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STK-Mesh Tutorial Minisymposium

SIAM Conference on
Computational Science and Engineering
February 28, 2011

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Four Parts:

- **Part 1: STK-Mesh Domain Model**
  - Comprehensive conceptual overview; no code
- **Part 2: STK-Mesh Computations**
  - How to perform computations; with code snippets
- **Part 3: STK-Mesh Modifications**
  - How to modify a mesh; with code snippets
- **Part 4: SIERRA Toolkit – beyond STK-Mesh**
  - Other modules / library components

STK-Mesh Domain Model

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What is a *Domain Model*?

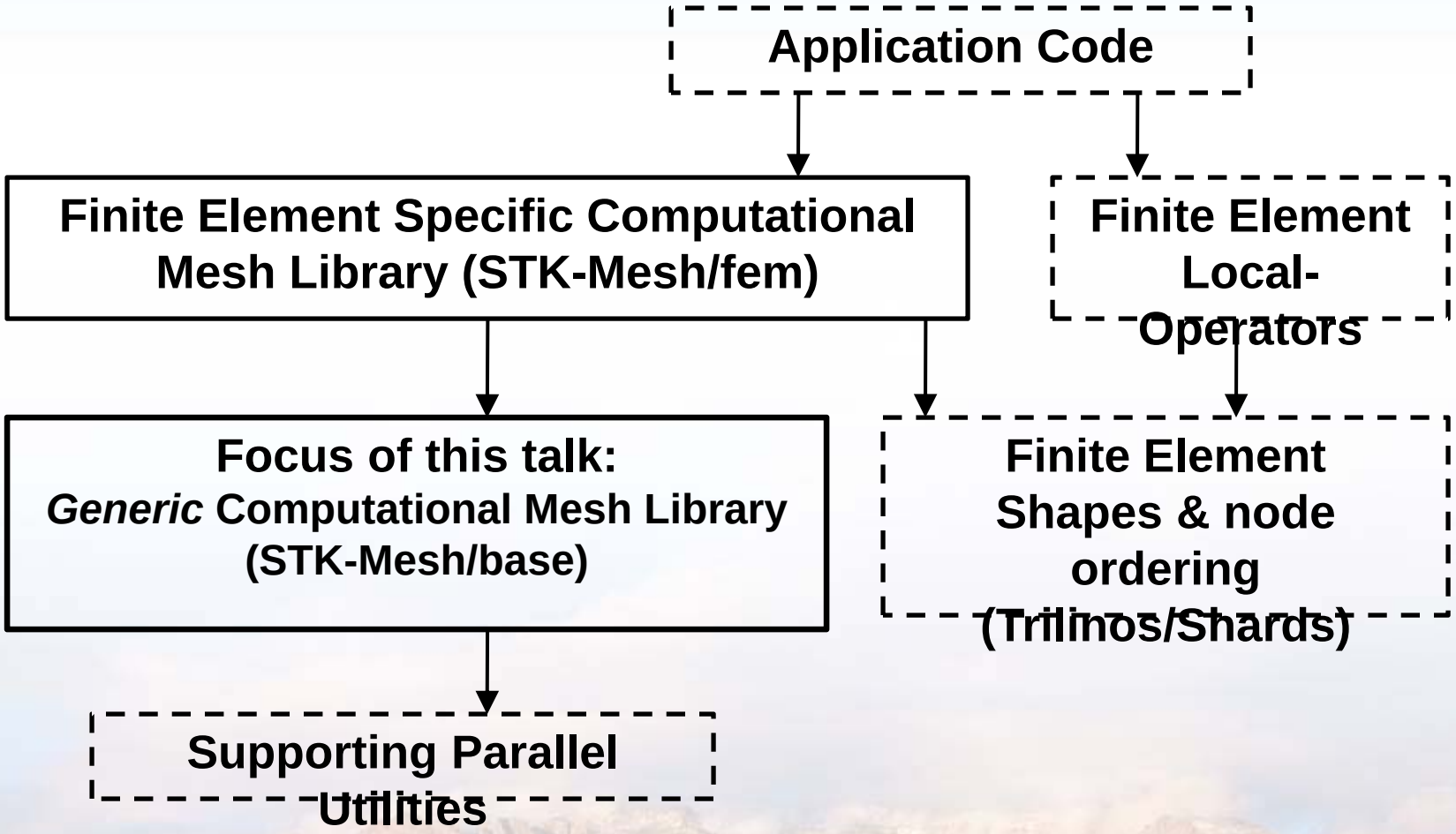
- **A formal expression of, and ubiquitous language for,**
  - Conceptual context
  - Software architecture
  - Software requirements framed within the conceptual context and software architecture context

- **"Domain-Driven Design; Tackling Complexity in the Heart of Software" by Eric Evans**
  - I highly recommend to developers of non-trivial CS&E software
  - Systematic and iterative approach to modeling a domain
  - Emphasis on managing complexity and mapping to software

The Challenging STK-Mesh *Domain*

- **An Unstructured Mesh**
  - "Weblike pattern or construction that fills a spatial domain Ω"
  - A discretization of a spatial domain Ω
  - Filled with arbitrary elemental subdomains; e.g., polyhedrons
- **Supporting Computations**
  - Simulations with multiphysics / heterogeneous phenomena
  - E.g., numerical solution of PDEs defined on the domain Ω
  - Computational data associated with entities of the discretization
- **That use Advanced Capabilities and Algorithms**
  - Massively parallel and hybrid parallel computations
  - Solution strategies that adapt the computations & discretization

Modular, Layered Architecture

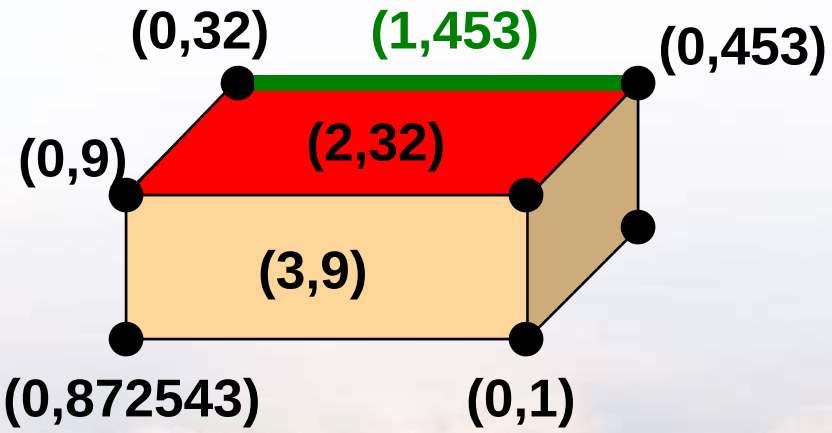


Computational Mesh Database

- **Computational Mesh**
  - Discretization data; e.g., nodes, elements, connectivity
  - Computation data; e.g., variables of the PDEs / models
- **Mesh Database Bulk-data**
  - Discretization and computation data of the problem to be solved
  - Size is proportional to the granularity of the discretization
  - Must be parallel-distributed for scalable computations
- **Mesh Database Meta-data**
  - *Description* of the bulk-data (a.k.a., the database's schema)
  - Size is proportional to the complexity of the discretization
  - Assumed to be parallel-duplicated for simplicity

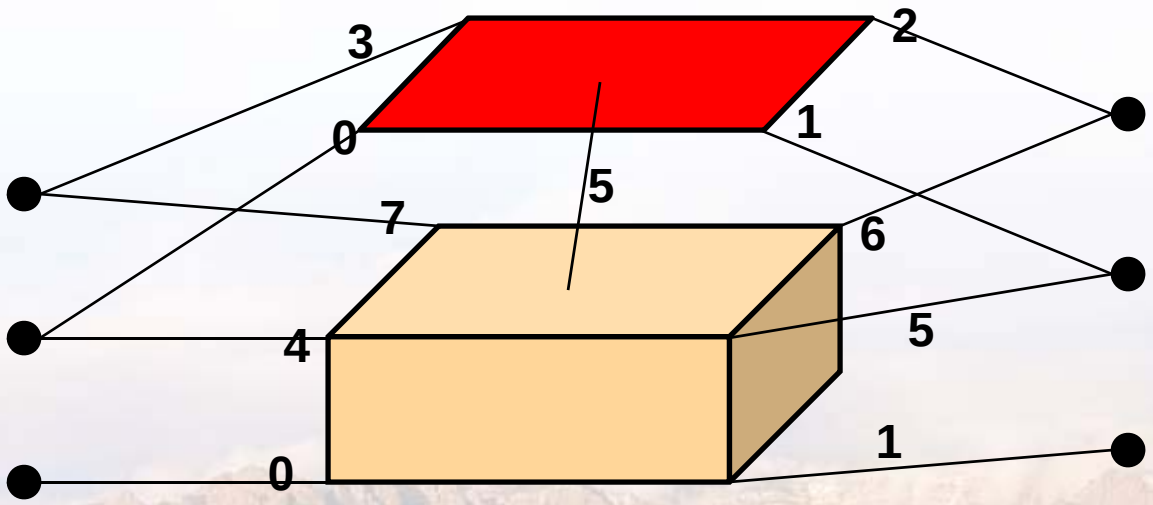
Mesh Bulk-Data: Discretization

- **Mesh Entity:** $entity_{GlobalID}^{Rank}$
  - The fundamental, atomic units of the discretization
  - E.g., finite element method's nodes, edges, faces, and elements
  - Ranking within the discretization; e.g., node < element
  - Globally unique and persistent identifier
    - Across parallel-distributed memory space
    - For the lifetime of the entity
    - Fully ordered
  - Unique: (Rank , Global-ID)



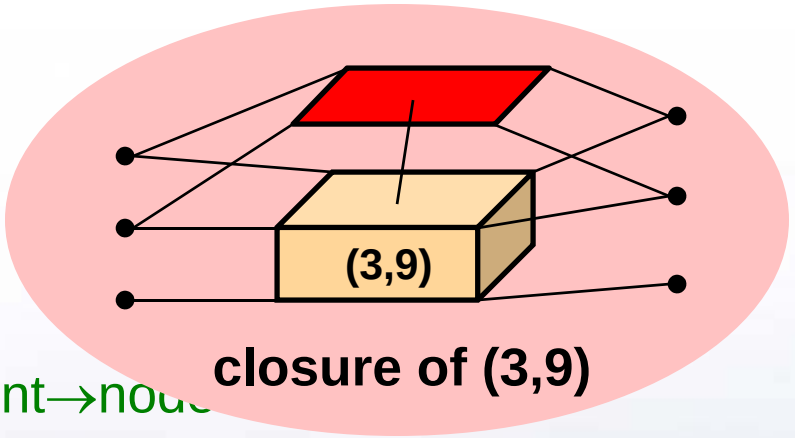
Mesh Bulk-Data: Discretization

- **Mesh Entity Relation:** $\left(entity_a^J, entity_b^K, relationID\right)$
  - Directed from higher to lower ranking entity
    - Rank J > Rank K : $entity_a^J \rightarrow entity_b^K$; required J ≠ K
  - E.g., an element is defined to be higher ranking than a node
  - Uniqueness when J > K: $\left(entity_a^J, K, relationID\right) \rightarrow entity_b^K$
    - … or does not exist



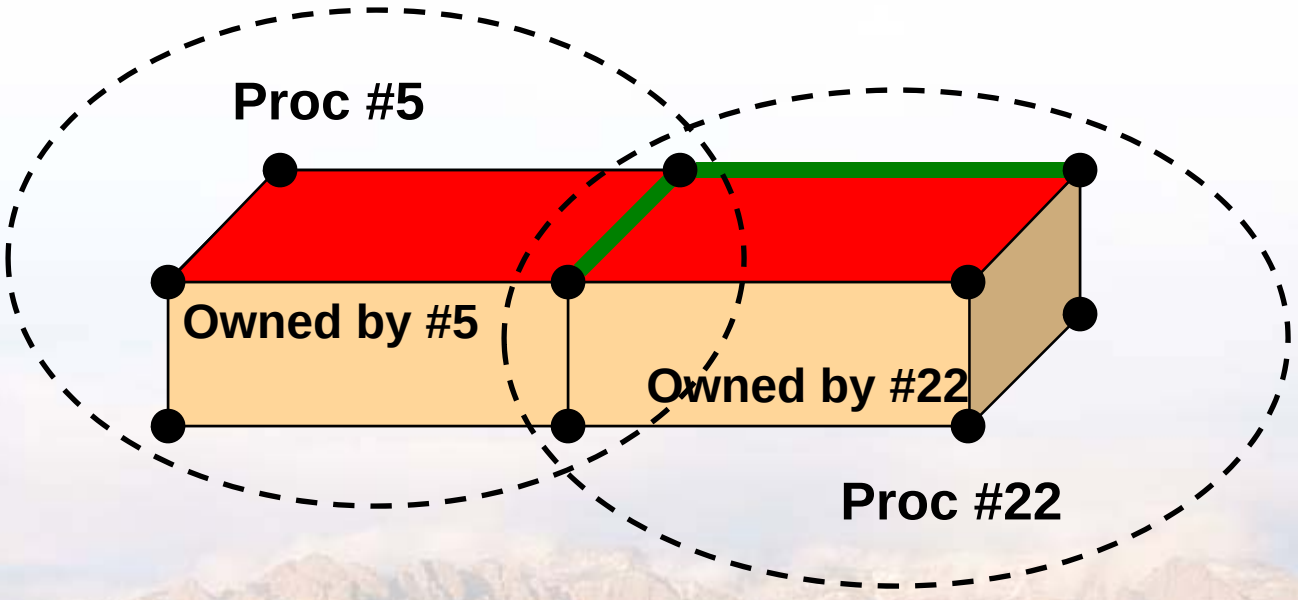
Mesh Bulk-Data: *Closure*

- **Directed Acyclic Graph (DAG)**
  - Entities are nodes of the graph
  - Relations are directed edges of the graph
  - Acyclic: directed relations higher→lower rank
  - Concept of “Closure”
- **Closure of a Mesh Entity:** $\overline{entity_a^J}$
  - Collection of entities and relations
    - Reachable from that entity
    - Following directed relations
  - E.g., an element, its nodes, and element→node
  - Assumption: The totality of computations performed on a given mesh entity require access to the closure of that mesh entity



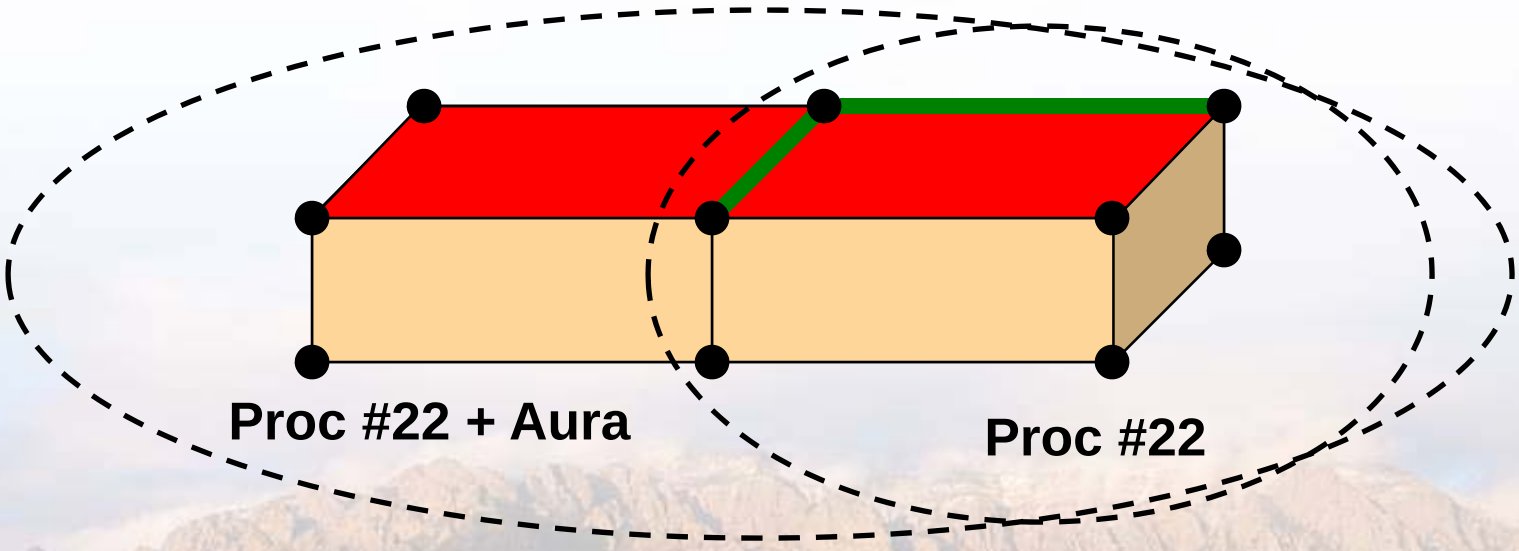
Mesh Bulk-Data: Parallel Distribution

- **Parallel distribution of mesh entities and relations**
  - Every mesh entity is uniquely owned by a parallel process
  - *Closure* of an owned mesh entity must reside on that process
  - This requires duplication (sharing) of mesh entities
  - $\overline{entity_a^J} \bigcap \overline{entity_b^J}$ is shared between the owning processes



Mesh Bulk-Data: Parallel Distribution

- **One Layer Ghosting (a.k.a., Ghosting Aura)**
  - If a mesh entity is shared by a process
  - Is in the closure of another mesh entity: $entity_b^K \in \overline{entity_a^J}$
  - Then that closure is also duplicated on the process
  - E.g., the closure of the elements connected to a shared node are ghosted on all processes on which the node is shared
  - Invaluable for neighborhood / patch accessing algorithms



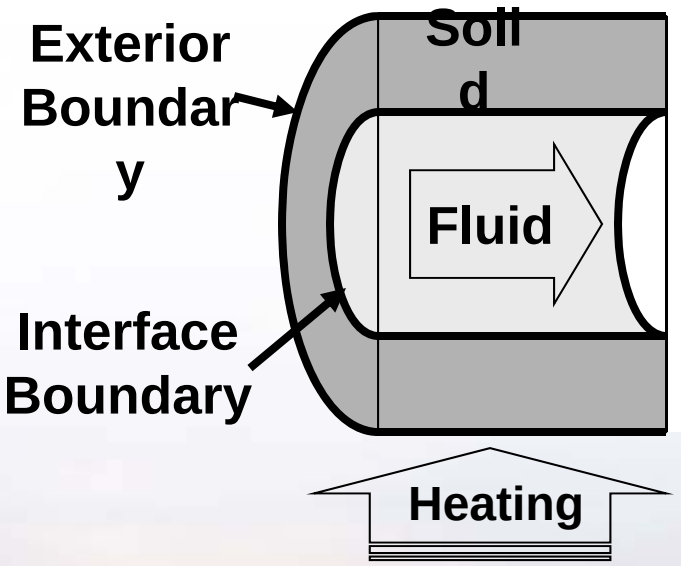
Mesh Meta Data: Defining Subsets

- **Multiphysics and Heterogeneity**
  - Different models and computations in different subdomains
  - Heterogeneous discretizations: shapes, polynomial degree, …

- **Mesh Part:** $Part_A$
  - **Define subdomains for different computations**
  - **Define collections of mesh entities with the same discretization**
  - **Define supersets of parts**

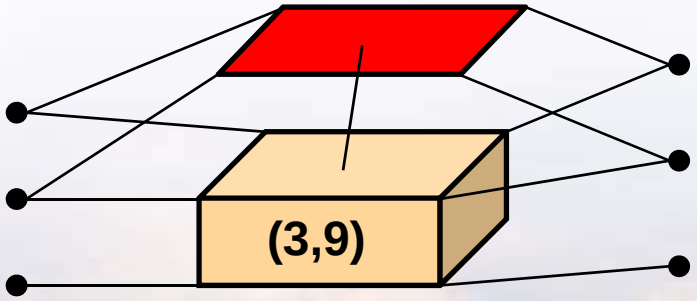
$$Part_X = Part_A \bigcup Part_B \bigcup Part_C$$

  - **# Mesh Parts depends upon heterogeneity (complexity) of the domain and computations**



Mesh Bulk-Data: Part Membership

- **A Mesh Entity is a Member of one or more Mesh Parts**
  - $entity_a^J \in Part_A \bigcap Part_C \bigcap Part_F$
  - Always a member of the universal part: $Part_\Omega$
- **Mesh Part Membership may be Induced**
  - If $entity_a^J \in Part_A$ and $entity_a^J \rightarrow entity_b^K$
  - Then $entity_b^K \in Part_A$ may be induced
  - Decision to induce membership is an attribute of the mesh part
- **Example:**
  - Entity (3,9) $\in$ Part "Block-2"
  - Nodes and face are *induced* members of Part "Block-2"

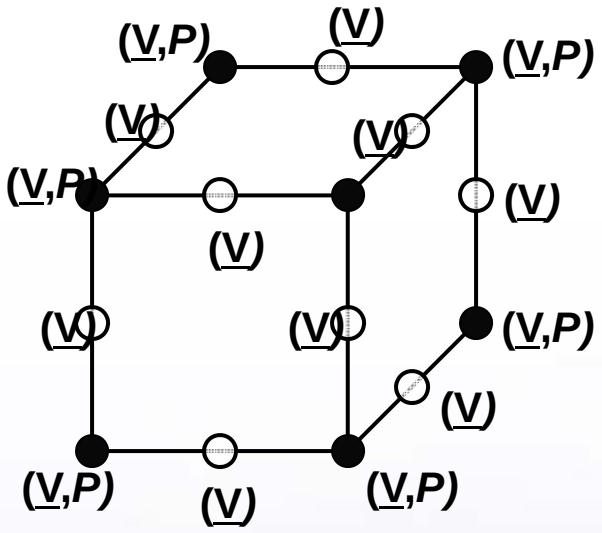


Field Data $\subset$ Computation Data

- **A *Computational* Mesh Supports Computations**
  - Computations require field data:
  - Data associated with mesh entities: $entity_a^J \rightarrow \{FieldData_X\}$
  - Heterogeneity: existence of field data varies with mesh entity
- **Field Declaration** $Field_X$
  - The *type* of the field; analogous to a 'C' or 'C++' *typedef*
  - A multidimensional array of a simple mathematical type
- **Field Restriction** $(Field_X, J, Part_A) \rightarrow [n_0, n_1, \cdots]$
  - A field exists for an $entity_a^J$
    - Which is of a specified rank J and
    - A member of a specified mesh part
  - Defines the dimensions of the multidimensional array value $entity_a^J \in Part_A$

Field Data Heterogeneity Example

- **Velocity field data on all nodes**
  - Velocity field declaration
  - Restriction $(velocity, 0, Part_{\Omega}) \rightarrow [3]$
- **Pressure field data only on vertices**
  - Pressure field declaration
  - Vertex node mesh part $Part_{VTX}$
  - Restriction $(pressure, 0, Part_{VTX}) \rightarrow 1$
  - Vertex nodes declared to be members of vertex node mesh part

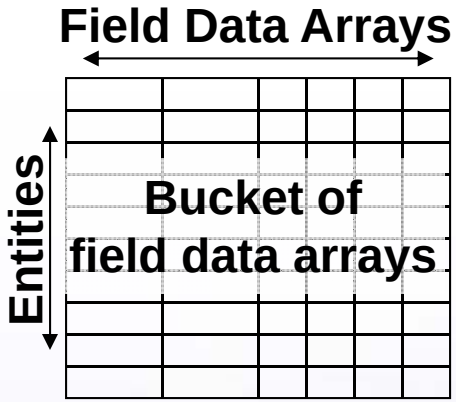


Heterogeneity Impacts Performance

- **Heterogeneous computations, heterogeneous field data**
  - Computations operate on subsets of Ω
    - Problem defined: e.g., fluid region, solid region, boundary
    - Discretization defined: e.g., hex, tet, linear, quadratic, shell
    - Parallel defined: e.g., owned by local process
  - Field data existence and dimensions can vary across Ω
- **Impact on Performance**
  - Want: Computations on nice contiguous arrays of field data
  - Have: Irregular computations and irregular field data
    - Selection logic in inner loops hurts performance, esp. GPGPU
    - Dense arrays with “ignore this entry” flags wastes memory
  - Solution: …

Field Data Arrays in *Buckets*

- **We have homogeneous subsets of mesh entities**
  - Same mesh entity rank and members of same mesh parts
  - ⇒ Have same field data of the same array dimensions
- **Buckets of homogeneous field data**
  - Contiguous arrays of field data
  - Bundled into a block of memory



- **Computations on buckets**
  - Outer loop to select buckets
  - Inner loop to computes on arrays in the selected bucket
  - Active R&D for portable thread-parallelism
    - Including GPGPU – buckets residing in device memory

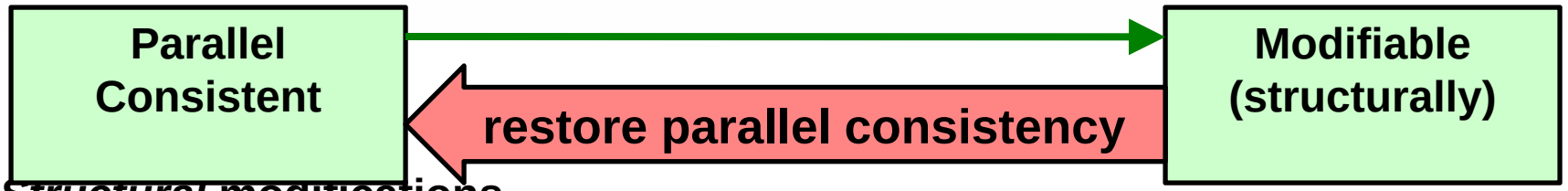
Constructing Mesh Meta-Data
(mesh database schema)

- **Declare Mesh Parts and Mesh Fields**
  - And mesh part superset-subset relationships $Part_A \subseteq Part_B$
  - And mesh field restrictions $(Field_X, J, Part_A) \rightarrow [n_0, n_1, \cdots]$
  - Detect and prohibit inconsistencies
    - Cyclic superset-subset relationships
    - Conflicting field array dimensions

- **Complete (Finalize) Mesh Meta-Data Construction**
  - Analogous to a database schema for the mesh bulk-data
  - Prohibit changes after mesh bulk-data is created …
  - Because it can be expensive and complex to edit a populated database's schema

Modifying Mesh Bulk-Data
(structural changes)

- **Two Mesh Bulk-Data Modification *States***



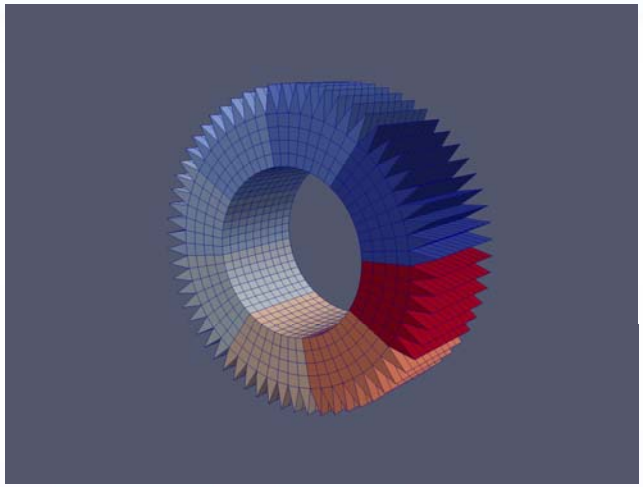
- ***Structural* modifications**
  - Declare and destroy mesh entities and relations
  - Change mesh entities' mesh part memberships
  - Local and parallel-inconsistent for shared or ghosted entities
- **Restore parallel consistency**
  - A single parallel collective operation
  - Very complex; good performance is especially hard
  - Incremental – only resolve what has been modified

STK-Mesh Finite Element Layer

- **Layer element concept onto "generic" mesh**
  - Element shapes and node ordering (a.k.a., cell topology)
    - Including element-sides and element-edges
  - Trilinos / Shards API and library of standard cell-topologies
- **Optionally Associate a Cell Topology with a Mesh Part**
  - $Part_{Tet\langle 4\rangle} \rightarrow Tetrahedron\langle 4\rangle$
  - All elements that are members of this part are tetrahedrons
- **Includes concept of element boundaries**
  - Sides & side neighbors, edges & edge neighbors
- **Foundation for finite element computations**
  - Basis functions, numerical integration, …

Conclusion

- **STK-Mesh is an active R&D effort**
  - Within the DOE ASC SIERRA Toolkit project at Sandia
  - Related R&D for field data arrays on multicore and GPGPU
  - Open source though Trilinos: http://trilinos.sandia.gov
- **Very complex domain and needs**
  - Parallel, heterogeneous, dynamically modifiable unstructured mesh
  - Computational performance requirements: field data buckets
- **Domain Modeling is Key to Managing Complexity**
  - Modular and layered architecture
  - “Lean and clean” modules, dependencies, and APIs
  - Minimize coupling between modules



STK-Mesh Example Computation Setup and Parallel Execution

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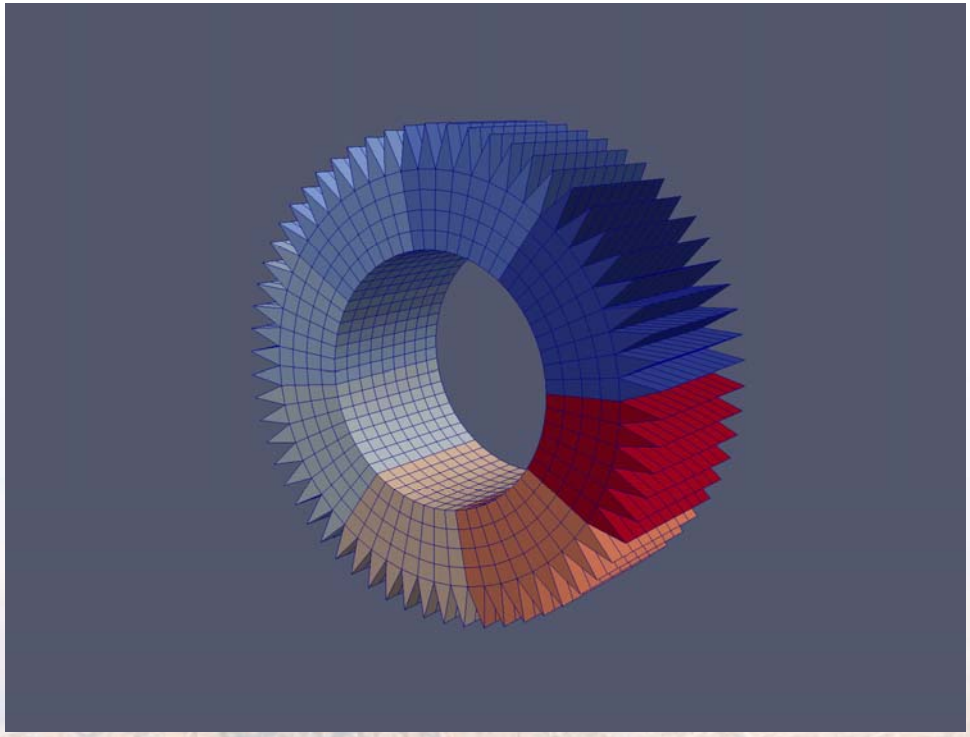
Outline

- Overview of Gear Fixture & features
- Setup of Meta Data
- Setup of Bulk Data
- Computational Kernel
- Movie

Description of Gears Demo

- Basis for movie at Super-Computing 2010
- Example is in STK sources and is used for testing



Overview of Gear Fixture

- **Located in source:**
  - http://trilinos.sandia.gov/
    - packages/stk/stk_mesh/stk_mesh/fixtures/GearsFixture
    - packages/stk/stk_mesh/stk_mesh/fixtures/Gear
    - packages/stk/stk_performance_tests/stk_mesh/GearsSkinning
- **Cylindrical gear body made up of Hexahedron<8> elements**
- **Gear Teeth made up of Wedge<6> elements**
- **Parallel distribution of elements and nodes**
- **Rotation of gear**

Gear Meta Data

- **Declare the following parts of the mesh**
  - Cylindrical coordinates part
  - Hex part
  - Wedge part
- **Declare the following fields:**
  - Cartesian coordinates field (x,y,z) on nodes
  - Displacement field (Δx,Δy,Δz) on nodes
  - Translation field on nodes
  - Cylindrical coordinates field (r,θ,z) on nodes
- **Restrict the fields to parts**

Fixture Declaration of Meta Data

```
typedef Field< double , Cylindrical>  CylindricalField;
typedef Field< double , Cartesian>    CartesianField;

class GearsFixture {
public:
  MetaData   meta_data;
  BulkData   bulk_data;
…
  Part & cylindrical_coord_part;
  Part & hex_part;
  Part & wedge_part;
  CartesianField    & cartesian_coord_field;
  CartesianField    & displacement_field;
  CartesianField    & translation_field;
  CylindricalField  & cylindrical_coord_field;
…
};
```

Fixture Construction: [MetaData]

- **Inside Gear Fixture constructor:**

```
const unsigned TWO_STATE = 2;
GearsFixture::GearsFixture( … ) :
  meta_data( fem::entity_rank_names(SpatialDimension) ),
  bulk_data( meta_data , parallel_machine ),
  …,
  cylindrical_coord_part(
     meta_data.declare_part("cylindrical_coord_part”,element_rank)
     ),
  displacement_field(
     meta_data.declare_field<CartesianField>("displacement", TWO_STATE)
     ), …
{
…
}
```

Restrict Fields to Parts: [MetaData]

- Field Restrictions: Entities in the part will have the field

- Example for cylindrical coordinate field and part:

```
GearsFixture::GearsFixture(…): [prev slide] {
  put_field(
        cylindrical_coord_field,
        node_rank,
        cylindrical_coord_part,
        SpatialDimension
        );
  …
}
```

Induced Part Membership

Simplified Mesh Maintenance

- **How to apply a field to nodes that are connected to elements of a particular type?**

- **Option A: Manually**
- **Option B: Automagically**
  1. Put elements in a Part of that type
  2. Restrict the nodal field to that part
  3. All nodes in closure of elements in this part will get this field

- **Cylindrical Part limited to Elements**
- **Cylindrical coordinates Field limited to Nodes**
- **Cylindrical coordinates field restricted to cylindrical part**

Gear Bulk Data Operations

- **Create Hex entities for gear body**
  - Place Hex entities in Hex part and Cylindrical part
  - Declare relations to nodes
- **Create Wedge entities for gear teeth**
  - Place Wedge entities in Wedge part and Cylindrical part
  - Declare relations to nodes
- **Initialize field data**
- **Skin mesh with faces**
  - Skinning function in fem

Initialize Field Data (entity-wise)

- Loop over nodes
- Assign Cartesian coordinates from cylindrical coordinates

```
loop over nodes {
    const double rad = … ;
    const double angle = … ;
    const double height = … ;

    double * const cartesian_data = field_data( cartesian_coord_field , node );

    cartesian_data[0] = rad * std::cos(angle);
    cartesian_data[1] = rad * std::sin(angle);
    cartesian_data[2] = height;
}
```

Gear Rotation Computation (bucket-wise)

- **Recall: Select buckets, iterate over buckets, compute**

```
Selector select = cylindrical_coord_part &
                  ( locally_owned_part | globally_shared_part );

BucketVector selected_node_buckets;

get_buckets(
    select,
    bulk_data.buckets(Node),
    selected_node_buckets
    );
```

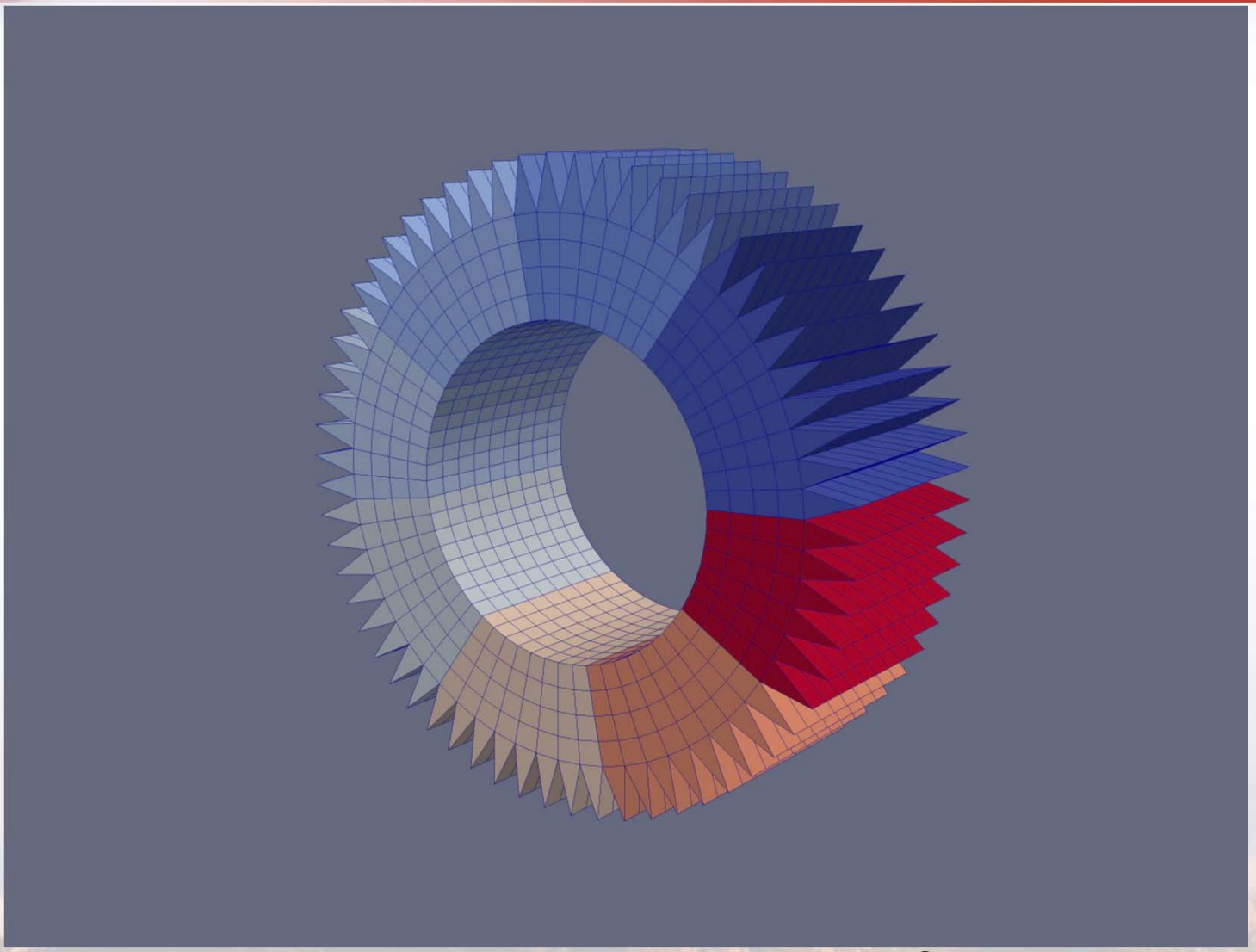
Gear Rotation Computation (bucket-wise)

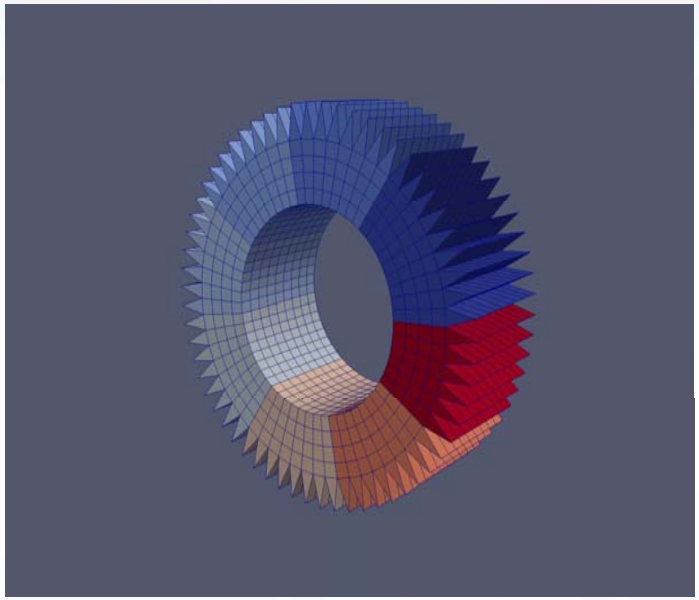
```
for (BucketVector::iterator b_itr = selected_node_buckets.begin();
      b_itr != selected_node_buckets.end();
      ++b_itr) {
  Bucket & b = **b_itr;

  const BucketArray<CartesianField>
      old_coordinate_data( cartesian_coord_field, b);
  BucketArray<CartesianField>
      displacement_data( displacement_field.field_of_state(StateNew), b);
  …

  for (size_t node_index = 0; node_index < b.size(); ++index) {
    // Compute new and old coordinate data and assign to displacements:
   displacement_data(0,index) = new_coordinate_data[0] – old_coordinate_data(0,index);
   displacement_data(1,index) = new_coordinate_data[1] – old_coordinate_data(1,index);
   displacement_data(2,index) = new_coordinate_data[2] – old_coordinate_data(2,index);
   …
  }
}
```

Hybrid Parallelism

- Alan's talk will cover hybrid parallelization of this example
- Basic Idea: Parallel For applied to bucket loops
- Also see the following example:
  stk_usecases/app/UseCase_blas_algs.hpp
  stk_usecases/app/UseCase_blas.cpp

Gears Demo (stk_mesh, epu, conjoin, paraview)





STK-Mesh Example Dynamic Mesh Modification

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Outline

- **The Meta-Data**
- **Modifying the Bulk-Data**
  - Maintaining Consistency
    - Bulk-Data State
    - Parallel Consistency
    - Local Consistency
    - Field Data
    - Atomic Modifications
- **Gear Demo**
  - Overview
  - Code snippets necessary to strip teeth off of the gear

Mesh Modification

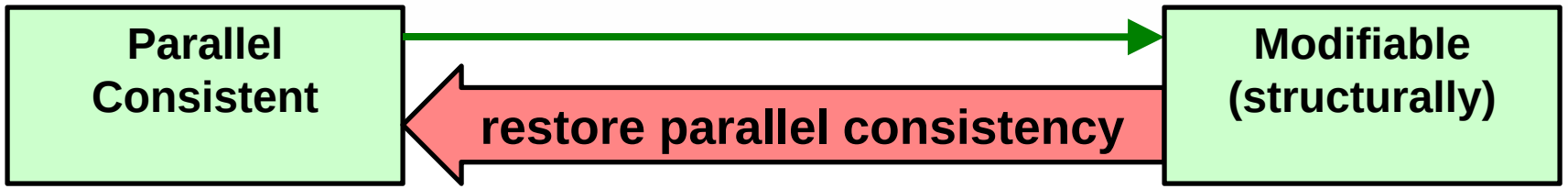
- **Meta-Data**
  - Equivalent to the schema of a database, the meta-data describes the problem domain
  - Freely modifiable before being committed
  - ***No*** modifications allowed after commit

Mesh Modification

Bulk-Data

- Contains the discretization of the problem
- Its meta-data ***must be*** committed before any function beside the bulk-data constructor can be called
  - *Meta-data check for global consistency will throw if the meta-data is not globally consistent*
- Bulk-data modifications are only allowed when the bulk-data is in a modifiable state.

Modification Cycle



- **Parallel Consistent**
  - **NO** Mesh modification allowed
- **Modifiable**
  - Guaranteed to be locally consistent
  - Atomic mesh modifications are allowed

*Parallel consistency is enforced when switching from **Modifiable** to **Parallel Consistent***

Maintaining Consistency

- The bulk-data state is transitioned by calling

```
bulk_data.modification_begin()
bulk_data.modification_end()
```

  - A new modification cycle begins whenever modification begin is called
  - Atomic mesh modifications mark affected entities and all their upward relations as *modified*
  - Parallel consistency is enforced at modification end by
    - Deleting all ghosts of modified entities
    - Resolving parallel ownership and sharing of created and destroyed entities
    - Resolving shared entities mesh part membership, entity relations, field data memory allocation, and bucket membership
    - Updating the one layer ghosted aura

Maintaining Consistency

- **The following operations are available through Atomic Mesh Modifications**
  - Creating and/or deleting entities
  - Changing entities' mesh part memberships
  - Changing entities' relations
  - Moving entities' ownership to another process

- **Atomic modifications are guaranteed to be *locally consistent***
  - Induced mesh part membership will change as necessary
  - Memory for field data will be created, resized, or deleted
  - Existing field data will move to the correct bucket

Maintaining Consistency

Field Data

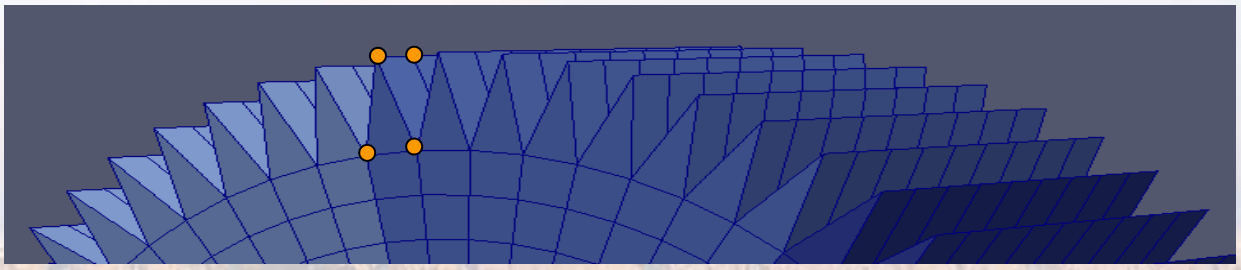
- Communicating field data **does not** modify the topology of the mesh and can happen at any time (i.e. not restricted to a modifiable bulk-data**)**
- Atomic mesh modifications will move existing field data to the correct bucket on the *local* process

  *When **changing entity owner** the field data is moved to the correct bucket on the remote process*
- After modification end space for field data of ghosted and shared entities has be allocated but the data *has not been copied* from the owner
- Field data values can be copied from owned to shared/ghosted at any time by calling

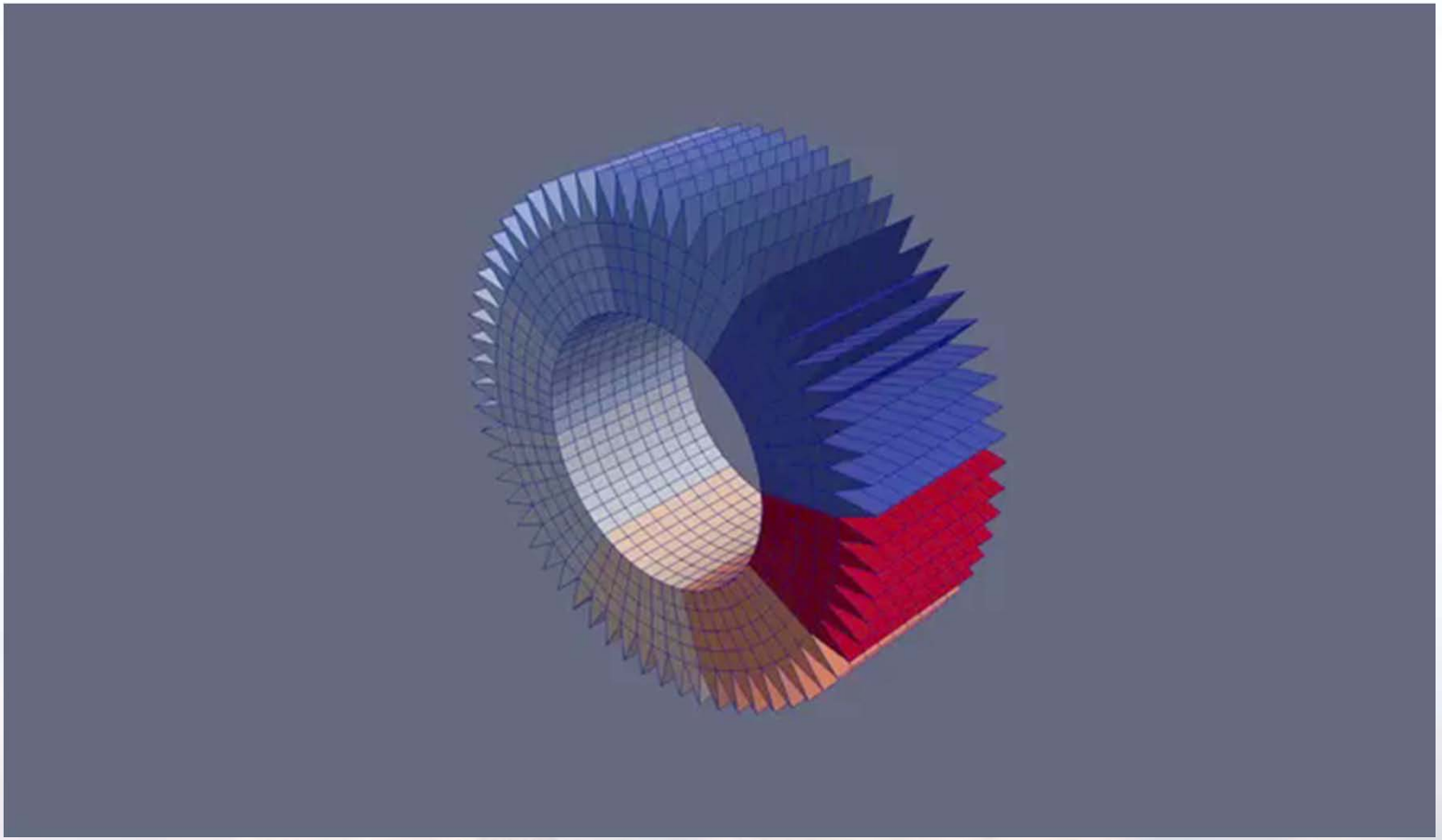
```
bulk_data.communicate_field_data(…);
```

Simple Mesh Modification Example

- **Breaking teeth off of the gear**
  - Distribute mesh over available processes
  - Create 6 new nodes to attach to the wedge
  - Destroy the relationship between the current nodes and the wedge
  - Attach the new nodes to the wedge
  - Copy the field data from the current nodes to the new nodes
    - The current nodes stay with the body gear



Putting it all together



Distribute mesh across available processes

- **Change entity owner (moving the entity to another process)**
  - The bulk data function change_entity_owner is a parallel collective call that ***gives away*** ownership of entities to other processes

```
//EntityProc is the pair
//(Entity *owned_entity, unsigned to_proc_id)
std::vector< stk::mesh::EntityProc> > move_entities;

// move the wedge to proc 2
if ( bulk_data.parallel_rank() ==  0) {
  move_entites.push_back( std::pair(&wedge,2));
}

// Parallel collective call
bulk_data.change_entity_owner( move_entities );

// The field data will also be moved with the wedge
```

Creating a new wedge

- **Creating new entities**
  - When new entities are created the creating process is the *owner* of the entity
  - If two or more processes create an entity with the same rank and identifier, the entity will be ***shared***

```
//Declare a new wedge element
stk::mesh::PartVector add_parts;
add_parts.push_back( wedge_part );
stk::mesh::Entity & wedge = bulk_data.declare_entity(
                                                      element_rank,
                                                      element_id,
                                                      add_parts
                                                    );
```

Creating new nodes

- **Generating new entities**
  - The bulk data function generate_new_entities is a parallel collective call that will create new entities of the requested ranks with *globally unique ids*

```
//create 6 nodes on process 0
std::vector<size_t> num_requested_entities(num_entities_rank,0);

if ( bulk_data.parallel_rank() == 0) {
        num_requested_entities[node_rank]=6;
}

stk::mesh::EntityVector requested_nodes;

//parallel collective call
bulk_data.generate_new_entities(
                                num_requested_entities,
                                request_nodes
                               );
```

Attaching the nodes to the wedge

- **Creating/Destroying entity relations**
  - Relations are directed from the higher ranking entity to the lower ranking entity, the converse relation is automatically inserted/deleted
  - Processes can only create/destroy relations when they own or share the higher ranking entity
  - Creating or deleting relations may change entity's induced mesh part membership

```
// declare relations from the wedge to the nodes
for ( size_t i=0; i<6; ++i) {
  bulk_data.declare_relation (
                        wedge, // from entity
         requested_nodes[i], // to entity
                            i  // relation identifer
                               );
}
```

Destroying nodes

- **Destroying entities**
  - A process may destroy its reference to an entity if the entity does not have a relation to a higher ranking entity in its owned closure.
  - If the owning process destroys an entity and another process *shares* the entity, ownership automatically transfers to a *sharing* process

```
// destroy the old nodes attached to the wedge
stk::mesh::PairIterRelations
    node_relations = wedge.relations(node_rank);

for ( size_t i=0; i<node_relations.size(); ++i) {
  stk::mesh::Entity * node = node_relations[i].entity();
  //destroy relation to wedge
  bulk_data.destroy_relation( wedge, *node );
  //destroy the entity
  bulk_data.destroy_entity( node );
}
```

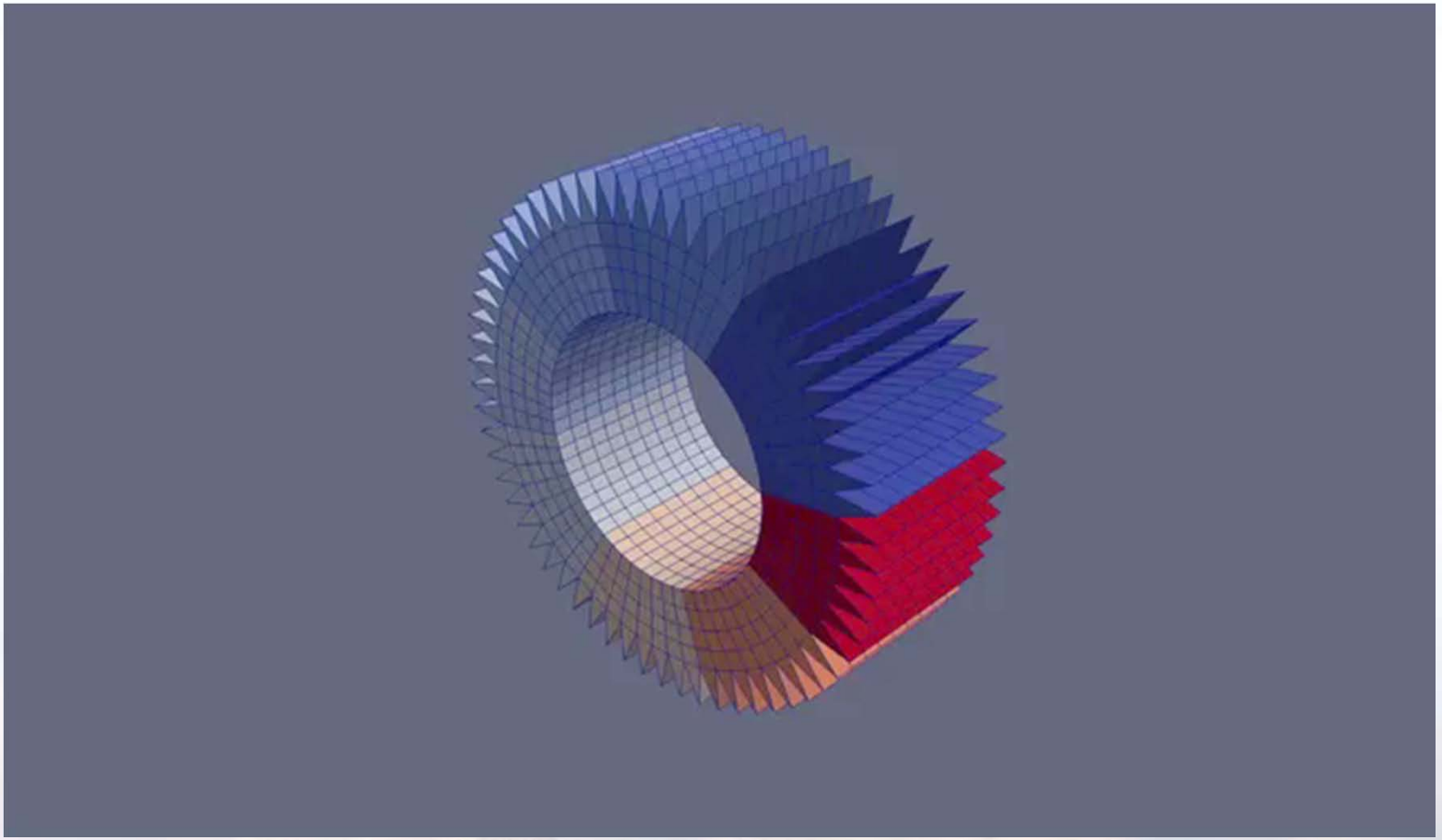
Changing mesh part membership

- Processes can only change part membership when they **own** or **share** the entity
- The entity will be moved to a different bucket
- The fields available to the entity will change to match the fields restrictions

```
// add the wedge to the cylindrical coordinate part
stk::mesh::PartVector add_parts, remove_parts;
add_parts.push_back( & cylindrical_coord_part );

bulk_data.change_entity_parts(
                                wedge,
                                add_parts,
                                remove_parts
                               );
// If cylindrical_coord_part was declare to be of rank element,
then the nodes will be induced into this part and the
cylindrical coordinate field will be available to the nodes
```

Gear Demo: Putting it all together



STK: Beyond stk-mesh
(what else is in STK?)

STK Tutorial

Carter Edwards, Todd Coffey,
Dan Sunderland, Alan Williams

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STK modules overview

Algorithm-Support (AlgSup)

- Multi-threaded execution of bucket-loop algorithms

Search

- Proximity, mesh independent

Linsys, IO, Rebalance

- Bridges from mesh-data to external capabilities
- Built optionally

Util

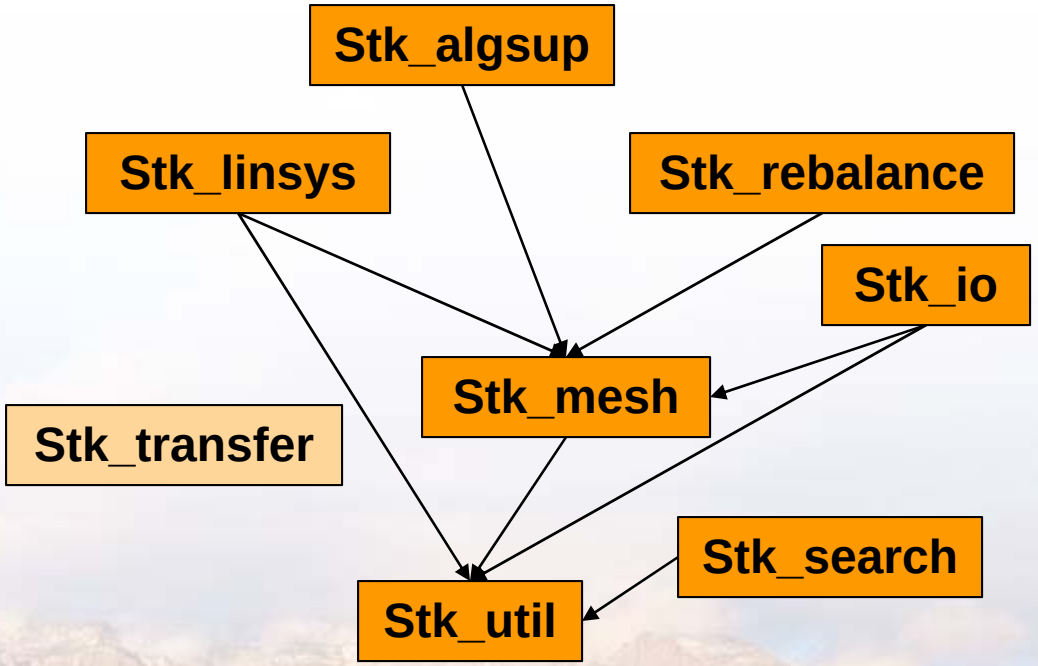
- Everything depends on util directly or indirectly

Transfer

- Not yet implemented

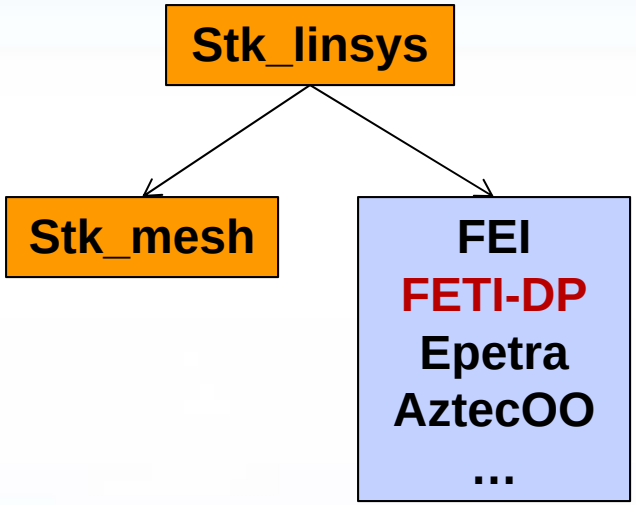
Dependency diagram:

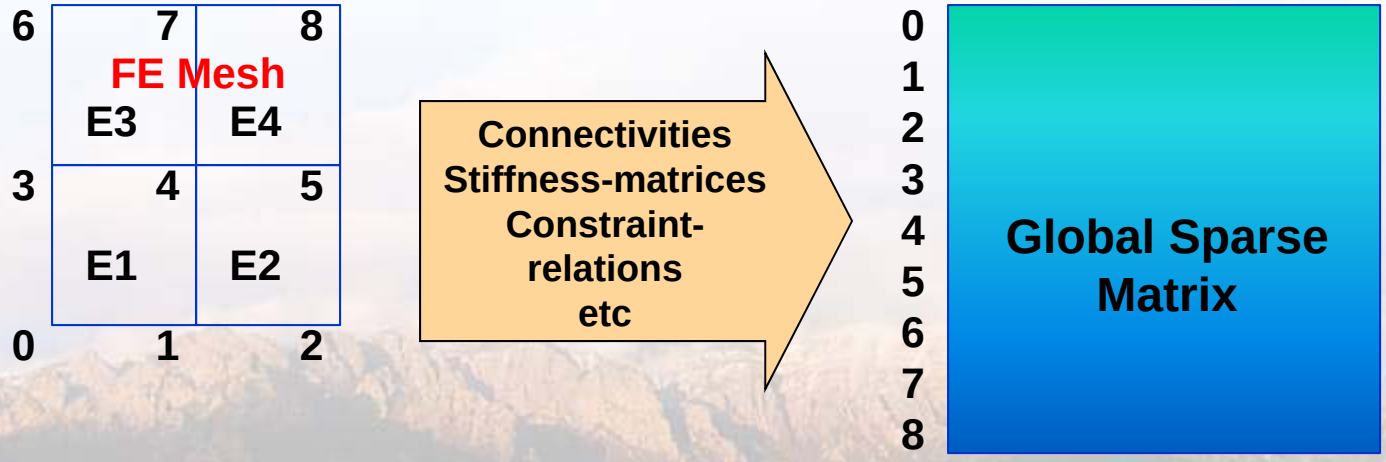
- Arrows point towards a module that is used (depended on) by another module.



STK linsys – bridge between mesh-data and linear-systems

Stk_linsys provides helpers for assembling linear-systems





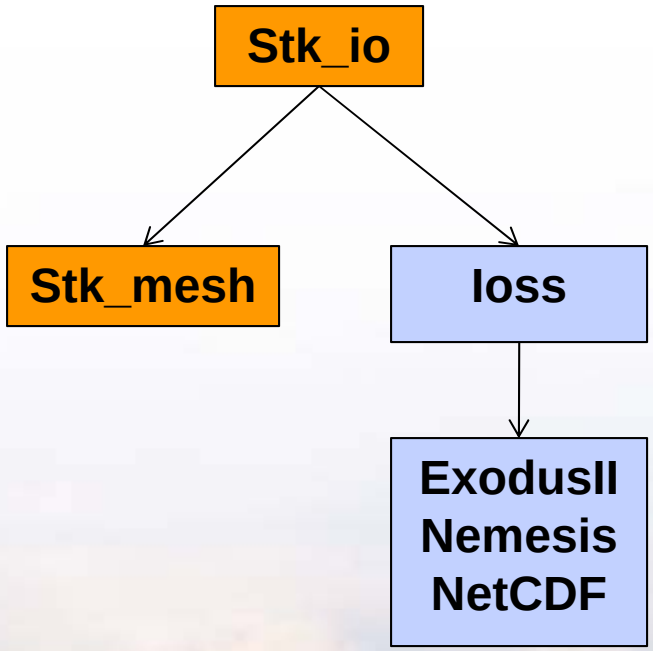
STK IO – Bridge between mesh-data and disk IO

IOSS: Abstract Finite Element mesh interface

- Object-Oriented
- Database-Independent
- ExodusII is primary output format
- Also supports XDMF, heartbeat, history, and pamgen

Stk_io is a Bridge layer that understands the interfaces of stk_mesh and Ioss.

- Provides functions for moving data to/from stk_io and Ioss.
- Provides high-level functions for creating a mesh input and/or results outputwith minimal code.
- Lower-level functions also provided for more control of the data movement.



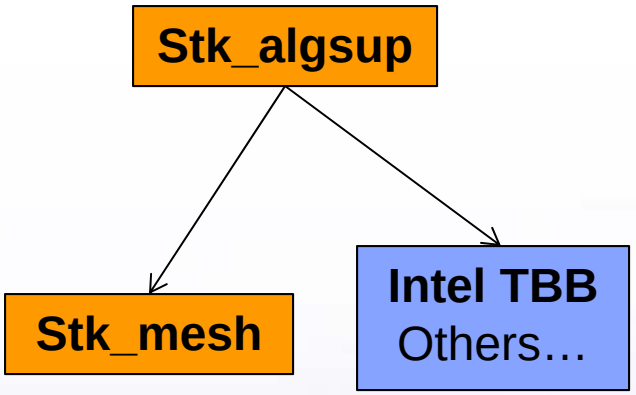
STK_AlgSup – Algorithm Support

Infrastructure for executing bucket-loop algorithms, including multi-threaded.

Recall the gears demo had loops for updating coordinates, etc.

In general, many algorithms on mesh data can be described as:

- create selector for desired parts
- get buckets
- for each bucket:
  - get field-data
  - perform computations



The bucket-loop is often compute-intensive and can benefit from thread-parallel (or GPU) execution.

Gear Rotation Computation (bucket-wise)

```
for (BucketVector::iterator b_itr = selected_node_buckets.begin();
      b_itr != selected_node_buckets.end(); ++b_itr)  {
    Bucket & b = **b_itr;

    const BucketArray<CartesianField> old_coord_data( cartesian_coord_field, b);
    BucketArray<CartesianField> displ_data(displacement_field.field_of_state(StateNew), b);
    …

    for (size_t node_index = 0; node_index < b.size(); ++index) {

      // Compute new and old coordinate data and assign to displacements:

      displ_data(0,index) = new_coord_data[0] – old_coord_data(0,index);
      …

    }
}
```

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STK_AlgSup – Algorithm Support (continued)

An Algorithm can be any class that has an 'apply' method…
(and the apply method contains the body of your bucket-loop**)**

```
struct My_Algorithm {

void apply(stk::mesh::Bucket::iterator begin,
           stk::mesh::Bucket::iterator end) const
{
  size_t num_nodes = std::distance(end – begin);

  const BucketArray<CartesianField> old_coord_data( cartesian_coord_field, begin, end
  BucketArray<CartesianField>
       displ_data(displacement_field.field_of_state(StateNew), begin, end);

  for (size_t node_index = 0; node_index < num_nodes; ++node_index) {
    // Compute new and old coordinate data and assign to displacements:

    displ_data(0,node_index) = new_coord_data[0] – old_coord_data(0,node_index);
    …
  }
}
 …
};
```

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STK_AlgSup – Algorithm Support

Example using Intel Thread Building Blocks (TBB)

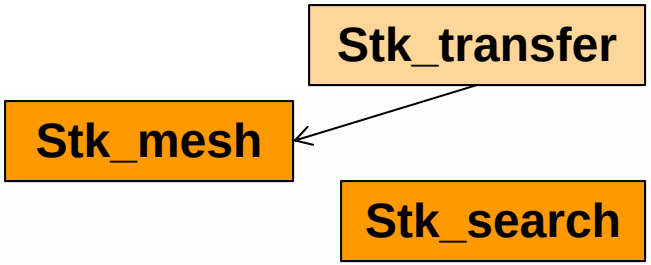
```
stk::AlgorithmRunnerInterface*
        alg_runner = stk::algorithm_runner_tbb(num_threads);

stk::mesh::Part& gear_part = …
stk::mesh::Selector select_nodes = gear_part & meta_data.locally_owned_part();

My_Algorithm alg;

alg_runner->run(select_nodes, …, bulk_data.buckets(NODE_RANK), alg);
```

The algorithm-runner implementation can launch buckets on different threads.

The goal is for application code (My_Algorithm) to be unaware of threading, as much as possible.
(Of course thread-safety issues must still be kept in mind…)

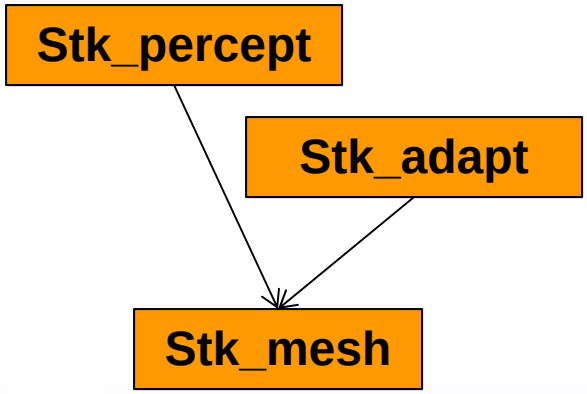
STK_Search, STK_Transfer

- Geometric proximity searches including: OctTree, BIH
- Proximity search doesn't depend on stk_mesh
  - Users provide lists of bounding boxes or bounding spheres
- Stk_transfer will use stk_search, and will depend on stk_mesh
- …but there will also be stk_mesh – to – non-stk_mesh transfers



STK_adapt, STK_percept

- Stk_percept
  - Verification tools, including:
    - Postprocessing
    - Error metrics (e.g. norms)
    - Manufactured solutions
- Stk_adapt
  - Extend/modify the discretization
    - Refine elements
    - Increase polynomial order
    - Convert topology (e.g. hex to tet)



STK_util - Utilities

STK_util doesn't depend on any other STK module

STK_util contains several subdirectories of related tools

- **Diag**
  - Timers
  - Ostream manipulators
- **Environment**
  - Error Reporting
  - Output Logging
- **Parallel**
  - Comm utils
  - Distributed-Index
- **Util**
  - String comparisons
  - Array Ops
  - etc

Future Modules

- **Stk_transfer:**
  - Mesh to mesh transfers
  - Including stk-mesh – to – non-stk-mesh transfers
- **Stk_parser:**
  - Input deck parsing
  - Sierra SDDM
- **Stk_coupling:**
  - Code coupling layer

Goals of the Toolkit Team

- **Clarity of code**
- **Use-case driven API & implementation**
- **Capability/Flexibility/Performance**
  - Growing collection of performance tests, use-cases, …
- **Modularity**
- **Highly unit-tested code**

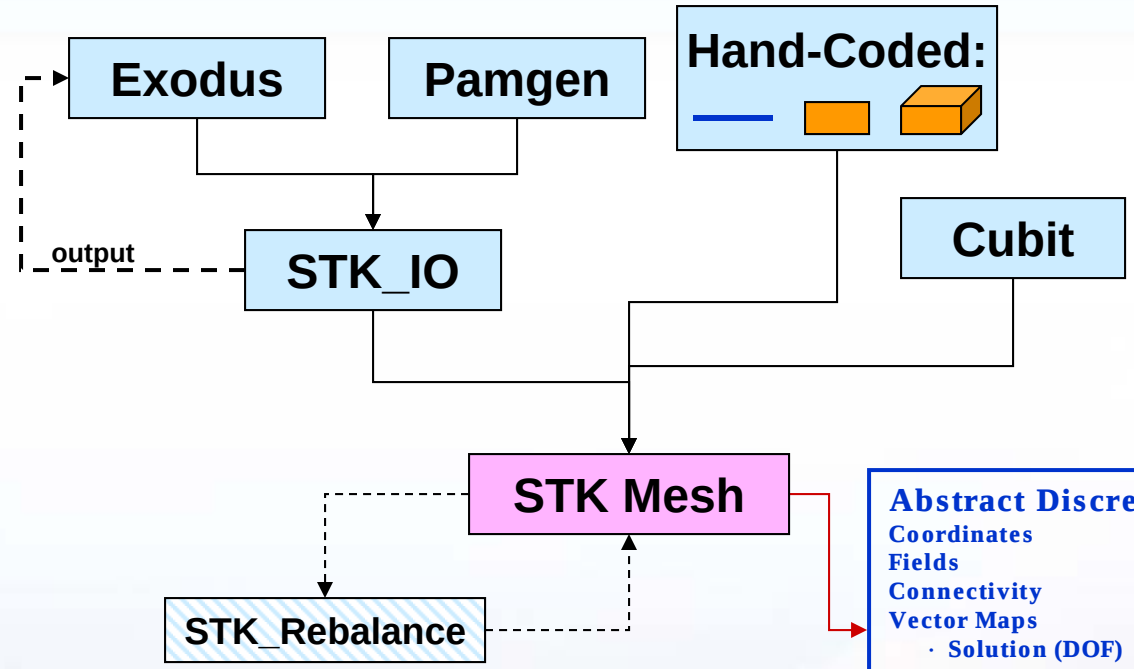
stk_mesh/stk_mesh/base		90.1 %	3272 / 3631
stk_mesh/stk_mesh/baseImpl		93.8 %	1099 / 1172

- **Threading/GPU support**
- **Facilitate external collaborations with Sierra**
- **Agile development**

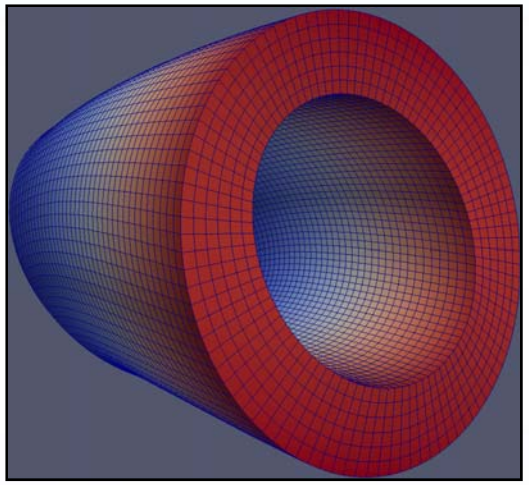
Current Users

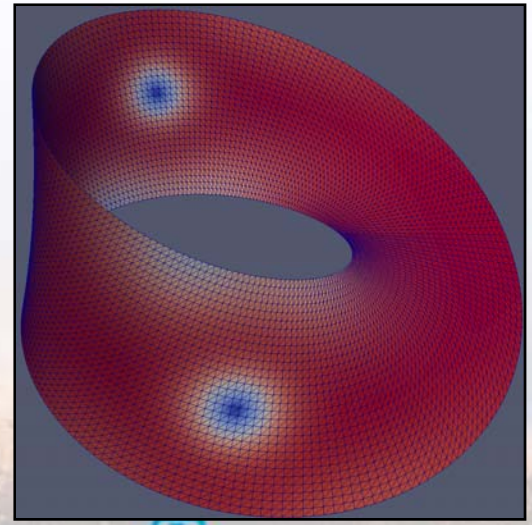
- Sierra (suite of finite-element analysis applications), SNL
- Cubit (Mesh generation)
  Steve Owen/Matt Staten, SNL
- Albany (Prototyping rapid PDE-application development)
  Andy Salinger, SNL
- Adaptive Mesh Refinement
  Ulrich Küttler, Technische Universität München
- Superconductivity simulations
  Nico Schloemer, University of Antwerp
- Fracture mechanics
  Joe Bishop, Fracture LDRD, SNL
- Charon (planned for FY11), SNL

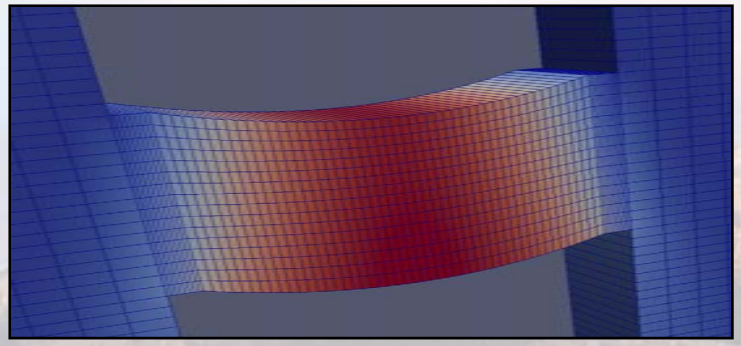
STK Capability in Albany



Abstract Discretization
- Coordinates
- Fields
- Connectivity
- Vector Maps
  - Solution (DOF)
  - Coordinate
  - Node
- Jacobian Graph
- Node Sets







Thank you!

- **For more information:**
  http://trilinos.sandia.gov/packages/stk/
  stk-users@software.sandia.gov email list

- **We want more feedback!**
  - Good clean clear APIs and code can't be achieved without user feedback!

- **Thanks for attending this tutorial!**

- **Developers:**
  Dave Baur, Todd Coffey, Carter Edwards,
  Jim Foucar, Russell Hooper, James Overfelt,
  Greg Sjaardema, Dan Sunderland, Alan Williams