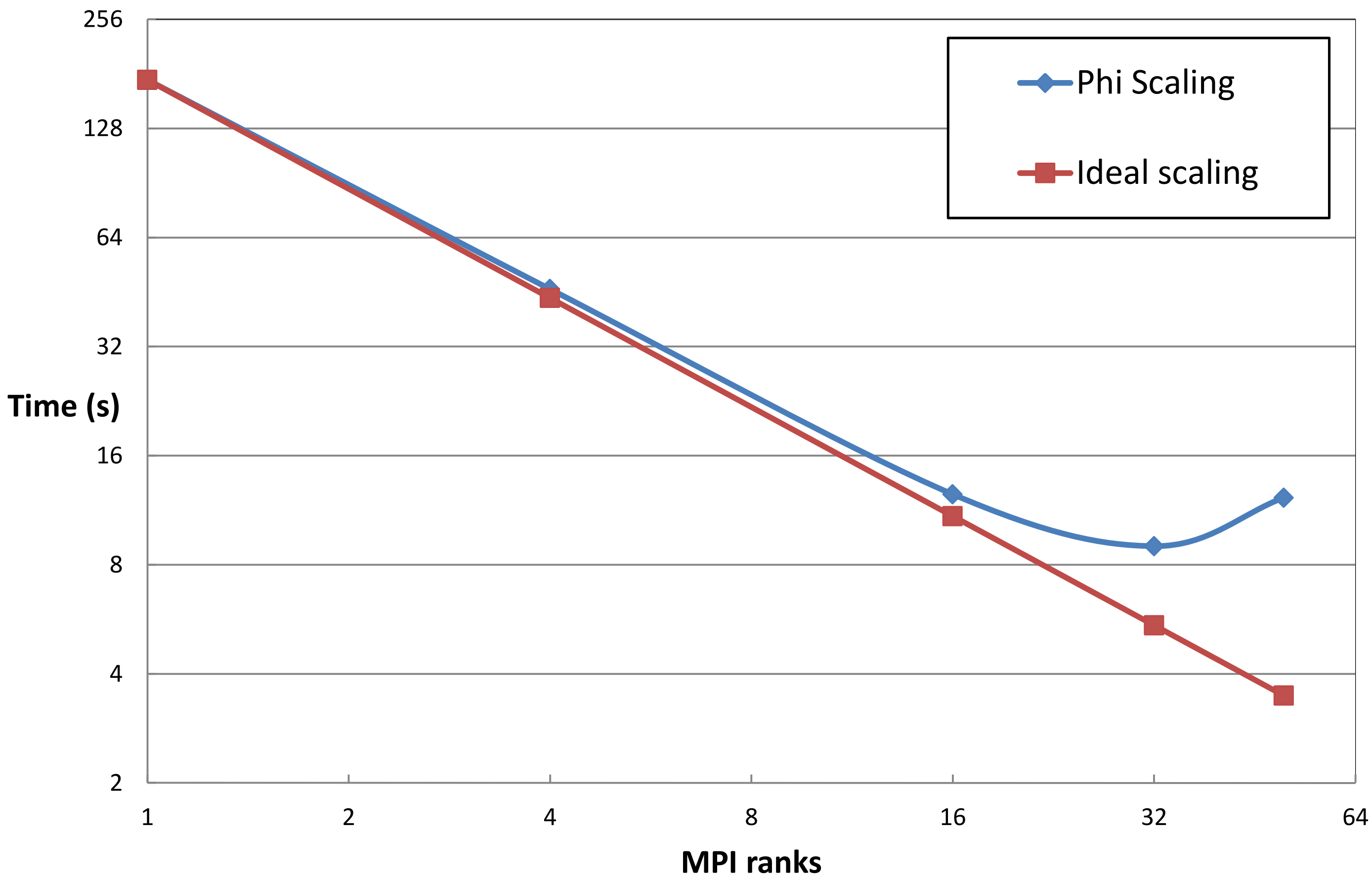
Call	Site	Time	App%	MPI%	COV
Allreduce	133	4.05e+06	3.90	17.46	0.09
Allreduce	168	4.01e+06	3.87	17.31	0.08
Barrier	53	3.4e+06	3.28	14.65	0.22
Allreduce	189	1.8e+06	1.74	7.78	0.00
Bcast	10	1.27e+06	1.22	5.48	0.01
Allreduce	167	1.19e+06	1.15	5.13	0.05
Bcast	98	5.68e+05	0.55	2.45	0.04

mpiP Top 5 MPI functions and call sites; 512 MPI tasks

Early KNC results

- Adagio compiles and runs on our test-bed KNC
- Scaling has proven difficult (with MPI and OpenMP)

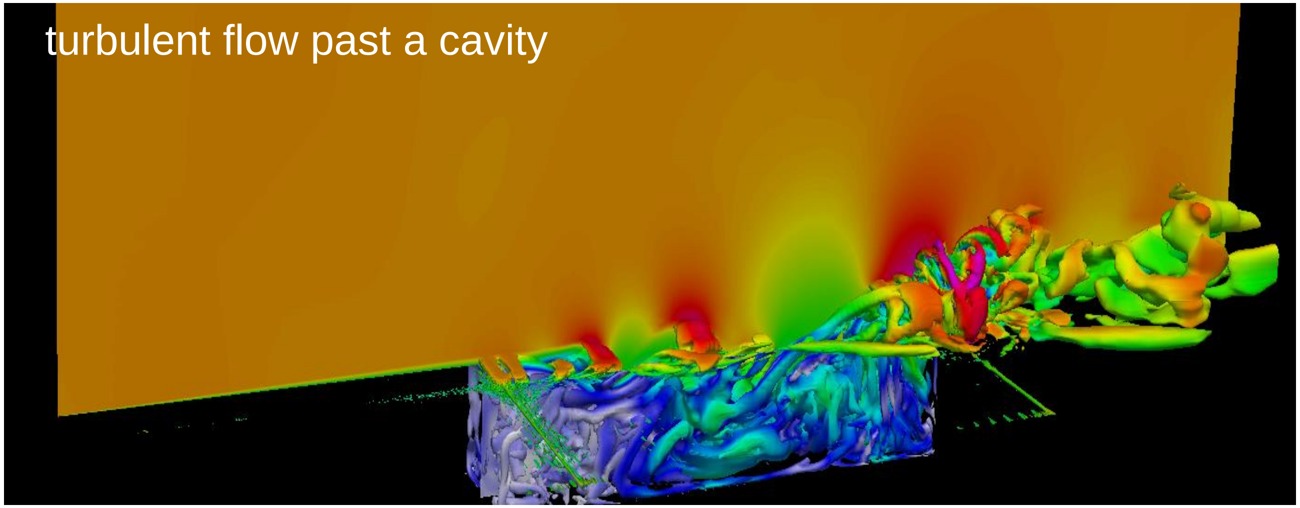


Adagio Performance Summary

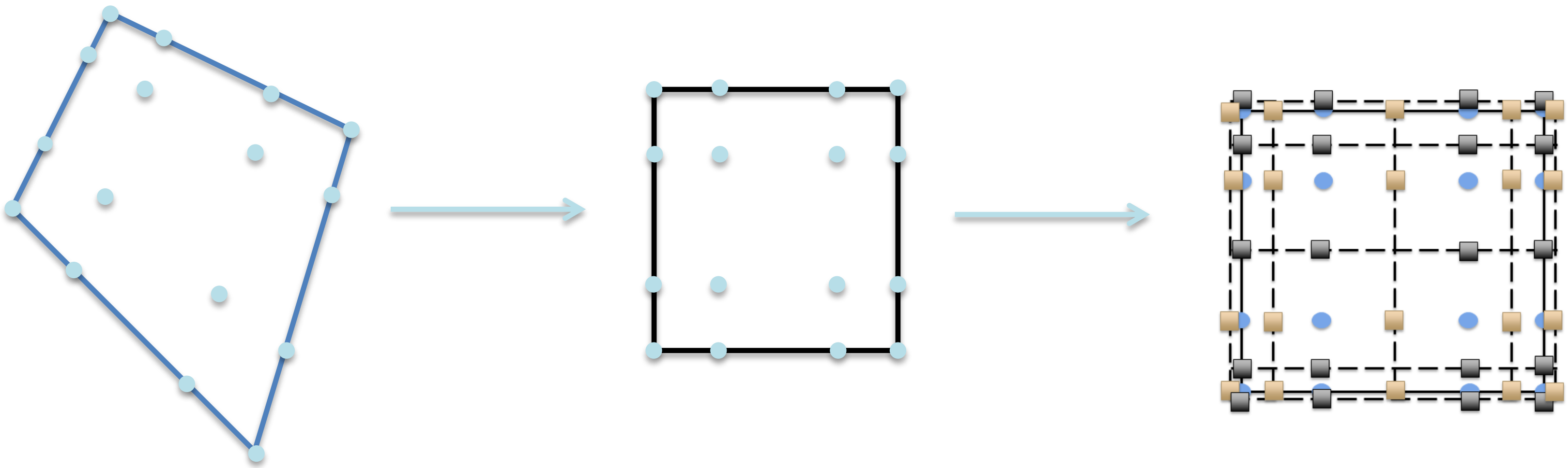
- Explicit dynamics dominated by MPI globals at scale
  – Try asynchronous collectives?
  – May benefit from optimization for small messages
- Quasi-statics
  – Need to investigate improvements after use of threading and vectorization with Pardiso / MKL
  – Leverage math library threading/vectorization

Summary of Sierra/Aero

- Unstructured meshes
- One and two equation turbulence models
- LES and Hybrid RANS
- Uses either FETI or Trilinos for sparse matrix operations and solvers.
- Assembly is substantial portion of the computational cost.



High-Order Unstructured Collocation



Unstructured Element | Standard Element | Flux-based Formulation

- Still under development
- Provably Entropy(Nonlinear) Stable
- Discontinouos formulation
- High computational intensity
- Accurate on unstructured topologies
- Trilinos Solvers for implicit solves

Trilinos Solver

- Uses Tpetra, Ifpack2 and Belos libraries
- For matrix assembly, preconditioning and solvers respectively.
- Symmetric Gauss-Seidel for preconditioner
- GMRES for solver

Aero Profile w/comments

|| 28.4% | 35715.2 | 545.8 | 1.5% |tftk::linsys::TpetraBaseBlockLinearSystem::sumInto

This function fills the actual linear system with values from the application code.

|| 19.9% | 25054.0 | 391.0 | 1.5% |Tpetra::Experimental::BlockCrsMatrix<double, int, long, KokkosClassic::SerialNode>::localGaussSeidel

This is the main work routine of the preconditioner (local on each process) that computes a smoothed solution for symmetric gauss-seidel. It is called twice for each linear iteration.

|| 14.5% | 18261.9 | 4939.1 | 21.5% |sierra::conchas::ElementFlux::operator()

This is the main computation of the residual and sensitivities for the linear system.

|| 13.7% | 17243.7 | 232.3 | 1.3% |Tpetra::Experimental::BlockCrsMatrix<double, int, long, KokkosClassic::SerialNode>::localApplyBlockNoTrans

This is a sparse matrix-vector multiply.

|| 2.9% | 3631.9 | 32.1 | 0.9% |tftk::linsys::TpetraBaseBlockLinearSystem::zeroSystem

This zeros the linear system.

|| 2.7% | 3427.8 | 39.2 | 1.1% |sierra::conchas::TpetraLinearSystem::scaleBlockMatrix

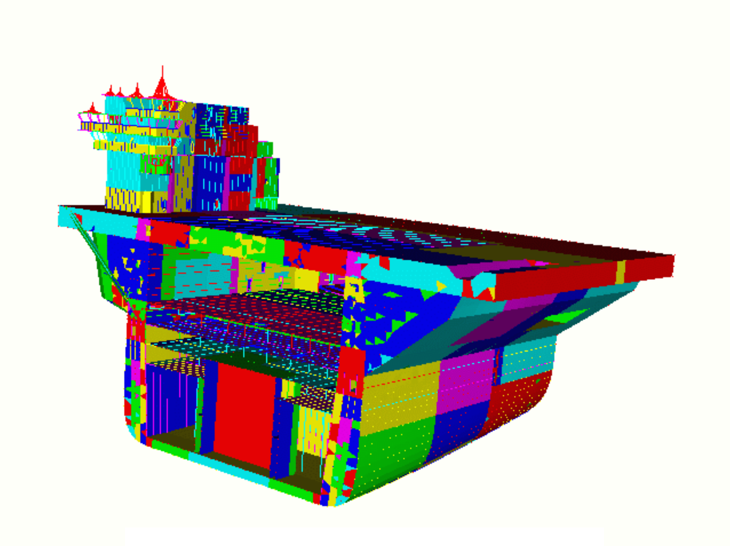
This modifies the linear system.

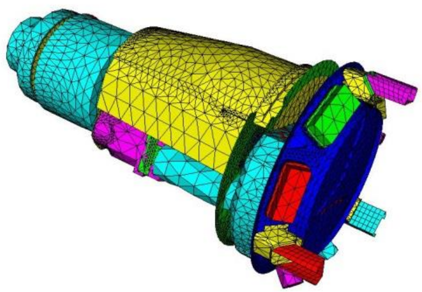
|| 1.6% | 2050.4 | 624.6 | 23.5% |sierra::conchas::FluxPenalty::operator()

This is the coupling terms for computing the residual and sensitivities for the linear system.

Domain Areas

- General Structural Dynamics, Finite Elements
  - Vibrations, normal modes, implicitly integrated transient dynamics, frequency response analysis
  - Shells, Solids, Beams, Point Masses
  - Complicated Large Structures
  - Typically many constraint equations
- Acoustics and Structural Acoustics
  - Even larger systems
  - More constraints
  - Infinite Elements (nonsymmetric)
- Optimization, UQ and Inverse Methods
  - Adjoint methods
  - Material and Parameter inversion
  - Verification and Validation





Sierra/SD Algorithms

- Domain Decomposition Linear Solvers
  - Sparse linear solver dependence
    - Threaded sparse solvers could play important future role
  - Alternative algorithms for new architectures
    - Flexibility in choice of subdomains, over-decomposition, …
- Eigen Solvers
  - Arpack current workhorse
    - Sparsekit sparse matrix utility package dependence
  - Trilinos/Anasazi
    - Could move in this direction going forward
  - Linear solver dependence
- Orthogonalization
  - Important to both linear and eigen solvers

Linear Solver Role

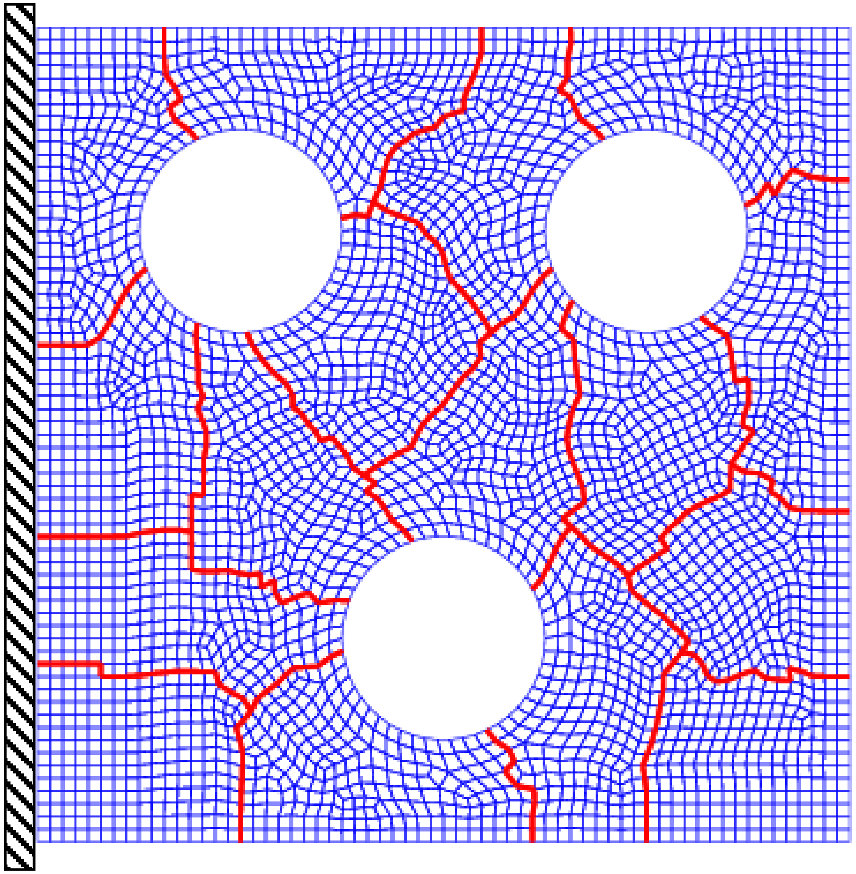
Selected Sierra-SD performance test results (chama)

Name	Analysis Type	Solve time/ Total time	Solve phase/ Solve time
mc2912	modal	0.96	0.90
nfn9	modal	0.98	0.97
endevco	transient	0.85	0.98
largerv	static	0.71	0.52

- Transient analysis (one solve for each time step)
- Modal analysis (multiple solves for each eigenmode)
- Each “solve” may take 10s to 100s of iterations

A lot of time in solve phase (initialization time often much smaller), final two columns can be even closer to 1 in practice

Domain Decomposition 101



- Partition into smaller subdomains
- Solve local (subdomain) problems
- Solve global (coarse) problem
- Combine local & global solutions
- Multilevel extensions
- Inexact solves
- Rich theory

B. Smith, P. Bjorstad, and W. Gropp, *Domain Decomposition: Parallel Multilevel Methods for Elliptic Partial Differential Equations*, Cambridge University Press, 1996.

A. Toselli and O. Widlund, *Domain Decomposition Methods: Algorithms and Theory*, Springer, 2005.

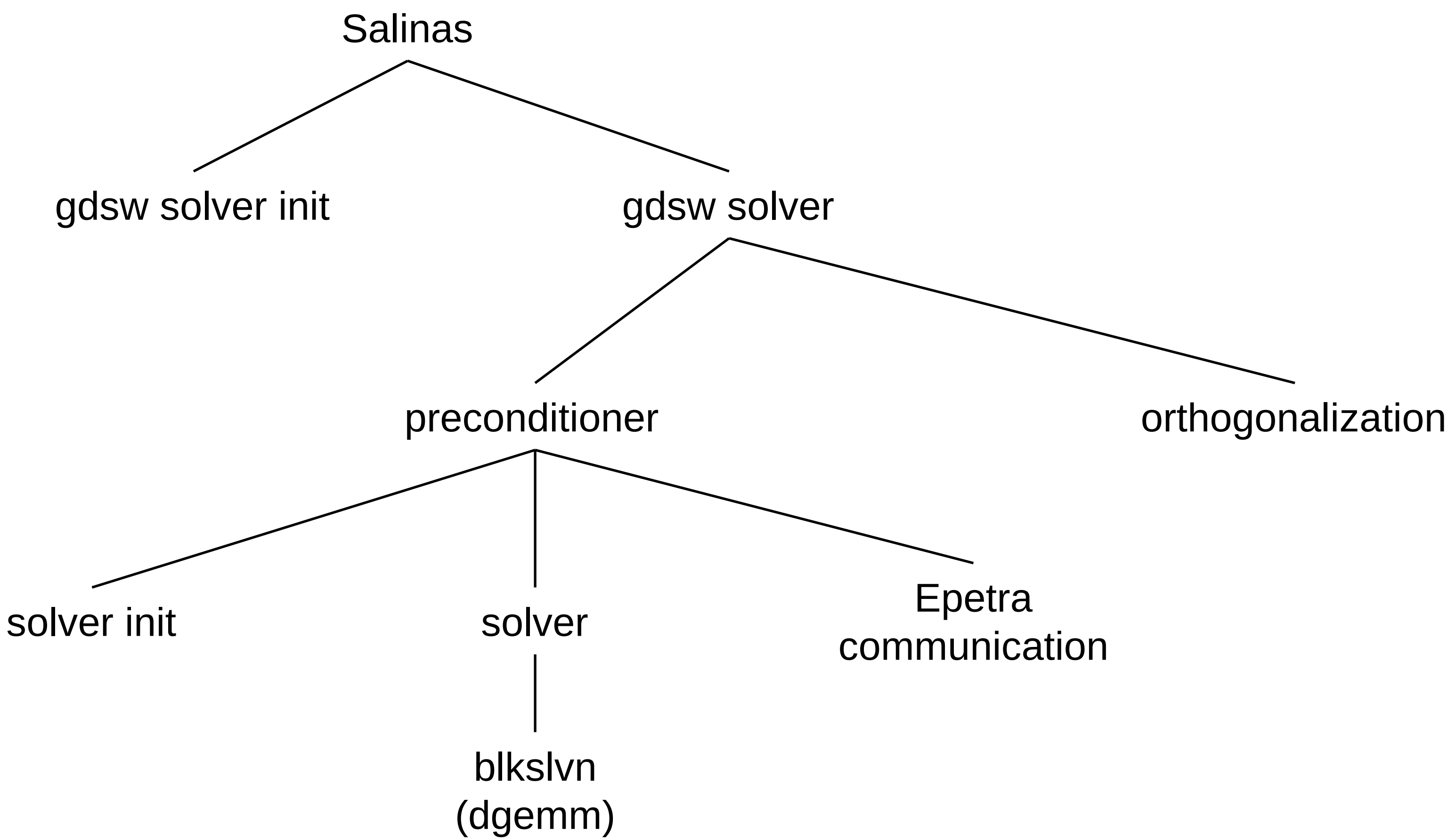
Sierra/SD TPLs

- Sparse Direct Solvers
  - SPRSBLKLLT (supernodal, left-looking, Ng & Peyton)
  - SuperLU (for complex frequency domain analysis)
  - Pardiso (option for Intel platforms, future importance?)
  - NoPivot (in-house code, left-looking, threads)
    - Movement to Trilinos/Amesos2
- Parallel Linear Algebra
  - Trilinos/Epetra movement to Trilinos/Tpetra for solver
- Dense Linear Algebra
  - BLAS, LAPACK, MKL, ScaLapack
- Graph Partitioning
  - (Par)Metis, Chaco, Zoltan/phg

Target Problems for CoE Focus

- NFN9 subsystem model
  - Currently runs on 120 processors
  - Refine mesh for scaling studies
  - OUO model
- Sparse Linear Solvers
  - Focus mainly on solve phase
  - Will provide representative linear systems
  - Evaluate performance of threaded and/or GPU accelerated solvers
- Goals:
  - Profile performance for improved speed, especially in solve phase
  - Identify problem areas
  - Suggestions for improvement
  - Reduce per-core memory footprint

Simplified Code Structure



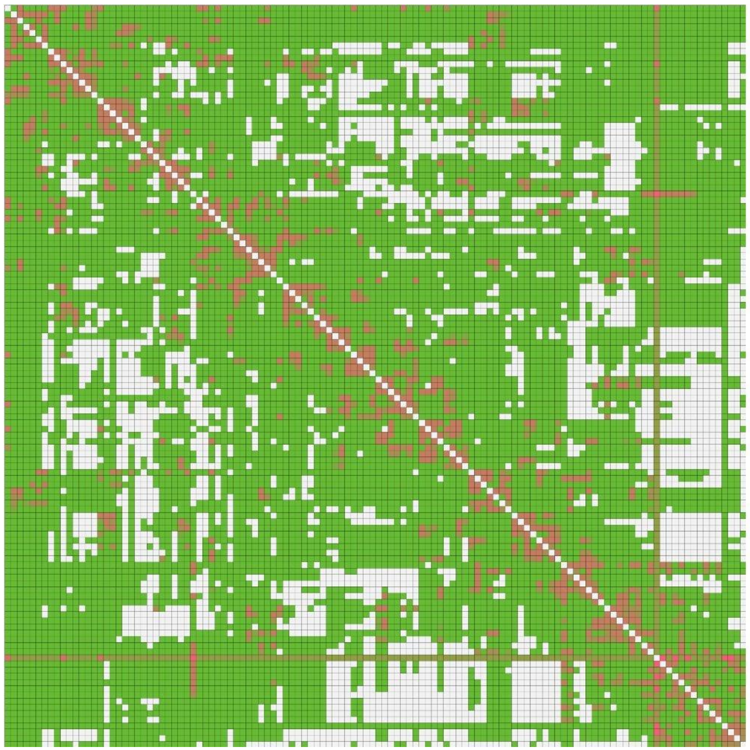
Overview

- Total time 1029.5 sec
  - User 538.5 sec (52.3%)
    - blkslvn 450.8 sec (43.7%)
  - MPI 9.6 sec (0.9%)
  - MPI_SYNC 481.4 sec (46.8%)
    - MPI_Barrier 352.3 sec (34.2%)
    - MPI_Allreduce 123.0 sec (11.9%)
- Total FLOPS 343.0e9 - double precision
  - 331.5 MFLOPs/rank (3.5% peak)

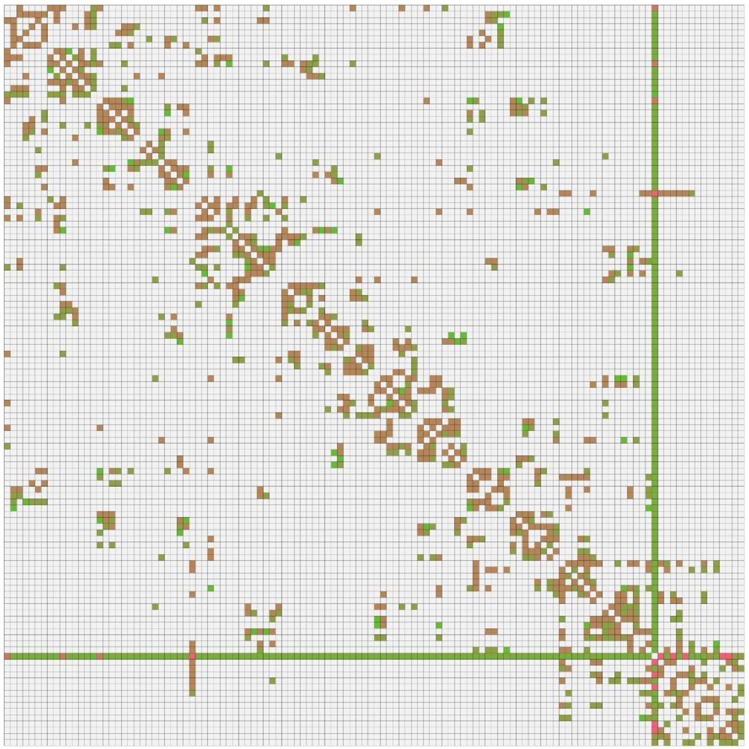
Preconditioner Solve

- On node backsolve
  - Shows 0 time when instrumented
  - called in .h file
- Calls blkslvn (FORTRAN)
- blkslvn called average of 6182 times
- calls dgemm
  - CrayPat loses connection to dgemm(shows up in call tree attached to root)
- Time for direct solve not in calling routines
- blkslvn takes 450.8 sec (83.7% of user time)

Communication Matrices



Whole Code



GDSW Solver

Summary

- Shown three applications from SIERRA Framework with performance profiling
- Significant time spent in two areas:
  - Solvers
  - Matrix Assembly
- Haswell performance should follow current processors
  - How to utilize the extra features of Haswell?
- Some experience with Knights Corner
  - How to translate to Knights Landing