

Computational Mesh Abstractions

Matthew Knepley and Dmitry Karpeev

Mathematics and Computer Science Division

Argonne National Laboratory

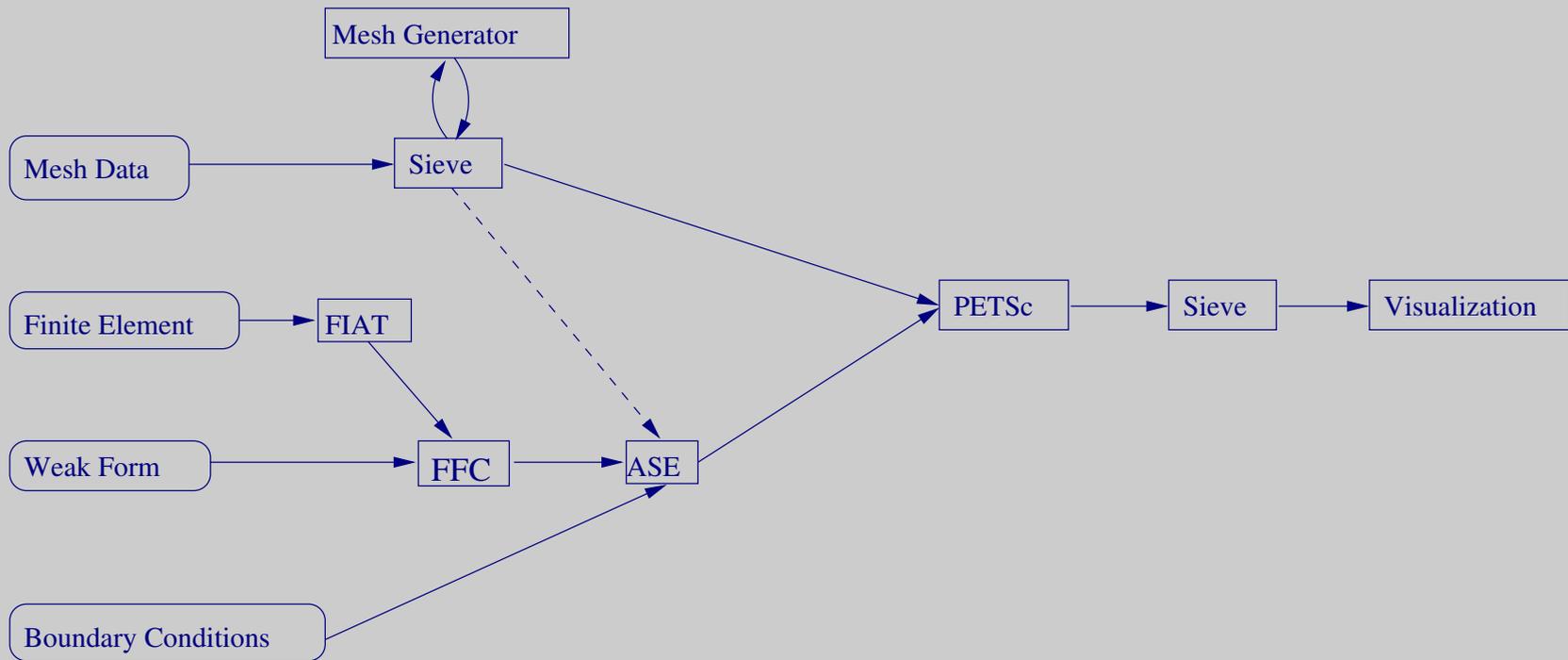
MOTIVATION

- Linear Algebra Abstractions
 - Allows reuse of iterative solvers (Krylov methods)
 - **Vec** and **Mat**
 - **KSP** uses **Vec** and **Mat** through interface only

HIERARCHY ABSTRACTIONS

- Expresses decomposition of space into progressively finer pieces
- Supports data overlays
 - Restriction to finer subspaces
 - Assembly to the whole space
 - Reduction: assembly-restriction
- Extensibility
 - User specifies local assembly/restriction
 - Hierarchy encodes data flow

TRIAL FRAMEWORK



The Sieve

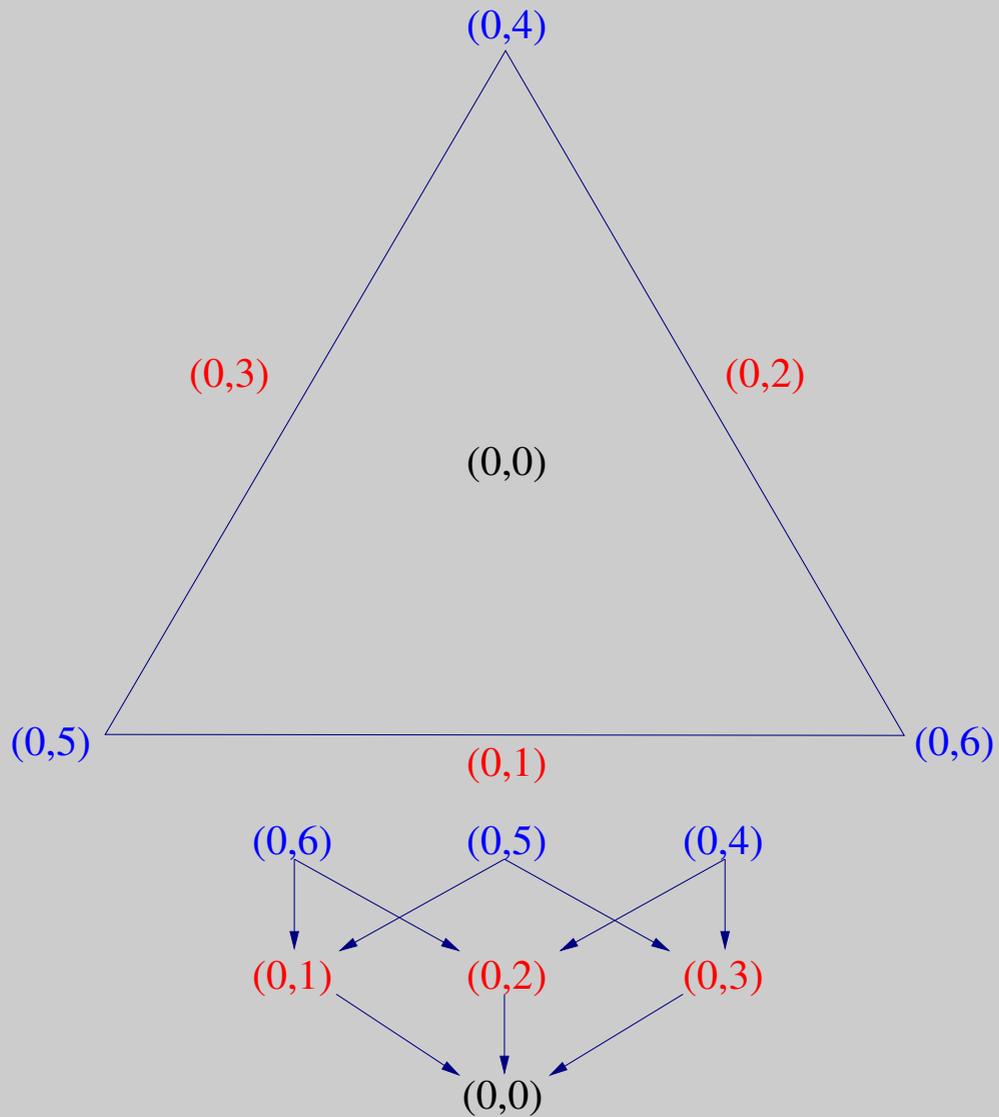
WHAT IS A SIEVE?

A Sieve encodes topology

- Category with arrows denoting a *covering* relation
 - We say that *cap* elements cover *base* elements
 - Any set of elements is called a *chain*
- Model for set theory
- Hierarchical geometric data
 - Finite element meshes
 - Multipole octree
- Clean separation between topology and data organized by the topology
 - Con-fused in most packages, e.g. PETSc Vec

SIMPLE SIEVE

Topological elements are encoded as (process, local id)



SIEVE PRIMITIVES

Cone: The set of cap elements covering a base element

$$\text{cone}(0, 0) = \{(0, 1), (0, 2), (0, 3)\}$$

Closure: The iterated cone

$$\text{closure}(0, 0) = \{(0, 1), (0, 2), (0, 3), (0, 4), (0, 5), (0, 6)\}$$

Support: The set of base elements covered by a cap element

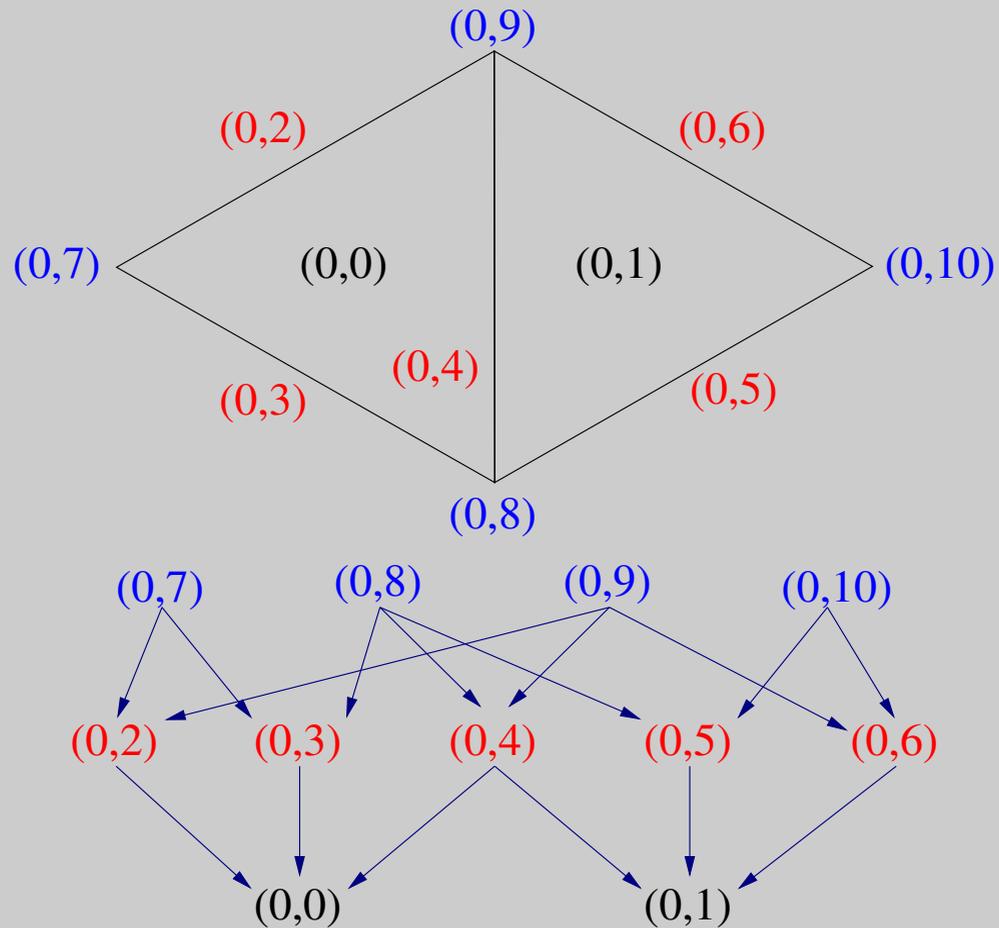
$$\text{support}(0, 4) = \{(0, 2), (0, 3)\}$$

Star: The iterated support

$$\text{star}(0, 4) = \{(0, 2), (0, 3), (0, 0)\}$$

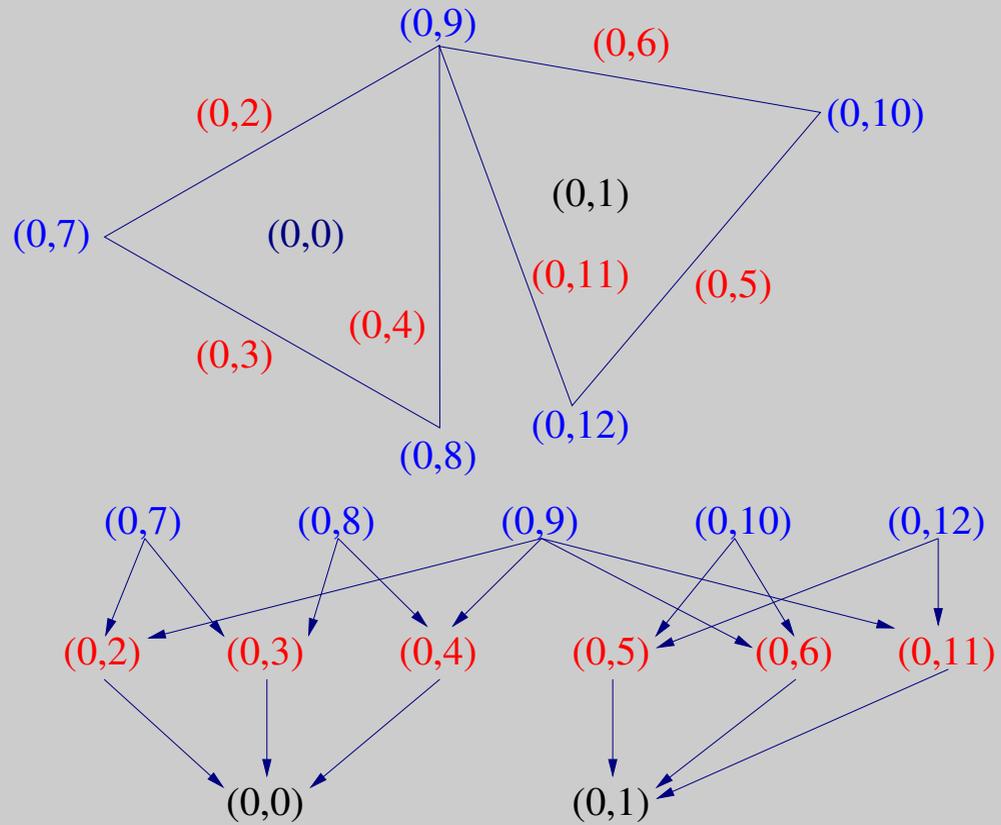
DOUBLET MESH

We can examine the meet and join using two adjacent elements

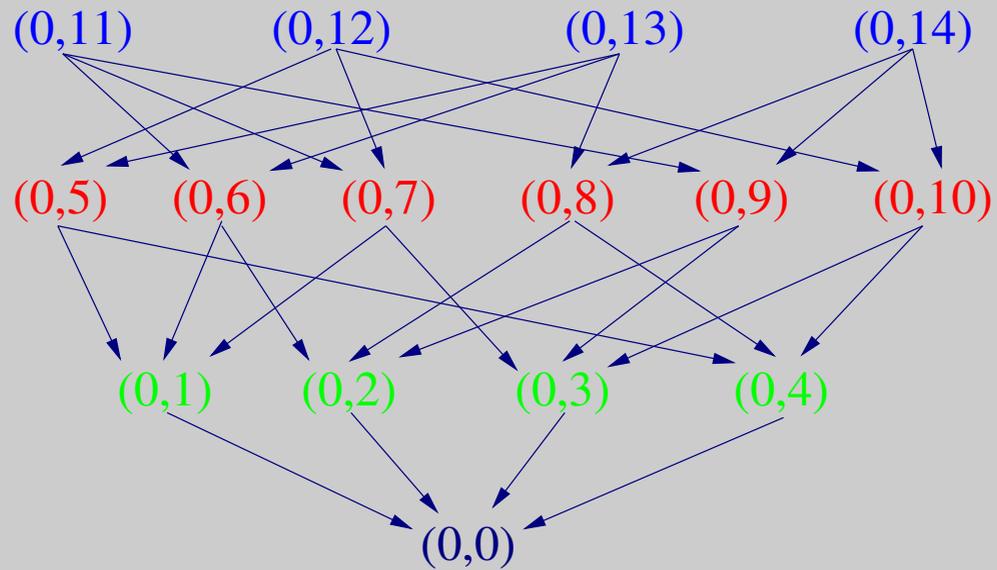
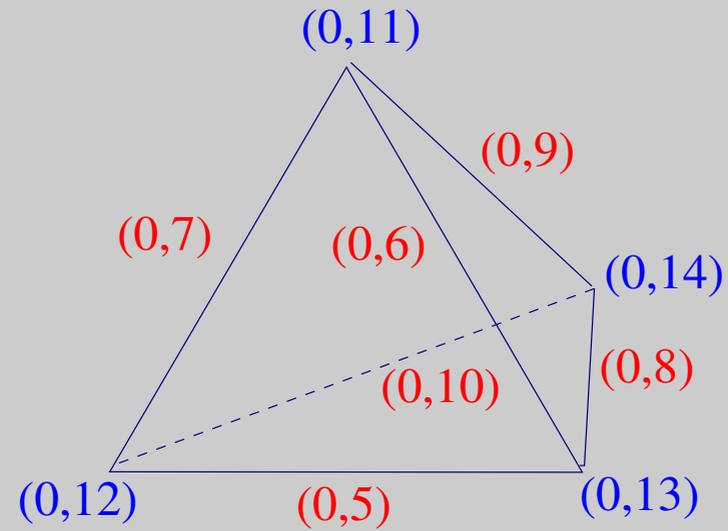


DOUBLET MESH II

These elements provide a different lattice



TETRAHEDRON MESH



LATTICE OPERATIONS

Meet: The smallest set of elements whose star contains the given chain

- Can be seen as the intersection of the closures of the chain elements
- For the doublet mesh, $meet((0, 0), (0, 1)) = (0, 4)$
- For the split doublet mesh, $meet((0, 0), (0, 1)) = (0, 9)$

Join: The smallest set of elements whose closure contain the given chain

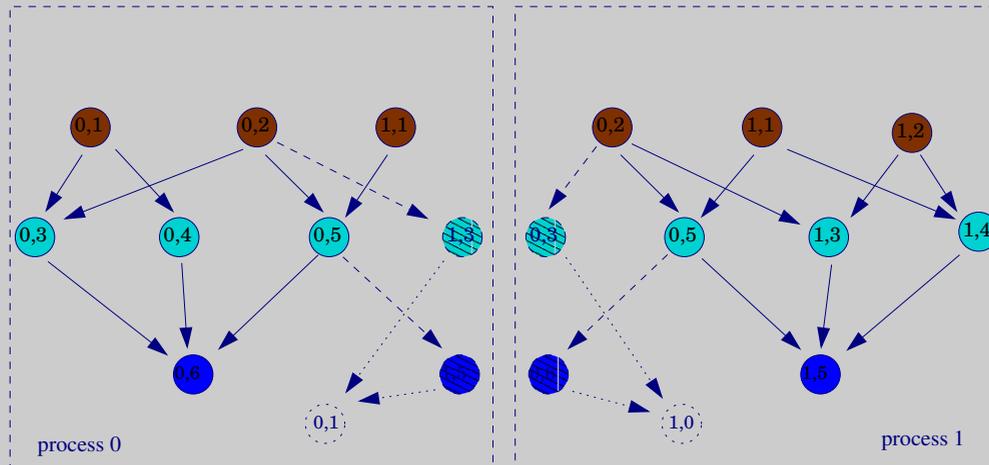
- Can be seen as the intersection of the supports of the chain elements
- For the doublet mesh, $join((0, 0), (0, 1)) = ((0, 0), (0, 1))$
- For the tetrahedron, $join((0, 5), (0, 7)) = (0, 1)$
- However, also for the tetrahedron, $join((0, 5), (0, 9)) = (0, 0)$

CONE COMPLETION

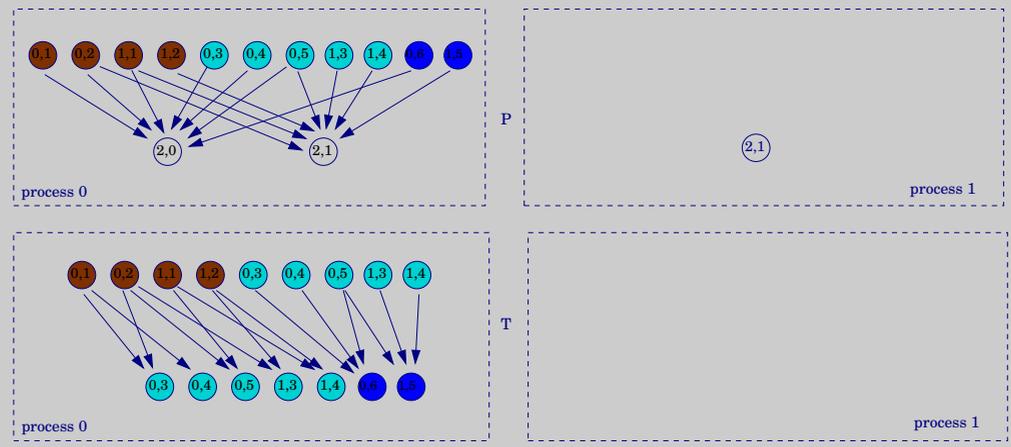
In a distributed Sieve, parts of an element's cone may lie on different processes. *Completion* constructs another local Sieve which contains the missing parts of each local cone.

- Dual operation of *support completion*
 - Uses the same communication routine
- Single parallel operation is sufficient for Sieve
- Enables many other parallel operations
 - Dual graph construction
 - Graph partitioning
 - Parallel and periodic meshing

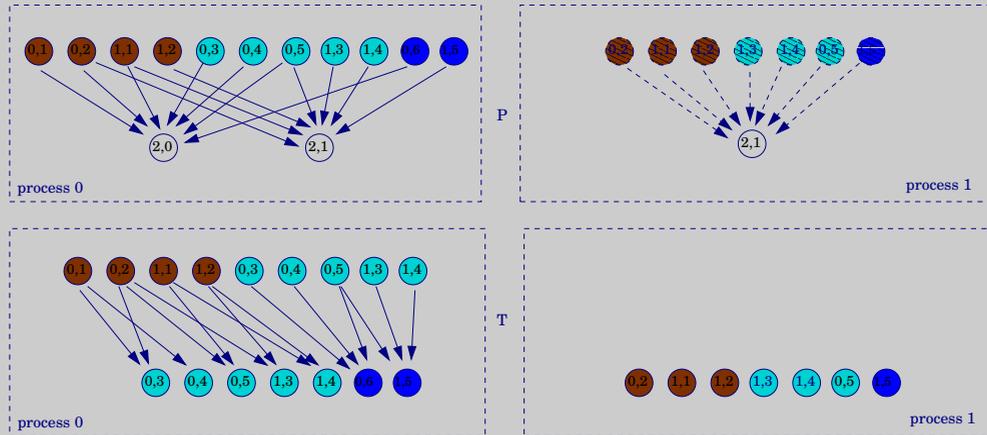
DOUBLET MESH COMPLETION



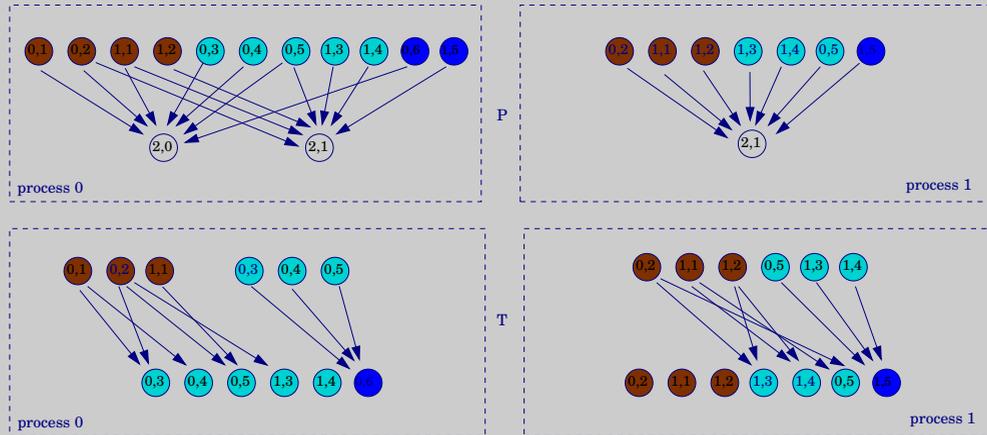
DOUBLET MESH DISTRIBUTION I



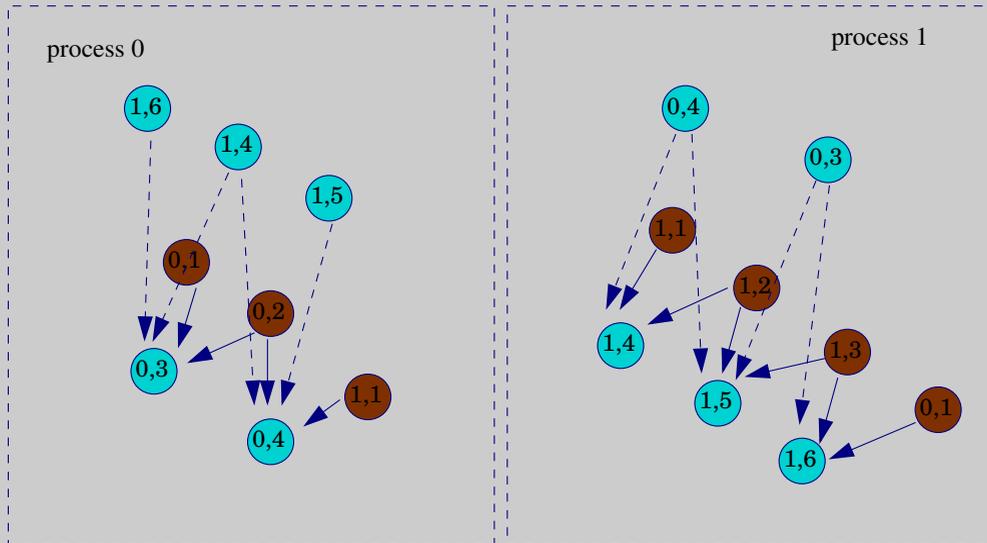
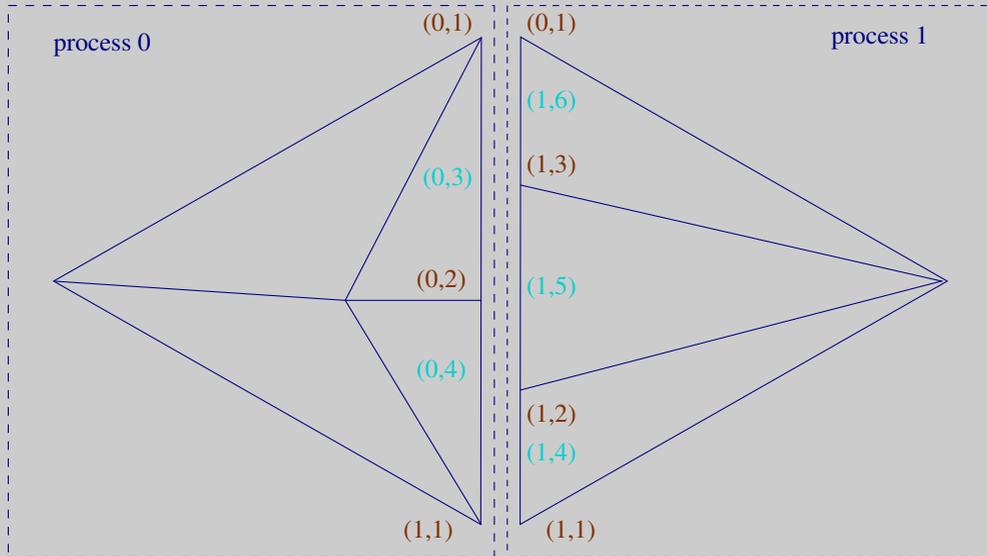
DOUBLET MESH DISTRIBUTION II



DOUBLET MESH DISTRIBUTION III



NONCONFORMING DOUBLET



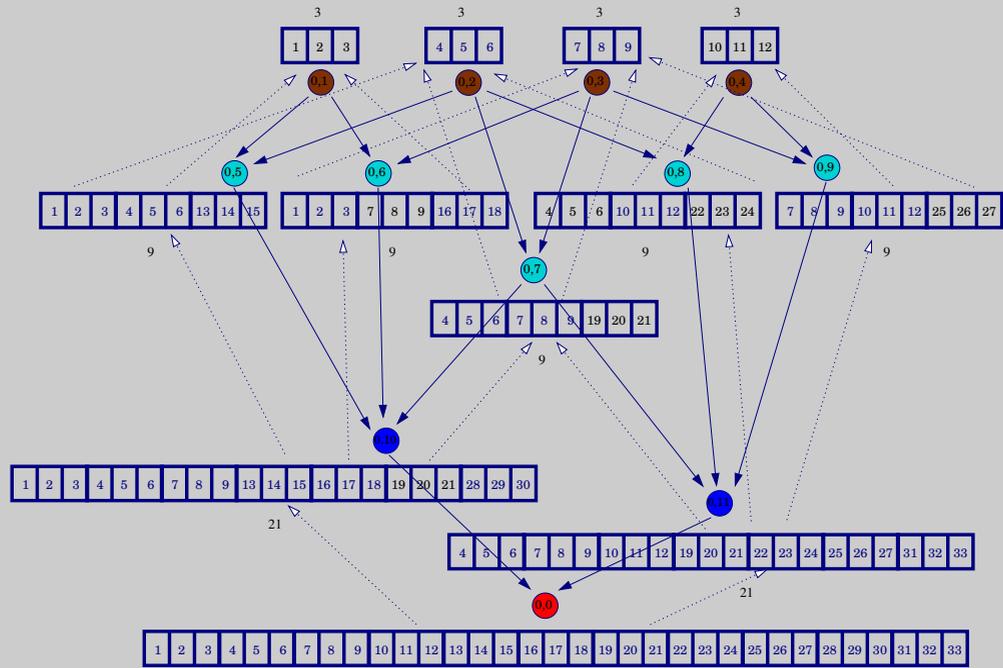
The Sieved Array

RESTRICTION

Restriction is the dual operation to covering

- Allows global fields to be manipulated locally
 - This is the heart of FEM
- Ties value storage to the topology (hierarchy)
- Can apply to any mesh subset (chain)
 - Single element
 - Mesh boundary
 - Local submesh
- Looks like indexing with elements

DOUBLET ARRAY



SIEVED ARRAYS

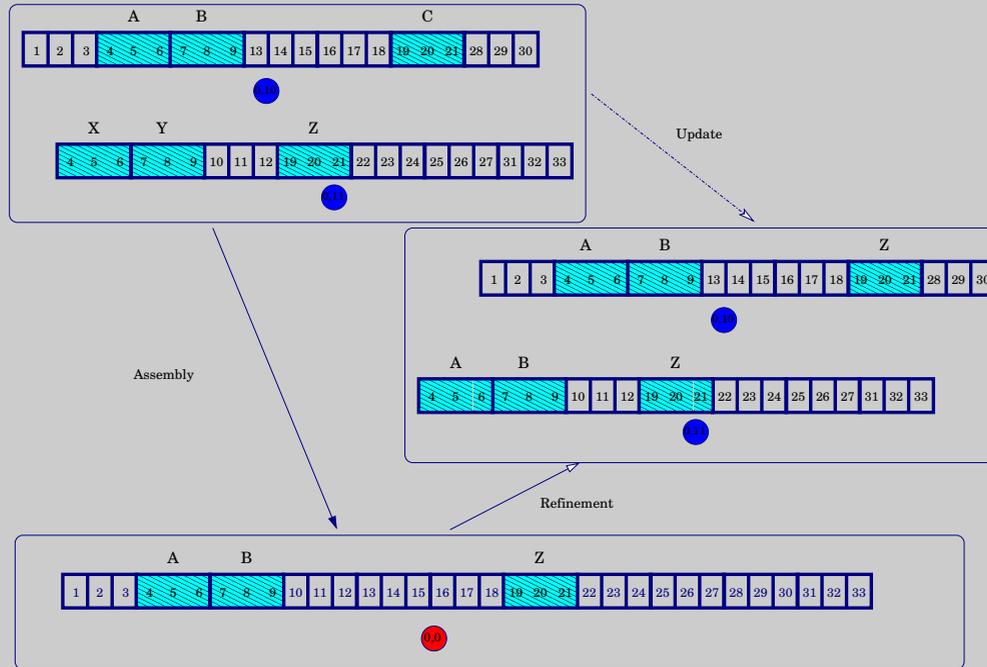
- Represent values organized by the underlying topology
 - Solution fields
 - Mesh geometry
 - Boundary markers
 - Chemical species
- Allows natural operations of restriction and prolongation (assembly)
 - Many different storage policies may be used
- Allows user to work completely locally, letting the Array handle assembly
 - Very similar to PETSc strategy for parallelism
- Arrays are sections of a fibre bundle over the mesh
 - Transition between chains is a (nontrivial) map between vector spaces

SIFTING

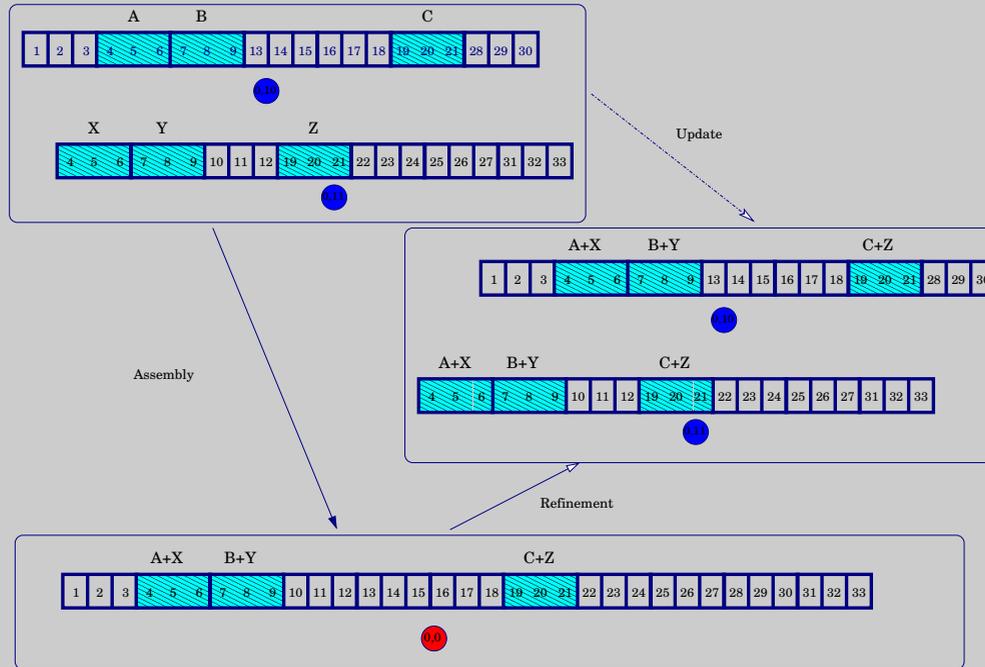
Sifting is the process of restricting or assembly of an Array

- Nontrivial assembly and restriction policies
 - replacement/preservation
 - addition
 - coordinate transformation
 - orientation using the input chain
 - Nonconforming overlapping grids
- Decouples storage/restriction policy from continuum mathematics
 - Vectors are **not** Arrays
- Seems to tied to the storage to factor out

DOUBLET ASSEMBLY I

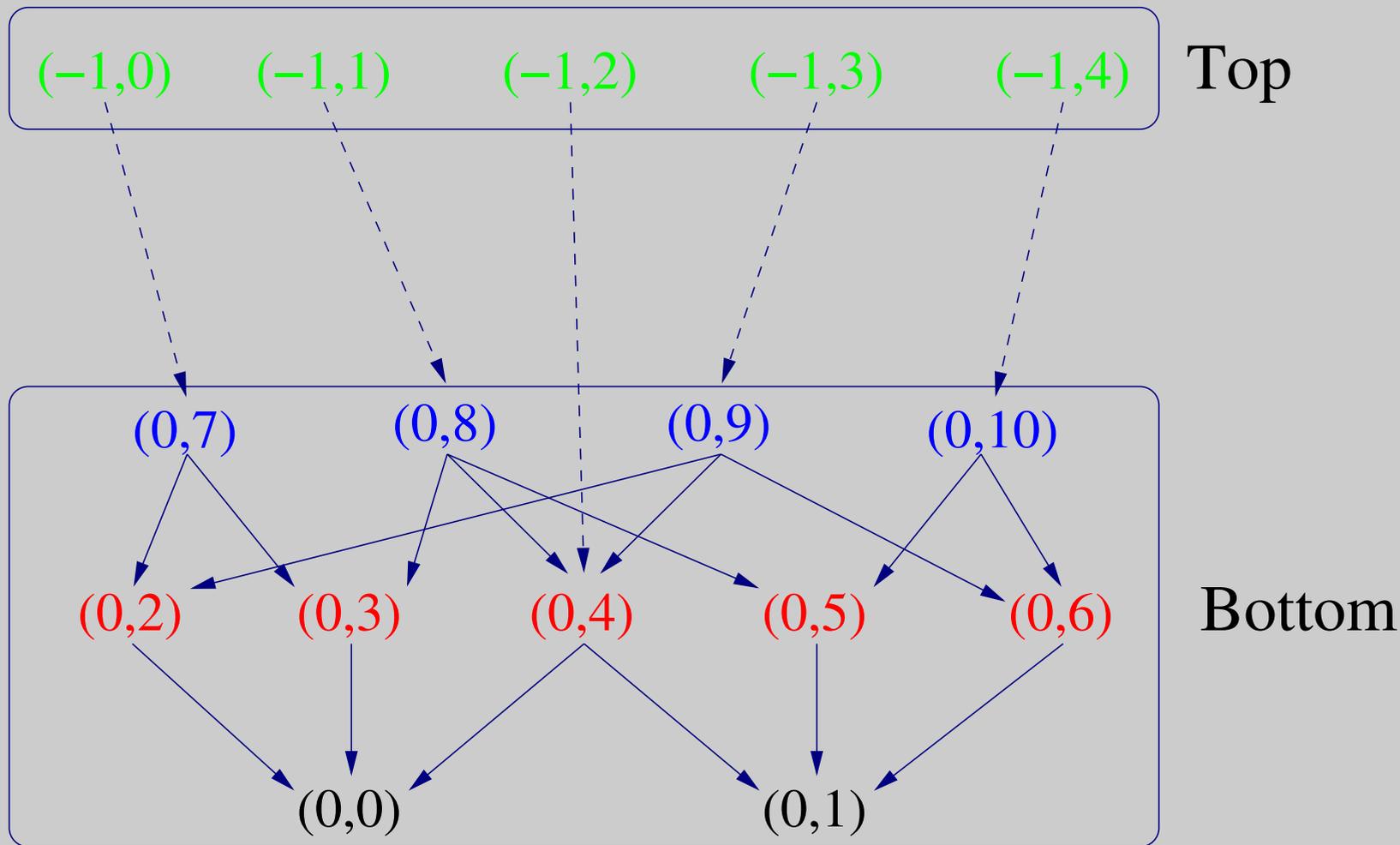


DOUBLET ASSEMBLY II



STACK

A *Stack* connects two Sieves with *vertical* arrows

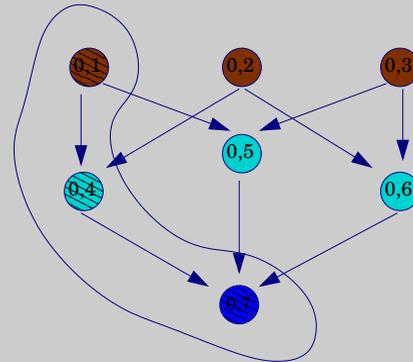
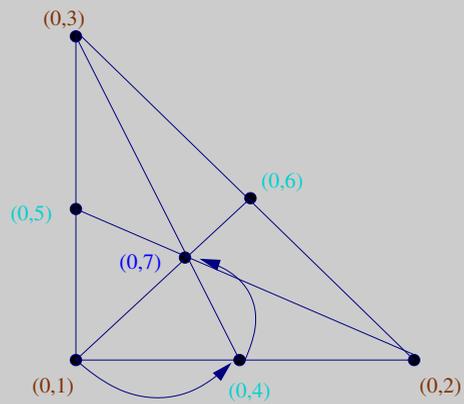


INDEX BUNDLE

Uses Stack to organize the degrees of freedom over a mesh

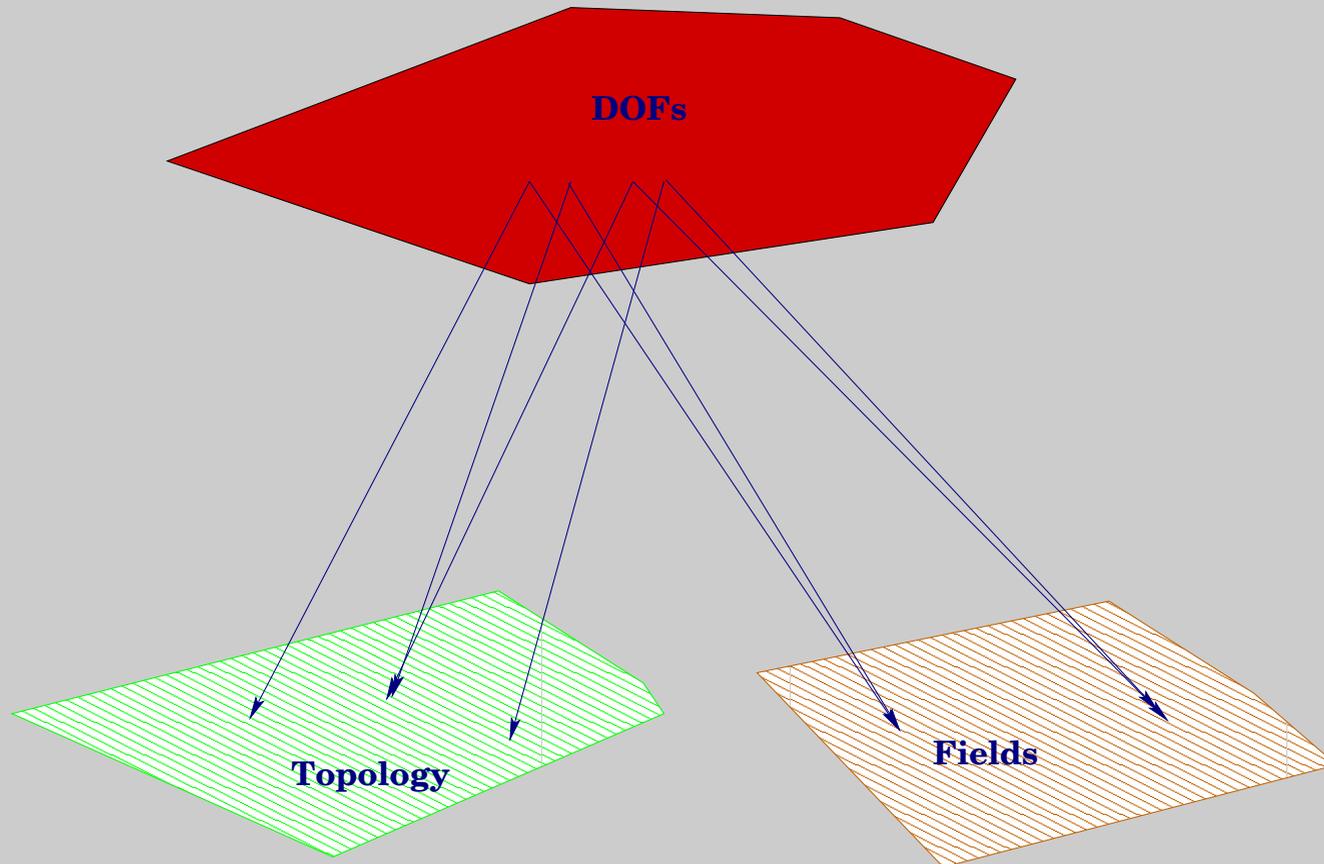
- The top (discrete) sieve contains the degrees of freedom
- The bottom sieve is the mesh topology
- Sieve operations now occur over vertical arrows
- Retrieves indices over a given chain
- Computes relative and ordered indices
- Computes indices on the overlap

ORDERED DATA



DEGREES OF FREEDOM FOR MULTIPLE FIELDS

Using a DOF and Field Stack with common top Sieve, we can extract the variables from a given field using the *meet* operation.



Examples

DUAL GRAPH CREATION

```
topology = mesh.getTopology()
# Loop over all edges
completion, footprint = topology.supportCompletion(supportFootprint)
for edge in topology.heightStratum(1):
    support = topology.support(edge)
    if len(support) == 2:
        dualTopology.addCone(support, edge)
    elif len(support) == 1 and completion.capContains(edge):
        cone = (support[0], completion.support(edge)[0])
        dualTopology.addCone(cone, edge)
dualMesh.setTopology(dualTopology)
```

MESH PARTITIONING

```
def partitionDoublet(self, topology):  
    if rank == 0:  
        topology.addCone(topology.closure((0, 0)), (-1, 0))  
        topology.addCone(topology.closure((0, 1)), (-1, 1))  
    else:  
        topology.addBasePoint((-1, rank))
```

MESH PARTITIONING

```
def genericPartition(self, comm, topology):  
    # Cone complete to move the partitions to the other processors  
    completion, footprint = topology.coneCompletion(footprintTypeCone)  
    # Merge in the completion  
    topology.add(completion)  
    # Cone complete again to build the local topology  
    completion, footprint = topology.coneCompletion(footprintTypeCone)  
    # Merge in the completion  
    topology.add(completion)  
    # Restrict to the local partition  
    topology.restrictBase(topology.cone((-1, rank)))  
    # Optional: Support complete to get the adjacency information
```

FEM NUMBERING

Start by creating the discretizations and a Stack

```
elements = [FIAT.Lagrange.Lagrange(FIAT.shapes.TRIANGLE, 2),  
            FIAT.Lagrange.Lagrange(FIAT.shapes.TRIANGLE, 3)]  
ranks = [1, 0]  
dof = ALE.Sieve.Sieve()  
numbering = ALE.Stack.Stack()  
numbering.setTop(dof)  
numbering.setBottom(topology)
```

FEM NUMBERING

```
def multipleFieldsStack(self, topology):
    completion, footprint = topology.supportCompletion(supportType)
    for p in topology.space():
        if completion.capContains(p):
            support = footprint.support([p]+list(completion.support(p)))
            if [0 for processTie in support if processTie[1] < rank]:
                continue
    indices = []
    for field in range(len(elements)):
        entityDof = len(dualBases[field].getNodeIDs(topology.depth(p))[0])
        tensorSize = entityDof*max(1, dim*ranks[field])
        var = [(-(rank+1), index+i) for i in range(tensorSize)]
        indices.extend(var); index += dof
        dof.addCone(var, (-1, field))
    numbering.addCone(var, p)
    completion, footprint = topology.coneCompletion(coneType)
```

FEM ASSEMBLY

```
elements = mesh.heightStratum(0)
elemU = u.restrict(elements)
# Loop over highest dimensional elements
for element in elements:
    # We want values over the element and all its coverings
    chain = mesh.closure(element)
    # Retrieve the field coefficients for this element
    coeffs = elemU.getValues([element])
    # Calculate the stiffness matrix and load vector
    K, f = self.integrate(coeffs, self.jacobian(element, mesh, space))
    # Place results in global storage
    elemF.setValues([chain], f)
    elemA.setValues([[chain], [chain]], K)
F = elemF.prolong([])
A = elemA.prolong([])
```

FEM ASSEMBLY

Notice that the prior code is independent of:

- dimension
- element type
- finite element
- sifting policy

CONCLUSIONS

Better mathematical abstractions bring concrete benefits:

- Vast reduction in complexity
 - Dimension independent code
 - Only a single communication routine to optimize
 - One relation handles all hierarchy
- Expansion of capabilities
 - Can handle hybrid meshes
 - Can handle complicated topologies (magnetization)
 - Can handle complicated structures (faults)