

# STK (Sierra Toolkit) Update

## Trilinos User Group meetings, 2014

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# Outline

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- What is STK
- STK vs STK\_classic
  - API differences
  - Performance differences
- STK plans for the coming year

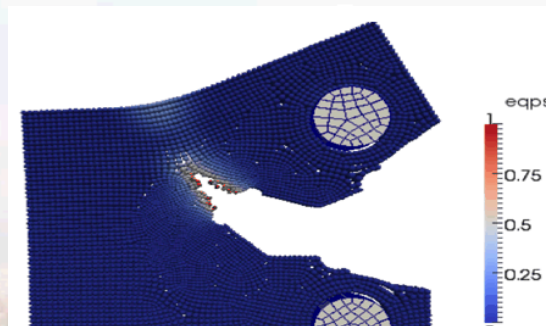
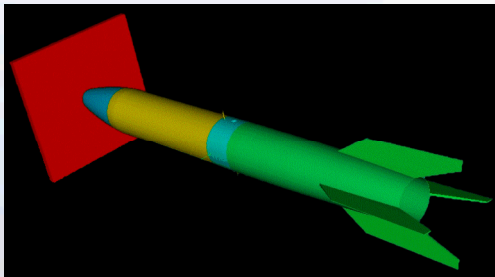
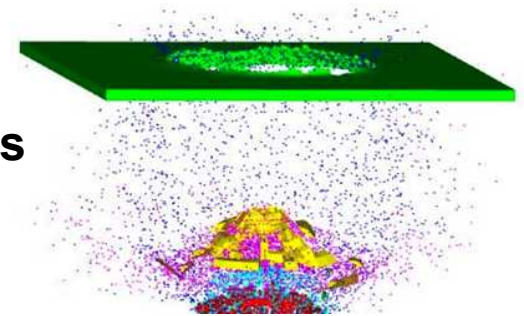


# What is STK

- STK is a collection of infrastructure modules supporting unstructured-mesh analysis applications.
- Developed in the SIERRA project

## Finite Element/Finite Volume Analysis Applications

- Solid Mechanics
- Structural Dynamics
- Thermal/Fluid Mechanics



# SIERRA / STK development environment

- The SIERRA project uses a build system based on “bjam” (of boost lineage).
- We monitor nightly and continuous builds/tests and valgrind reports on cdash dashboards.
- STK modules are updated into Trilinos periodically (thanks Brent!) and at that point the sources are built/tested using cmake/ctest support.



Dashboard

Calendar

Previous

Current

Project

Trac Site

Rally Site

External SQA

Team Views

Other GUIs

SierraNightly

No file changed as of Tuesday, October 14 2014 - 18:00 MDT

Switch to colorblind-friendly palette

Hide Filters

Advanced View

Auto-refresh

Help

Filters

Match the following rule:

Label

contains

TK

Limit results to 0 rows (0 for unlimited)

Apply

Clear

Create Hyperlink

Production - TLCC2

| Site         | Build Name   | Update<br>Files | Build |      |                | Test |      |                          | Build Time |
|--------------|--|-----------------|-------|------|----------------|------|------|--------------------------|------------|
|              |  |                 | Error | Warn | NotRun/Skipped | Fail | Pass |                          |            |
| sierra102    | master-intel-12.1-debug-openmpi-1.6.4-mkl              |                 | 0     | 0    | 0              | 0    | 257  | Oct 14, 2014 - 18:00 MDT |            |
| uno-login3   | master-intel-12.1-release-openmpi-1.6-mkl              |                 | 0     | 0    | 0              | 0    | 243  | Oct 14, 2014 - 18:00 MDT |            |
| chama-login8 | master-intel-12.1-release-openmpi-1.6-mkl              |                 | 0     | 0    | 0              | 0    | 248  | Oct 14, 2014 - 18:00 MDT |            |
| chama-login8 | master-intel-12.1-release-openmpi-1.6-mkl-installation |                 |       |      |                |      |      | Oct 14, 2014 - 18:00 MDT |            |
| sierra101    | master-intel-12.1-release-openmpi-1.6.4-mkl            |                 | 0     | 0    | 0              | 0    | 257  | Oct 14, 2014 - 18:00 MDT |            |

Production - TLCC

| Site         | Build Name   | Update<br>Files | Build |      |                | Test |      |                          | Build Time |
|--------------|--|-----------------|-------|------|----------------|------|------|--------------------------|------------|
|              |  |                 | Error | Warn | NotRun/Skipped | Fail | Pass |                          |            |
| glory-login2 | master-intel-12.1-release-openmpi-1.4.3-mkl              |                 |       |      |                |      |      | Oct 14, 2014 - 18:00 MDT |            |
| glory-login2 | master-intel-12.1-release-openmpi-1.4.3-mkl-installation |                 |       |      |                |      |      | Oct 14, 2014 - 18:00 MDT |            |

Production - RedSky

| Site          | Build Name   | Update<br>Files | Build |      |                | Test |      |                          | Build Time |
|---------------|--|-----------------|-------|------|----------------|------|------|--------------------------|------------|
|               |  |                 | Error | Warn | NotRun/Skipped | Fail | Pass |                          |            |
| redsky-login4 | master-intel-12.1-release-openmpi-1.6-mkl              |                 | 0     | 0    | 0              | 0    | 252  | Oct 14, 2014 - 18:00 MDT |            |
| redsky-login4 | master-intel-12.1-release-openmpi-1.6-mkl-installation |                 |       |      |                |      |      | Oct 14, 2014 - 18:00 MDT |            |

Production - Cleio

| Site       | Build Name  | Update<br>Files | Build |      |                | Test |      |                          | Build Time |
|------------|---|-----------------|-------|------|----------------|------|------|--------------------------|------------|
|            |   |                 | Error | Warn | NotRun/Skipped | Fail | Pass |                          |            |
| mzlogin01e | master-intel-12.1.xe6-release-vendor              |                 | 0     | 0    | 0              | 1    | 172  | Oct 14, 2014 - 18:00 MDT |            |
| mzlogin01e | master-intel-12.1.xe6-release-vendor-installation |                 |       |      |                |      |      | Oct 14, 2014 - 18:00 MDT |            |

Production - Sequoia

| Site | Build Name | Update<br>Files | Build |      |                | Test |      |  | Build Time |
|------|------------|-----------------|-------|------|----------------|------|------|--|------------|
|      |            |                 | Error | Warn | NotRun/Skipped | Fail | Pass |  |            |



# Sierra ToolKit (STK) modules overview

## Parallel-consistent Mesh database

- Heterogeneous element types
- Unstructured

## Search

- Proximity, mesh independent

## IO

- Bridge from mesh-data to external capability
- Built optionally

## Topology

- Entity-local definitions for node orderings, etc

## Util

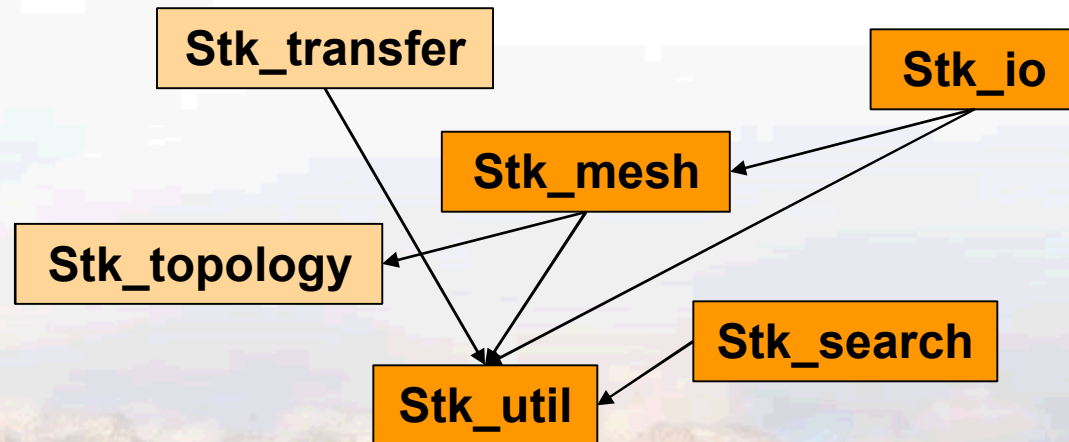
- Nearly everything depends on util directly or indirectly

## Transfer

- New

## Dependency diagram:

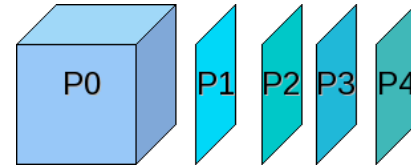
- Arrows point towards a module that is used (depended on) by another module.



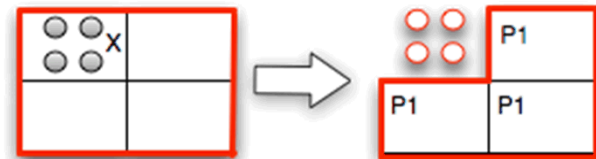


# STK Mesh

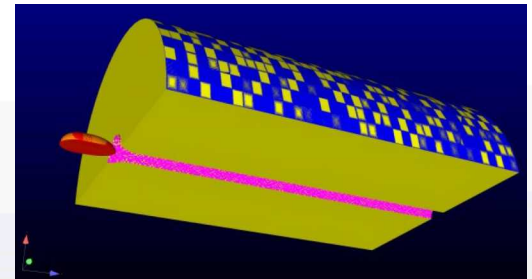
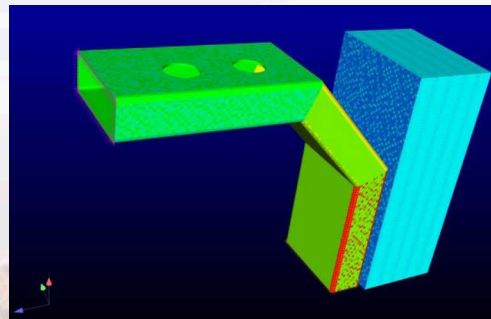
- Parallel distributed, parallel consistent



- Heterogeneous element types and field types

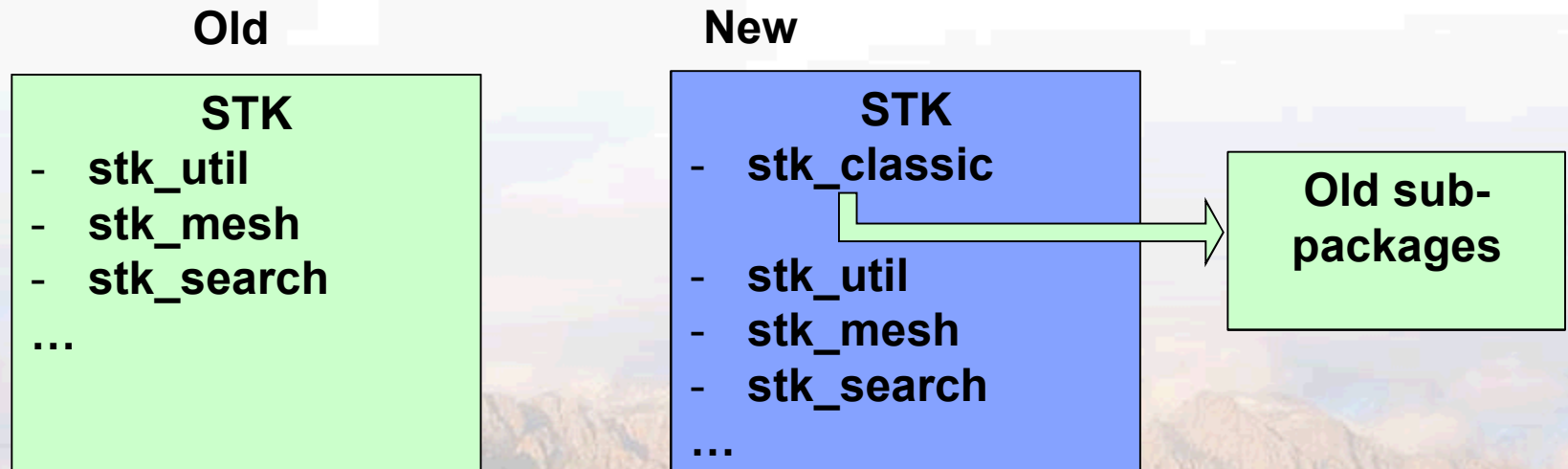


- Unstructured grid



# STK vs STK\_classic

- Starting a couple years ago, we made major changes to the STK package, changing APIs and data-structures, etc.
  - Almost all changes are in `stk_mesh`...
- We froze the STK package in Trilinos, performed development in the SIERRA repository, and have now brought the new code back into Trilinos.





# STK vs STK\_classic: API changes

## Entity

- Entity changed from an object with methods, to an index.
- To do anything with an Entity now, you need a BulkData.

### Example

Old

```
EntityId id = node.identifier();
```

New

```
EntityId id = bulkdata.identifier(node);
```



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# STK vs STK\_classic: API changes (continued)

## Relations / Connectivity: Entities are connected...

- Previously, Entity held arrays of Relations.
- Relation class held connected entity, ordinal (local-id) and other data
- These items are now held in separate 'raw' arrays.

Example: connected nodes of an element

Old

```
PairIterRelation node_relations = element.relations(NODE_RANK);  
Loop { Entity node = node_relations[i].entity();
```

New

```
unsigned num_nodes = bulkdata.num_nodes(element);  
const Entity* nodes = bulkdata.begin_nodes(element);  
Loop { Entity node = nodes[i];
```





## STK vs STK\_classic: API changes (continued)

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- Fields can only be associated with 1 entity rank
  - improved performance, reduced complexity
- IO: **MeshReadWriteUtils** replaced by **StkMeshIoBroker**
  - several API differences, see example materials
- **Shards** (topology definitions) is being replaced by **stk\_topology**
  - we will maintain mappings back and forth for users who continue to use Shards.





## STK vs STK\_classic: API changes (continued)

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- More detail is covered in a conversion guide written by Jim Foucar (thanks Jim!)
- Also see documentation tests which illustrate usage of a lot of the new STK code-base.  
See `stk/stk_doc_tests`





# STK vs STK\_classic: Performance improvements

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- Entity changes and connectivity storage changes improved cache efficiency of connectivity traversal
- Restricting fields to a single entity-rank improved speed of field-data access (removed pointer hop(s))
- Selector caching improved speed of bucket access
- Scalable entity creation
  - `stk::mesh::create_edges(mesh)...`
  - ...was reported as a scalability bottleneck for runs using large numbers of MPI ranks



# STK vs STK\_classic: Performance Improvements (continued)

naluEdge\_40x40x40\_hs\_master\_2013-02-06-13-50-08

Hotspots - Hotspots

Analysis Target Analysis Type Summary Bottom-up

Grouping: Function / Call Stack

| Function / Call Stack                        | CPU Time |
|--|----------|
| ▶ Epetra_BlockMap::LID                       | 9.269s   |
| ▶ Epetra_CrsMatrix::GeneralMV                | 5.279s   |
| ▶ stk::mesh::impl::EntityImpl::relations     | 4.548s   |
| ▶ LAY16_Loop_M16gas_1                        | 3.180s   |
| ▶ Epetra_CrsMatrix::SumIntoGlobalValues      | 3.071s   |
| ▶ LAX16_N4_Loop_M16gas_1                     | 2.941s   |
| ▶ AZ_precondition                            | 1.360s   |
| ▶ sierra::stk_nalu::AssembleMomentumEdgeSo   | 1.260s   |
| ▶ Epetra_Util_binary_search                  | 0.921s   |
| ▶ sierra::stk_nalu::AssembleNodalGradEdgeAl  | 0.790s   |
| ▶ Epetra_Vector::SumIntoGlobalValues         | 0.630s   |
| ▶ sierra::stk_nalu::AssembleCourantReynolds  | 0.540s   |
| ▶ sierra::stk_nalu::AssembleContinuityEdgeSo | 0.531s   |
| ▶ sierra::stk_nalu::EpetraLinearSystem::sumI | 0.500s   |
| ▶ sierra::stk_nalu::AssembleScalarEdgeSolver | 0.421s   |
| ▶ opal_memory_ptmalloc2_int_malloc           | 0.360s   |
| ▶ sierra::stk_nalu::ComputeMdotEdgeAlgorith  | 0.360s   |
| ▶ Epetra_CrsMatrix::NormInf                  | 0.270s   |
| ▶ std::__introsort_loop<__gnu_cxx::__normal_ | 0.260s   |
| ▶ sierra::stk_nalu::AssembleNodalGradUEdge   | 0.240s   |
| ▶ stk::mesh::induced_part_membership         | 0.209s   |
| ▶ Epetra_CrsGraph::ExtractMyRowCopy          | 0.201s   |
| ▶ Epetra_BlockMap::FirstPointInElement       | 0.180s   |

Selected 1 row(s): 9.269s

naluEdge\_40x40x40\_hs\_migration\_2013-02-06-13-51-01

Hotspots - Hotspots



Analysis Target Analysis Type Summary Bottom-up

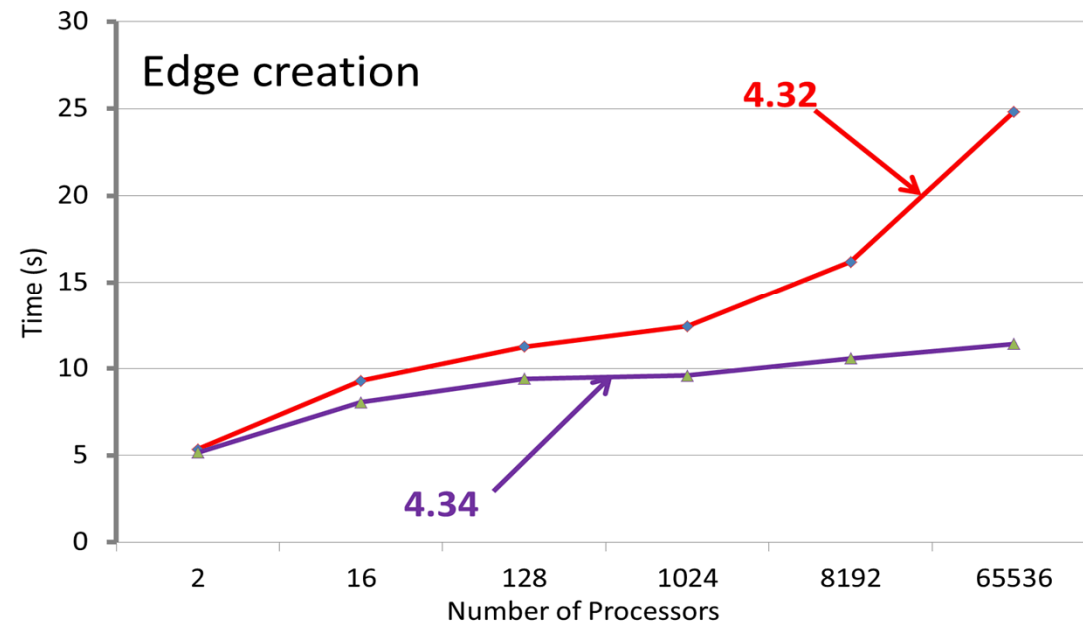
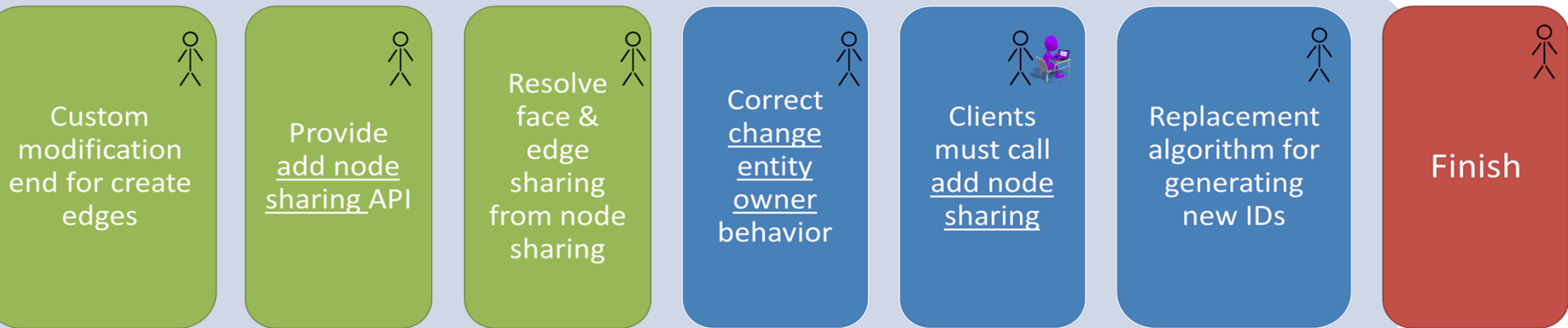
Grouping: Function / Call Stack

| Function / Call Stack                          | CPU Time |
|--|----------|
| ▶ Epetra_BlockMap::LID                         | 7.937s   |
| ▶ Epetra_CrsMatrix::GeneralMV                  | 4.971s   |
| ▶ LAY16_Loop_M16gas_1                          | 2.770s   |
| ▶ LAX16_N4_Loop_M16gas_1                       | 2.710s   |
| ▶ Epetra_CrsMatrix::SumIntoGlobalValues        | 2.351s   |
| ▶ sierra::stk_nalu::AssembleMomentumEdgeSo     | 1.240s   |
| ▶ AZ_precondition                              | 1.240s   |
| ▶ Epetra_Util_binary_search                    | 0.971s   |
| ▶ sierra::stk_nalu::AssembleScalarEdgeSolverA  | 0.680s   |
| ▶ Epetra_Vector::SumIntoGlobalValues           | 0.560s   |
| ▶ sierra::stk_nalu::AssembleCourantReynoldsE   | 0.490s   |
| ▶ sierra::stk_nalu::AssembleNodalGradEdgeAlg   | 0.420s   |
| ▶ sierra::stk_nalu::EpetraLinearSystem::sumInt | 0.370s   |
| ▶ sierra::stk_nalu::AssembleContinuityEdgeSolv | 0.370s   |
| ▶ Epetra_CrsMatrix::NormInf                    | 0.280s   |
| ▶ Epetra_BlockMap::GID64                       | 0.270s   |
| ▶ sierra::stk_nalu::ComputeMdotEdgeAlgorithm   | 0.260s   |
| ▶ std::__introsort_loop<__gnu_cxx::__normal_it | 0.230s   |
| ▶ stk::mesh::Bucket::internal_move_entity      | 0.221s   |
| ▶ Epetra_FE_CrsMatrix::SumIntoGlobalValues     | 0.210s   |
| ▶ sierra::stk_nalu::AssembleNodalGradUEdgeAl   | 0.200s   |
| ▶ Epetra_CrsGraph::ExtractMyRowCopy            | 0.190s   |
| ▶ stk::mesh::induced_part_membership           | 0.190s   |
| ▶ opal_memory_ptmalloc2_free_hook              | 0.180s   |
| ▶ pow  | 0.170s   |

Selected 1 row(s): 7.937s

# Scalable Entity Creation

 STK person  
 App person



- Make sure all internal code is using `generate_new_ids`
- Obtain new scalability data on Cielo





# STK plans for the coming year

## Feature Development, enhancements

Scalable  
Entity  
Creation

IO

Ghosting

Arbitrary  
Relations

Balance/R  
ebalance

IO Auto  
Decomp

Batch Mesh  
Modification

## Research

- Next generation platforms
- Threading, GPUs, Kokkos?
- Data Structures
- Hierarchical Decomposition



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