Finite Element Implementation

Matthew Knepley

Mathematics and Computer Science Division
Argonne National Laboratory

Institute for Computational Engineering and Sciences Seminar
University of Texas at Austin
July 17, 2008

Outline

Problems

The biggest problem in scientific computing is programmability:

- Lack of usable implementations of modern algorithms
  - Unstructured Multigrid
  - Fast Multipole Method
- Lack of comparison among classes of algorithms
  - Meshes
  - Discretizations

We should reorient thinking from

- characterizing the solution (FEM)
  - "what is the convergence rate (in h) of this finite element?"

to

- characterizing the computation (FErari)
  - "how many digits of accuracy per flop for this finite element?"

Problems

The biggest problem in scientific computing is programmability:

- Lack of widespread implementations of modern algorithms
  - Unstructured Multigrid
  - Fast Multipole Method
- Lack of comparison among classes of algorithms
  - Meshes
  - Discretizations

We should reorient thinking from

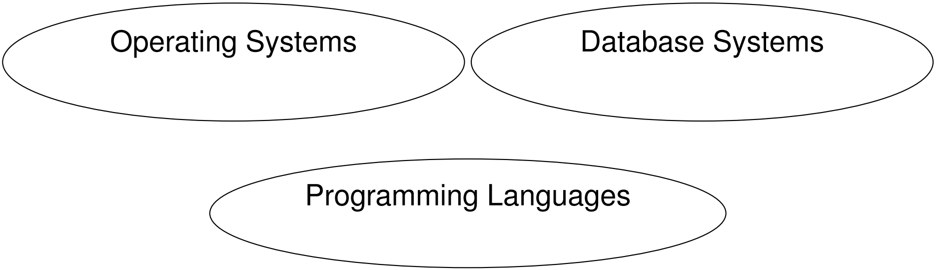
- characterizing the solution (FEM)
  - “what is the convergence rate (in *h*) of this finite element?”

to

- characterizing the computation (FErari)
  - “how many digits of accuracy per flop for this finite element?”

Interaction with Systems

We have to bridge the gap with Systems
to enable Scientific Computing



Interaction with Systems

We have to bridge the gap with Systems
to enable Scientific Computing

Operating Systems
Distributed Computing

Database Systems

Programming Languages

Interaction with Systems

We have to bridge the gap with Systems
to enable Scientific Computing

Operating Systems
Distributed Computing

Database Systems
Datamining

Programming Languages

Interaction with Systems

We have to bridge the gap with Systems
to enable Scientific Computing

Operating Systems
Distributed Computing

Database Systems
Datamining

Programming Languages
Code Generation

Future Compilers

I think compilers are victims of their own success (ala Rob Pike)

- Efforts to modularize compilers retain the same primtives
  - compiling on the fly (JIT)
  - **L**ow **L**evel **V**irtual **M**achine
- Raise the level of abstraction
  - **F**enics **F**orm **C**ompiler (variational form compiler)
  - Mython (**D**omain **S**pecific **L**anguage generator)

Representation Hierarchy

Divide the work into levels:

- Model
- Algorithm
- Implementation

Representation Hierarchy

Divide the work into levels:

- Model
- Algorithm
- Implementation

Spiral Project:

- **D**iscrete **F**ourier **T**ransform (DSP)
- **F**ast **F**ourier **T**ransform (SPL)
- C Implementation (SPL Compiler)

Representation Hierarchy

Divide the work into levels:

- Model
- Algorithm
- Implementation

FLAME Project:

- Abstract LA (PME/Invariants)
- Basic LA (FLAME/FLASH)
- Scheduling (SuperMatrix)

Representation Hierarchy

Divide the work into levels:

- Model
- Algorithm
- Implementation

FEniCS Project:

- Navier-Stokes (FFC)
- Finite Element (FIAT)
- Integration/Assembly (FErari)

Representation Hierarchy

Divide the work into levels:

- Model
- Algorithm
- Implementation

Treecodes:

- Kernels with decay (Coulomb)
- Treecodes (PetFMM)
- Scheduling (PetFMM-GPU)

Representation Hierarchy

Divide the work into levels:

- Model
- Algorithm
- Implementation

Treecodes:

- Kernels with decay (Coulomb)
- Treecodes (PetFMM)
- Scheduling (PetFMM-GPU)

Each level demands a strong abstraction layer

Outline

Outline

Form Decomposition

Element integrals are decomposed into analytic and geometric parts:

$$\int_{\mathcal{T}} \nabla\phi_i(\mathbf{x}) \cdot \nabla\phi_j(\mathbf{x}) d\mathbf{x} \quad (1)$$

$$= \int_{\mathcal{T}} \frac{\partial\phi_i(\mathbf{x})}{\partial x_\alpha} \frac{\partial\phi_j(\mathbf{x})}{\partial x_\alpha} d\mathbf{x} \quad (2)$$

$$= \int_{\mathcal{T}_{\mathrm{ref}}} \frac{\partial\xi_\beta}{\partial x_\alpha} \frac{\partial\phi_i(\xi)}{\partial\xi_\beta} \frac{\partial\xi_\gamma}{\partial x_\alpha} \frac{\partial\phi_j(\xi)}{\partial\xi_\gamma} |J| d\mathbf{x} \quad (3)$$

$$= \frac{\partial\xi_\beta}{\partial x_\alpha} \frac{\partial\xi_\gamma}{\partial x_\alpha} |J| \int_{\mathcal{T}_{\mathrm{ref}}} \frac{\partial\phi_i(\xi)}{\partial\xi_\beta} \frac{\partial\phi_j(\xi)}{\partial\xi_\gamma} d\mathbf{x} \quad (4)$$

$$= G^{\beta\gamma}(\mathcal{T}) K^{ij}_{\beta\gamma} \quad (5)$$

Coefficients are also put into the geometric part.

Element Matrix Formation

- Element matrix K is now made up of small tensors
- Contract all tensor elements with each the geometry tensor $G(\mathcal{T})$

3 0 0 0	0 -1 0 0	1 1 0 0	-4 -4 0 0	0 4 0 0	0 0 0 0
0 0 -1 0	0 0 0 3	0 0 1 1	0 0 0 0	0 0 4 0	0 0 -4 -4
1 0 1 0	0 1 0 1	3 3 3 3	-4 0 -4 0	0 0 0 0	0 -4 0 -4
-4 0 -4 0	0 0 0 0	-4 -4 0 0	8 4 4 8	0 -4 -4 -8	0 4 4 0
0 0 4 0	0 4 0 0	0 0 0 0	0 -4 -4 -8	8 4 4 8	-8 -4 -4 0
0 0 0 0	0 -4 0 -4	0 0 -4 -4	0 4 4 0	-8 -4 -4 0	8 4 4 8

Element Matrix Computation

- Element matrix K can be precomputed
  - FFC
  - SyFi
- Can be extended to nonlinearities and curved geometry
- Many redundancies among tensor elements of K
  - Could try to optimize the tensor contraction...

Abstract Problem

Given vectors $v_i \in \mathbb{R}^m$, minimize *flops*$(v^T g)$ for arbitrary $g \in \mathbb{R}^m$

- The set v_i is not at all random
- Not a traditional compiler optimization
- How to formulate as an optimization problem?

Outline

2 Operator Assembly
- Problem Statement
- Plan of Attack
- Results
- Mixed Integer Linear Programming

Complexity Reducing Relations

$$\text{If } v_i^T g \text{ is known, is } flops(v_j^T g) < 2m - 1?$$

We can use binary relations among the vectors:

- Equality
  - If $v_j = v_i$, then $flops(v_j^T g) = 0$
- Colinearity
  - If $v_j = \alpha v_i$, then $flops(v_j^T g) = 1$
- Hamming distance
  - If $dist_H(v_j, v_i) = k$, then $flops(v_j^T g) = 2k$

Algorithm for Binary Relations

- Construct a weighted graph on v_i
  - The weight $w(i, j)$ is $flops(v_j^T g)$ given $v_i^T g$
  - With the above relations, the graph is symmetric
- Find a minimum spanning tree
  - Use Prim or Kruskal for worst case $O(n^2 \log n)$
- Traverse the MST, using the appropriate calculation for each edge
  - Roots require a full dot product

Coplanarity

- Ternary relation
  - If $v_k = \alpha v_i + \beta v_j$, then $flops(v_k^T g) = 3$
  - Does not fit our undirected graph paradigm
- SVD for vector triples is expensive
  - Use a randomized projection into a few $\mathbb{R}^3$s
- Use a hypergraph?
  - MST algorithm available
- Appeal to geometry?
  - Incidence structures

Outline

FErari

Finite Element rearragement to automaically reduce instructions

- Open source implementation http://www.fenics.org/wiki/FErari
- Build tensor blocks $K^{ij}_{m,m'}$ as vectors using FIAT
- Discover dependencies
  - Represented as a DAG
  - Can also use hypergraph model
- Use minimal spanning tree to construct computation

Preliminary Results

Order	Entries	Base MAPs	FErari MAPs
1	6	24	7
2	21	84	15
3	55	220	45
4	120	480	176
5	231	924	443
6	406	1624	867

Outline

2. Operator Assembly
   - Problem Statement
   - Plan of Attack
   - Results
   - Mixed Integer Linear Programming

Modeling the Problem

- Objective is cost of dot products (tensor contractions in FEM)
  - Set of vectors V with a given arbitrary vector g
- The original MINLP has a nonconvex, nonlinear objective
- Reformulate to obtain a MILP using auxiliary binary variables

Modeling the Problem

Variables

$$\begin{aligned} \alpha_{ij} &= \text{Basis expansion coefficients} \\ y_i &= \text{Binary variable indicating membership in the basis} \\ s_{ij} &= \text{Binary variable indicating nonzero coefficient } \alpha_{ij} \\ z_{ij} &= \text{Binary variable linearizes the objective function (equivalent to } y_i y_j) \\ U &= \text{Upper bound on coefficients} \end{aligned}$$

Constraints

$$\begin{aligned} Eq.\ (6b) &: \text{Basis expansion} \\ Eq.\ (6c) &: \text{Exclude nonbasis vector from the expansion} \\ Eq.\ (6d) &: \text{Remove offdiagonal coefficients for basis vectors} \\ Eq.\ (7c) &: \text{Exclude vanishing coefficients from cost} \end{aligned}$$

Original Formulation

MINLP Model

$$\text{minimize} \quad \sum_{i=1}^{n} \left\{ y_i(2m-1) + (1-y_i)\left(2\sum_{j=1, j\neq i}^{n} y_j - 1\right)\right\} \tag{6a}$$

subject to

$$v_i = \sum_{j=1}^{n} \alpha_{ij} v_j \qquad i = 1, \ldots, n \tag{6b}$$

$$-Uy_j \leq \alpha_{ij} \leq Uy_j \qquad i, j = 1, \ldots, n \tag{6c}$$

$$-U(1-y_i) \leq \alpha_{ij} \leq U(1-y_i) \qquad i, j = 1, \ldots, n, \tag{6d}$$

$$y_i \in \{0, 1\} \qquad i = 1, \ldots, n. \tag{6e}$$

Original Formulation

Equivalent MILP Model: $z_{ij} = y_i \cdot y_j$

$$\text{minimize} \quad 2m \sum_{i=1}^{n} y_i + 2 \sum_{i=1}^{n} \sum_{j=1, j \neq i}^{n} (y_j - z_{ij}) - n \tag{6a}$$

$$\text{subject to} \quad v_i = \sum_{j=1}^{n} \alpha_{ij} v_j \qquad i = 1, \ldots, n \tag{6b}$$

$$-Uy_j \leq \alpha_{ij} \leq Uy_j \qquad i, j = 1, \ldots, n \tag{6c}$$

$$-U(1 - y_i) \leq \alpha_{ij} \leq U(1 - y_i) \qquad i, j = 1, \ldots, n, \ i \neq j \tag{6d}$$

$$z_{ij} \leq y_i, \quad z_{ij} \leq y_j, \quad z_{ij} \geq y_i + y_j - 1, \qquad i, j = 1, \ldots, n \tag{6e}$$

$$y_i \in \{0, 1\}, \quad z_{ij} \in \{0, 1\} \qquad i, j = 1, \ldots, n. \tag{6f}$$

Sparse Coefficient Formulation

- Take advantage of sparsity of α_{ij} coefficient
- Introduce binary variables s_{ij} to model existence of α_{ij}
- Add constraints $-Us_{ij} \leq \alpha_{ij} \leq Us_{ij}$

Sparse Coefficient Formulation

MINLP Model

$$\text{minimize} \quad \sum_{i=1}^{n} \left\{ y_i(2m-1) + (1-y_i)\left(2\sum_{j=1,j\neq i}^{n} s_{ij} - 1\right)\right\} \tag{7a}$$

$$\text{subject to} \quad v_i = \sum_{j=1}^{n} \alpha_{ij} v_j \qquad i = 1,\ldots,n \tag{7b}$$

$$-Us_{ij} \leq \alpha_{ij} \leq Us_{ij} \qquad i,j = 1,\ldots,n \tag{7c}$$

$$-U(1-y_i) \leq \alpha_{ij} \leq U(1-y_i) \qquad i,j = 1,\ldots,n \tag{7d}$$

$$s_{ij} \leq y_j \qquad i,j = 1,\ldots,n \tag{7e}$$

$$y_i \in \{0,1\}, \quad s_{ij} \in \{0,1\} \qquad i,j = 1,\ldots,n \tag{7f}$$

Sparse Coefficient Formulation

Equivalent MILP Model

$$\text{minimize} \quad 2m\sum_{i=1}^{n} y_i + 2\sum_{i=1}^{n}\sum_{j=1,j\neq i}^{n}(s_{ij} - z_{ij}) - n \tag{7a}$$

$$\text{subject to} \quad v_i = \sum_{j=1}^{n} \alpha_{ij} v_j \qquad i = 1,\dots,n \tag{7b}$$

$$-Us_{ij} \le \alpha_{ij} \le Us_{ij} \qquad i,j = 1,\dots,n \tag{7c}$$

$$-U(1-y_i) \le \alpha_{ij} \le U(1-y_i) \qquad i,j = 1,\dots,n,\ i \neq \tag{7d}$$

$$z_{ij} \le y_i, \quad z_{ij} \le s_{ij}, \quad z_{ij} \ge y_i + s_{ij} - 1, \qquad i,j = 1,\dots,n \tag{7e}$$

$$y_i \in \{0,1\}, \quad z_{ij} \in \{0,1\}, \quad s_{ij} \in \{0,1\} \qquad i,j = 1,\dots,n. \tag{7f}$$

Results

Initial Formulation

- Initial formulation only had sparsity in the α_{ij}
- MINTO was not able to produce some optimal solutions
  - Report results after 36000 seconds

Element	Default	MILP			Sparse Coef. MILP		
	Flops	Flops	LPs	CPU	Flops	LPs	CPU
P_1 2D	42	42	33	0.10	34	187	0.43
P_2 2D	147	147	2577	37.12	67	6030501	36000
P_1 3D	170	166	79	0.49	146	727	3.97
P_2 3D	935	935	25283	36000	829	33200	36000

Results

Formulation with Sparse Basis

- We can also take account of the sparsity in the basis vectors
- Count only the flops for nonzero entries
    - Significantly decreases the flop count

Elements	Sparse Coefficient Flops	Sparse Basis Flops
P_1 2D	34	12
P_1 3D	146	26

Outline

Outline

Sieve

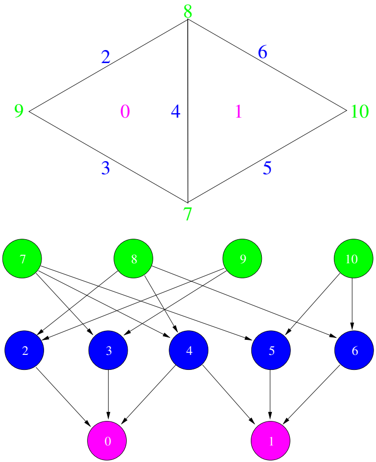
Sieve is an interface for

- general topologies
- functions over these topologies (bundles)
- traversals

One relation handles all hierarchy

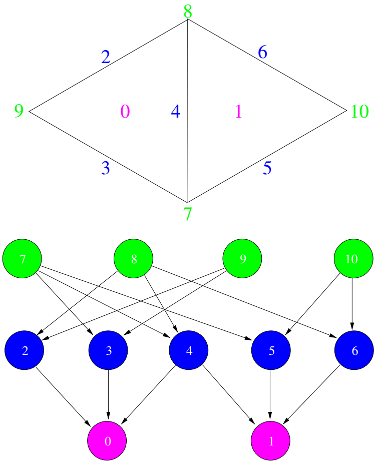
- Vast reduction in complexity
  - Dimension independent code
  - A single communication routine to optimize
- Expansion of capabilities
  - Partitioning and distribution
  - Hybrid meshes
  - Complicated structures and embedded boundaries
  - Unstructured multigrid

Doublet Mesh



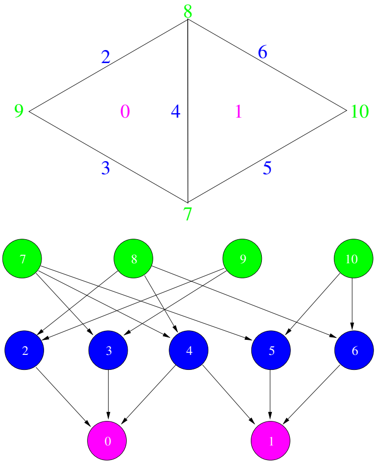
- Incidence/covering arrows
- *cone*(0) = {2, 3, 4}
- *support*(7) = {2, 3}

Doublet Mesh



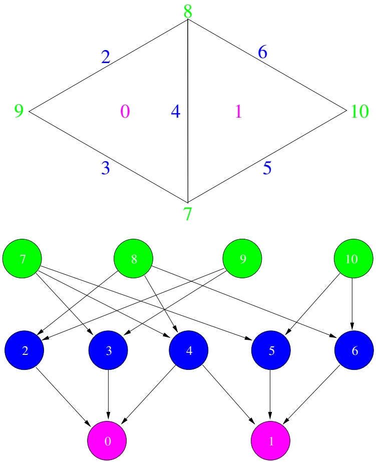
- Incidence/covering arrows
- *cone*$(0) = \{2, 3, 4\}$
- *support*$(7) = \{2, 3\}$

Doublet Mesh



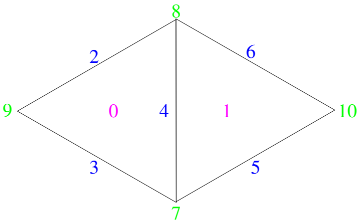
- Incidence/covering arrows
- *cone*(0) = {2, 3, 4}
- *support*(7) = {2, 3}

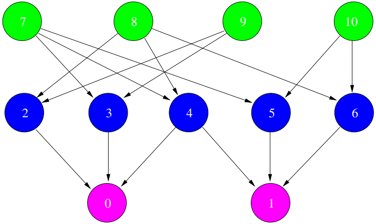
Doublet Mesh



- Incidence/covering arrows
- *closure*(0) = {0, 2, 3, 4, 7, 8, 9}
- *star*(7) = {7, 2, 3, 0}

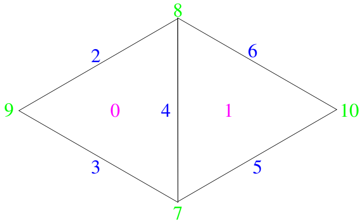
Doublet Mesh

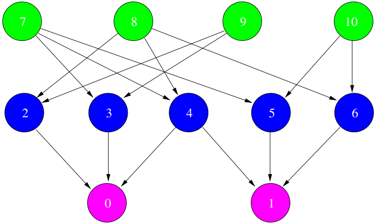




- Incidence/covering arrows
- $closure(0) = \{0, 2, 3, 4, 7, 8, 9\}$
- $star(7) = \{7, 2, 3, 0\}$

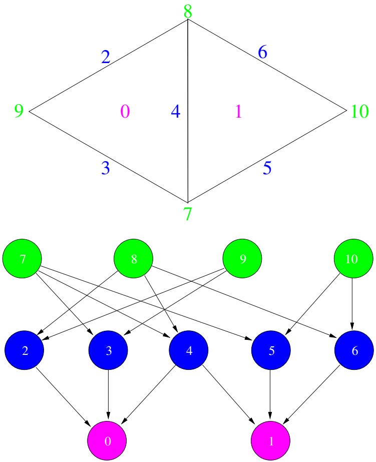
Doublet Mesh





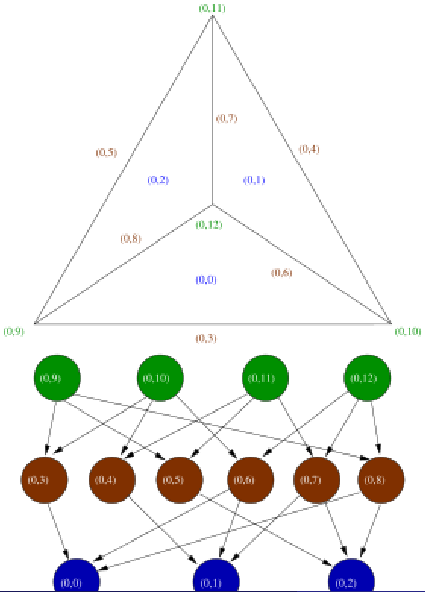
- Incidence/covering arrows
- *meet*(0, 1) = {4}
- *join*(8, 9) = {4}

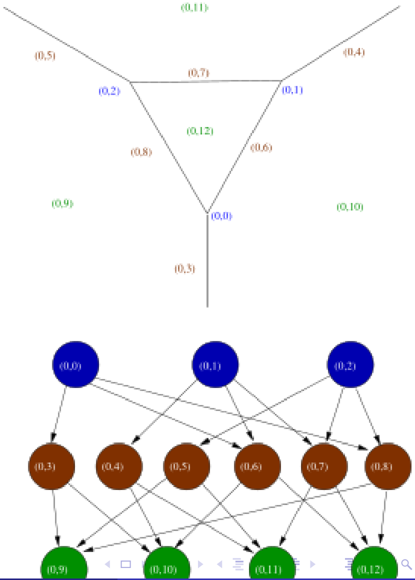
Doublet Mesh



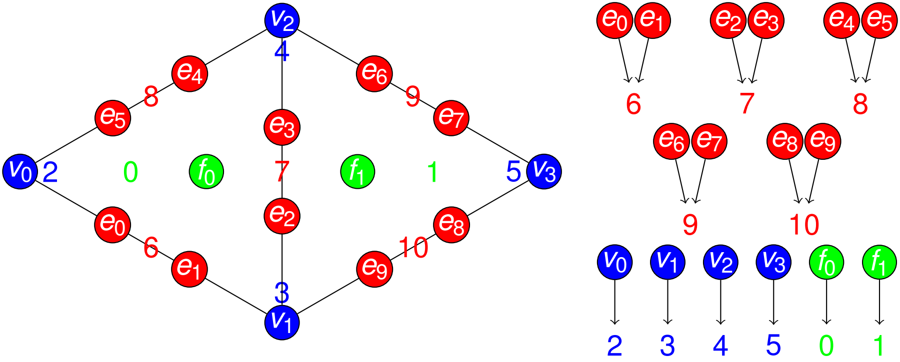
- Incidence/covering arrows
- $meet(0, 1) = \{4\}$
- $join(8, 9) = \{4\}$

The Mesh Dual



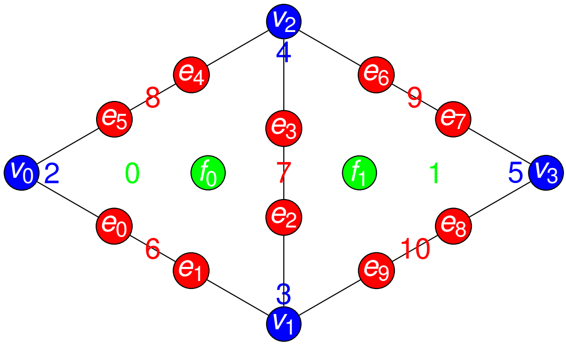


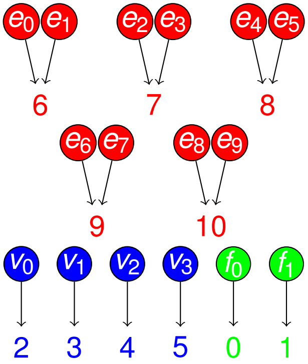
Doublet Section



- **Section** interface
  - $restrict(0) = \{f_0\}$
  - $restrict(2) = \{v_0\}$
  - $restrict(6) = \{e_0, e_1\}$

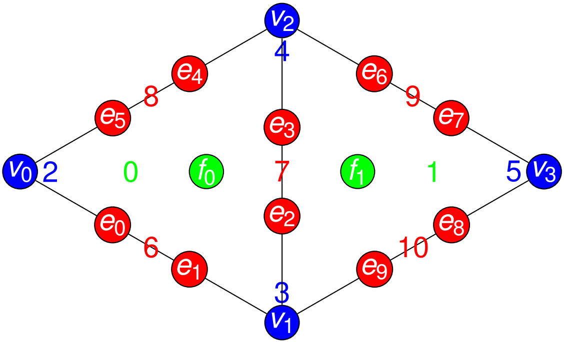
Doublet Section

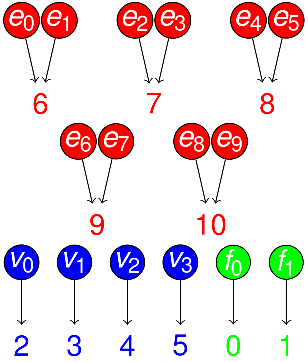




- **Section** interface
  - $restrict(0) = \{f_0\}$
  - $restrict(2) = \{v_0\}$
  - $restrict(6) = \{e_0, e_1\}$

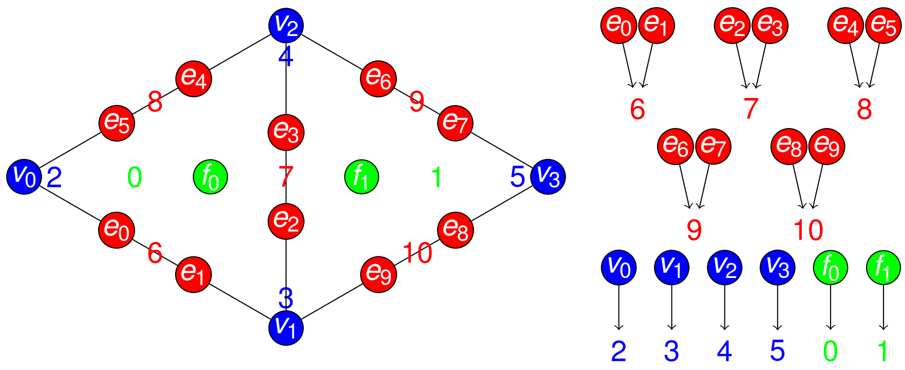
Doublet Section





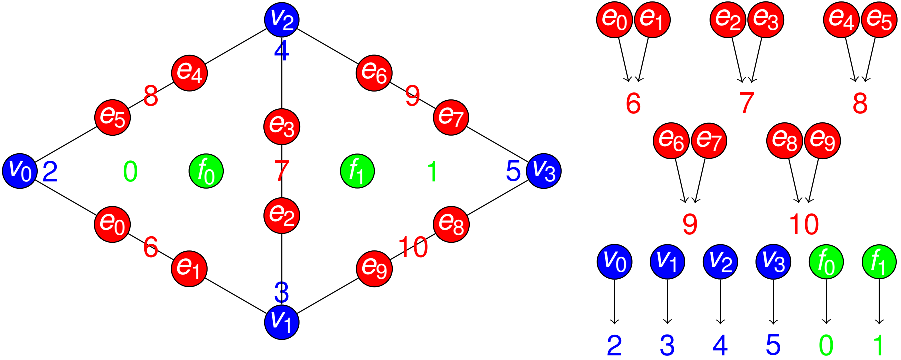
- **Section** interface
  - $restrict(0) = \{f_0\}$
  - $restrict(2) = \{v_0\}$
  - $restrict(6) = \{e_0, e_1\}$

Doublet Section



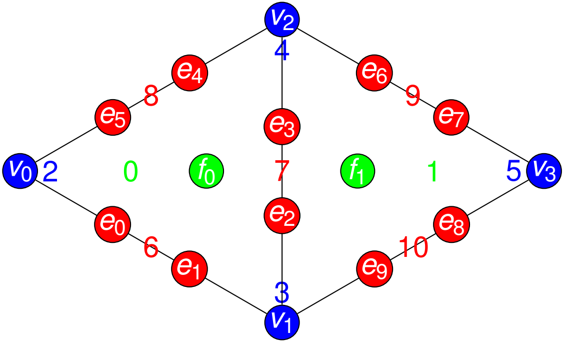
- **Section** interface
  - $restrict(0) = \{f_0\}$
  - $restrict(2) = \{v_0\}$
  - $restrict(6) = \{e_0, e_1\}$

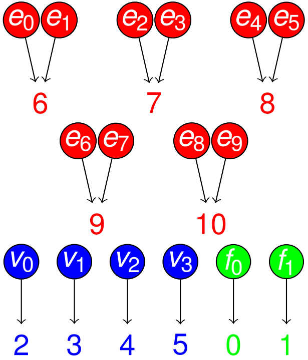
Doublet Section



- Topological traversals: follow connectivity
  - *restrictClosure*(0) $= \{f_0\, e_0\, e_1\, e_2\, e_3\, e_4\, e_5\, v_0\, v_1\, v_2\}$
  - *restrictStar*(7) $= \{v_0\, e_0\, e_1\, e_4\, e_5\, f_0\}$

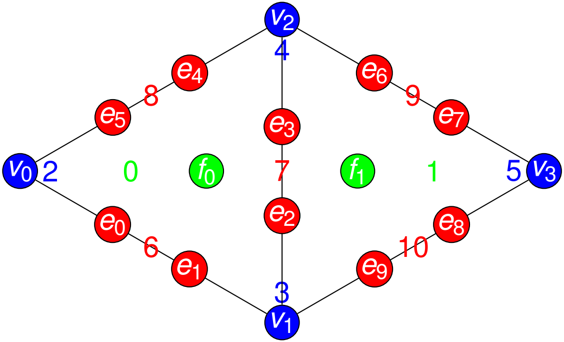
Doublet Section

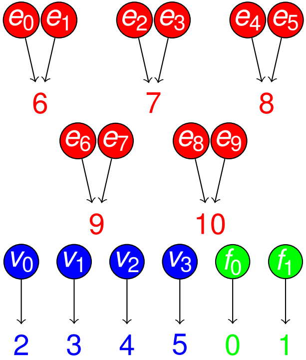




- Topological traversals: follow connectivity
  - *restrictClosure*(0) $= \{f_0\, e_0\, e_1\, e_2\, e_3\, e_4\, e_5\, v_0\, v_1\, v_2\}$
  - *restrictStar*(7) $= \{v_0\, e_0\, e_1\, e_4\, e_5\, f_0\}$

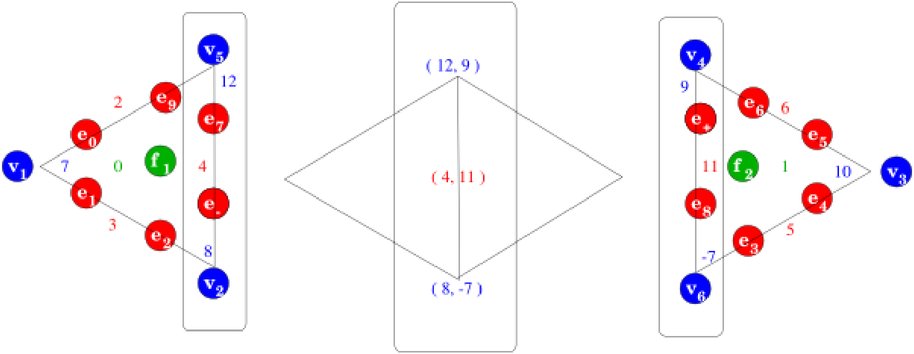
Doublet Section





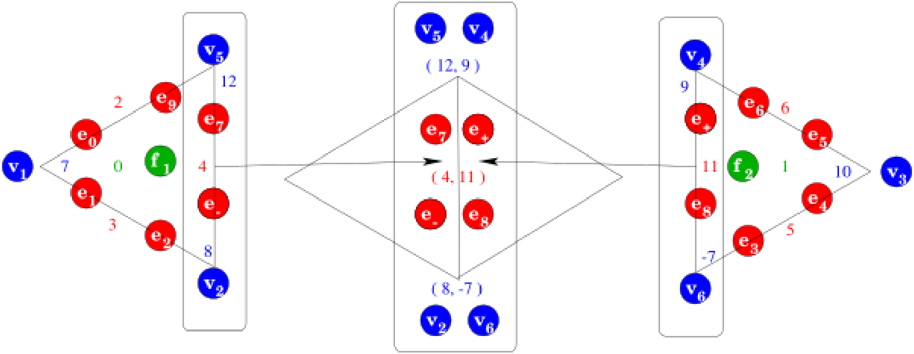
- Topological traversals: follow connectivity
  - $restrictClosure(0) = \{f_0\, e_0\, e_1\, e_2\, e_3\, e_4\, e_5\, v_0\, v_1\, v_2\}$
  - $restrictStar(7) = \{v_0\, e_0\, e_1\, e_4\, e_5\, f_0\}$

Restriction



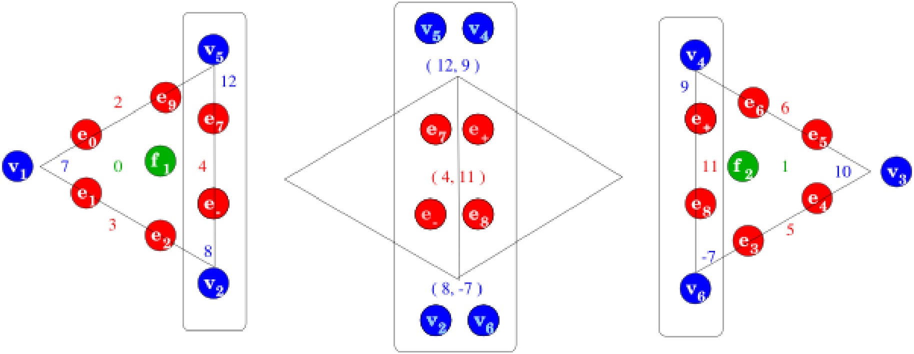
- Localization
  - Restrict to patches (here an edge closure)
  - Compute locally

Delta



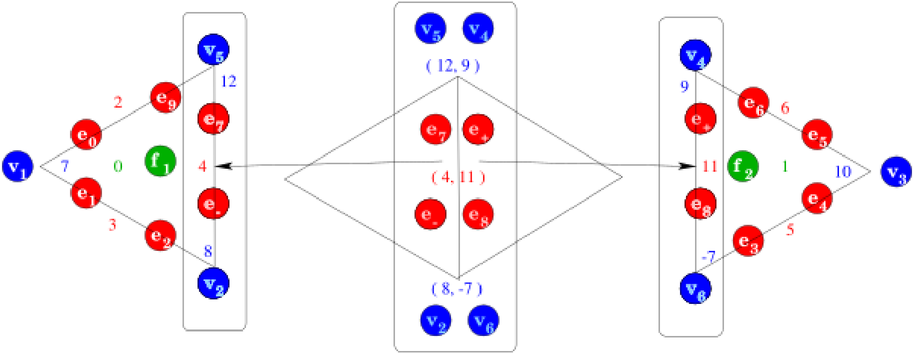
- `Delta`
  - Restrict further to the overlap
  - `Overlap` now carries twice the data

Fusion



- Merge/reconcile data on the overlap
  - Addition (FEM)
  - Replacement (FD)
  - Coordinate transform (Sphere)
  - Linear transform (MG)

Update



- Update
  - Update local patch data
  - Completion = restrict ⟶ fuse ⟶ update, <u>in parallel</u>

Uses

Completion has many uses:

FEM accumulating integrals on shared faces

FVM accumulating fluxes on shared cells

FDM setting values on ghost vertices

- distributing mesh entities after partition
- redistributing mesh entities and data for load balance
- accumlating matvec for a partially assembled matrix

Uses

Completion has many uses:

FEM accumulating integrals on shared faces

FVM accumulating fluxes on shared cells

FDM setting values on ghost vertices

- distributing mesh entities after partition
- redistributing mesh entities and data for load balance
- accumlating matvec for a partially assembled matrix

Uses

Completion has many uses:

FEM accumulating integrals on shared faces

FVM accumulating fluxes on shared cells

FDM setting values on ghost vertices

- distributing mesh entities after partition
- redistributing mesh entities and data for load balance
- accumlating matvec for a partially assembled matrix

Uses

Completion has many uses:

FEM accumulating integrals on shared faces

FVM accumulating fluxes on shared cells

FDM setting values on ghost vertices

- distributing mesh entities after partition
- redistributing mesh entities and data for load balance
- accumlating matvec for a partially assembled matrix

Uses

Completion has many uses:

FEM accumulating integrals on shared faces

FVM accumulating fluxes on shared cells

FDM setting values on ghost vertices

- distributing mesh entities after partition
- redistributing mesh entities and data for load balance
- accumlating matvec for a partially assembled matrix

Uses

Completion has many uses:

FEM accumulating integrals on shared faces

FVM accumulating fluxes on shared cells

FDM setting values on ghost vertices

- distributing mesh entities after partition
- redistributing mesh entities and data for load balance
- accumlating matvec for a partially assembled matrix

Uses

Completion has many uses:

FEM accumulating integrals on shared faces

FVM accumulating fluxes on shared cells

FDM setting values on ghost vertices

- distributing mesh entities after partition
- redistributing mesh entities and data for load balance
- accumlating matvec for a partially assembled matrix

Outline

3. Mesh Distribution
   - Sieve
   - Distribution
   - Interfaces
   - More on Assembly

Mesh Distribution

Distributing a mesh means

- distributing the topology (Sieve)
- distributing data (Section)

However, a Sieve can be interpreted as a Section of `cone()`s!

Mesh Distribution

Distributing a mesh means

- distributing the topology (Sieve)
- distributing data (Section)

However, a Sieve can be interpreted as a Section of `cone()`s!

Mesh Distribution

Distributing a mesh means

- distributing the topology (Sieve)
- distributing data (Section)

However, a Sieve can be interpreted as a Section of `cone()`s!

Mesh Distribution

Distributing a mesh means

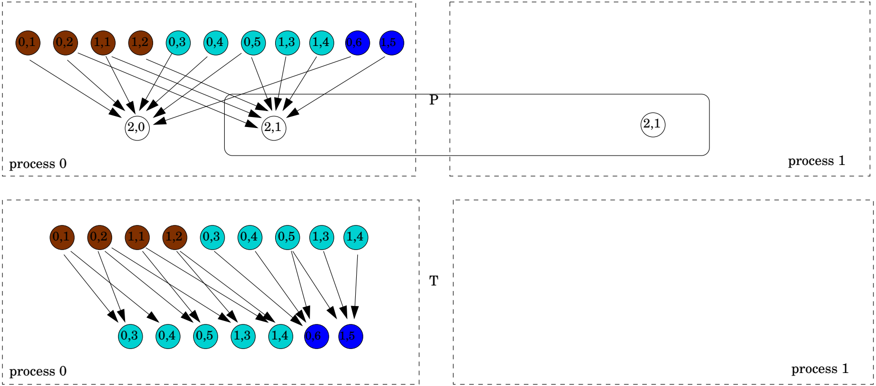
- distributing the topology (Sieve)
- distributing data (Section)

However, a Sieve can be interpreted as a Section of `cone()`s!

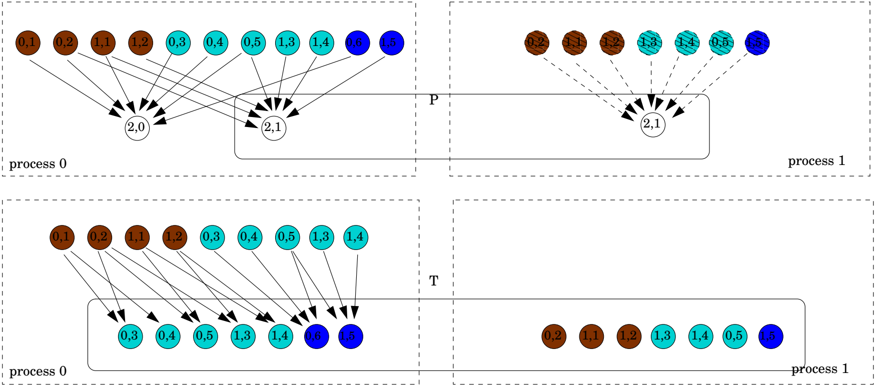
Mesh Partition

- 3rd party packages construct a vertex partition
- For FEM, partition dual graph vertices
- For FVM, construct hyperpgraph dual with faces as vertices
- Assign `closure(v)` and `star(v)` to same partition

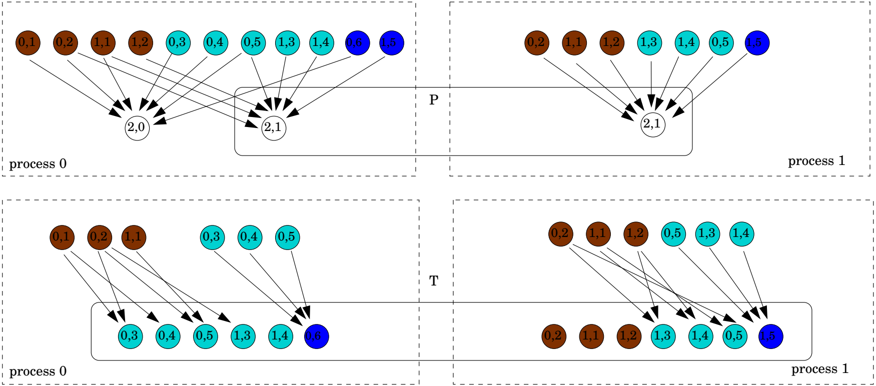
Doublet Mesh Distribution



Doublet Mesh Distribution

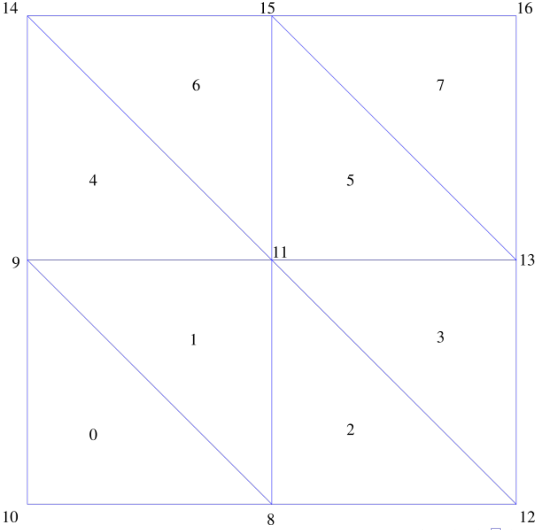


Doublet Mesh Distribution



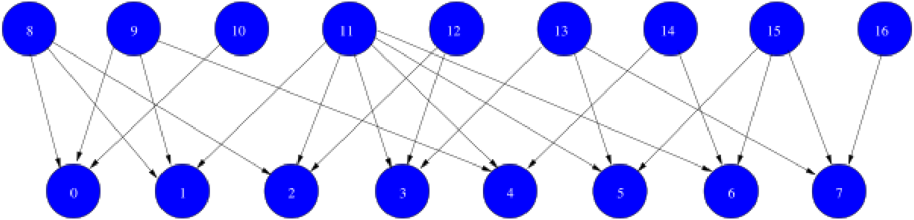
2D Example

A simple triangular mesh



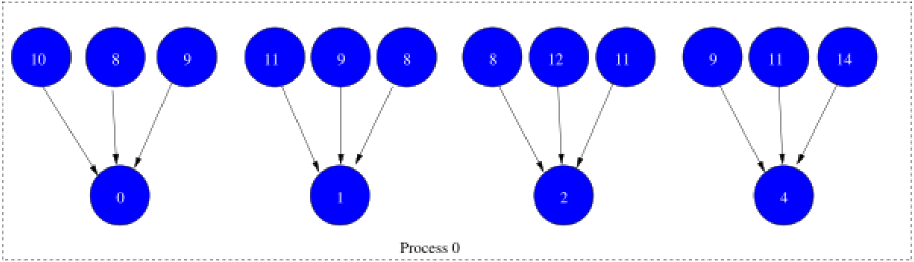
2D Example

Sieve for the mesh



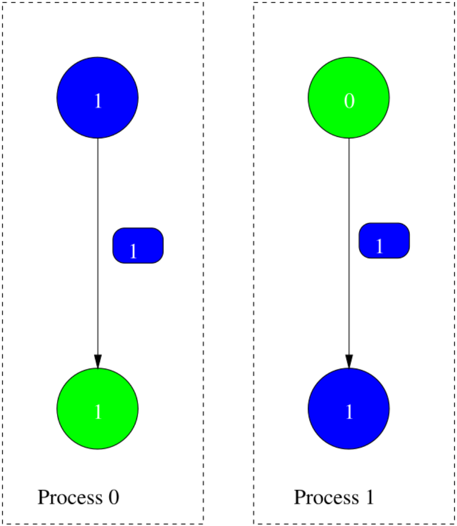
2D Example

Local sieve on process 0



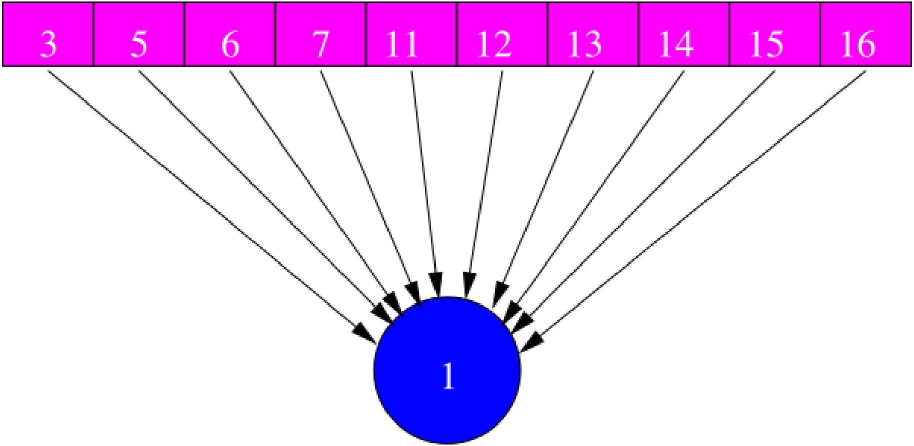
2D Example

Partition Overlap



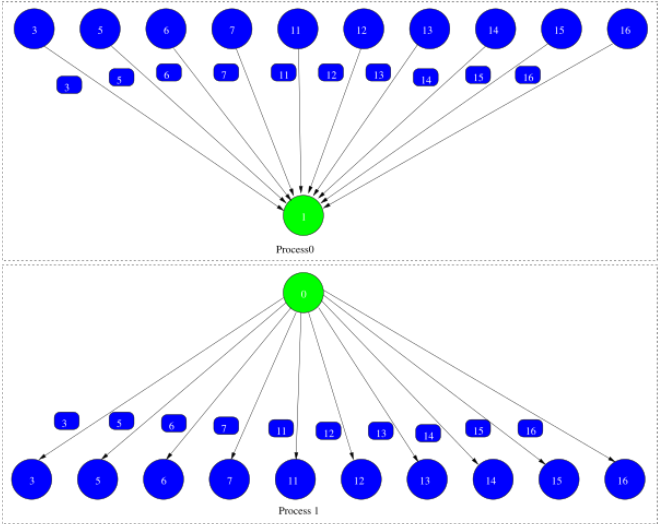
2D Example

Partition Section



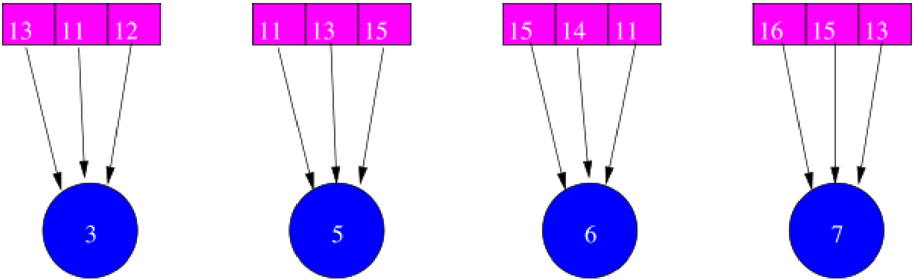
2D Example

Updated Sieve Overlap



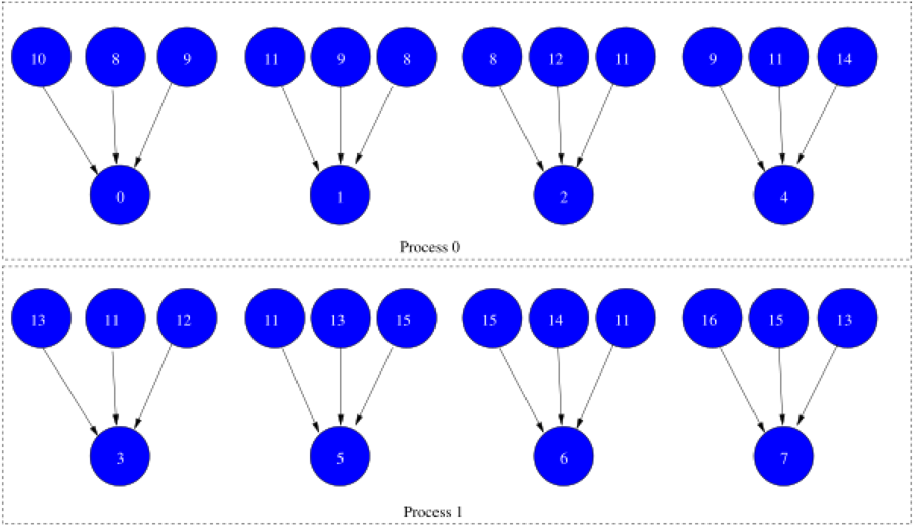
2D Example

Cone Section



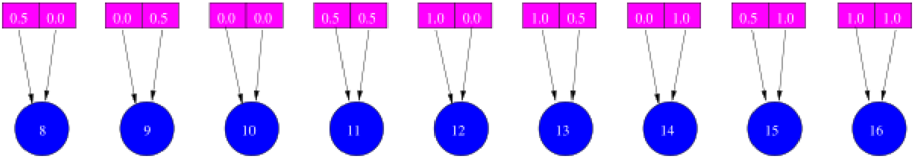
2D Example

Distributed Sieve



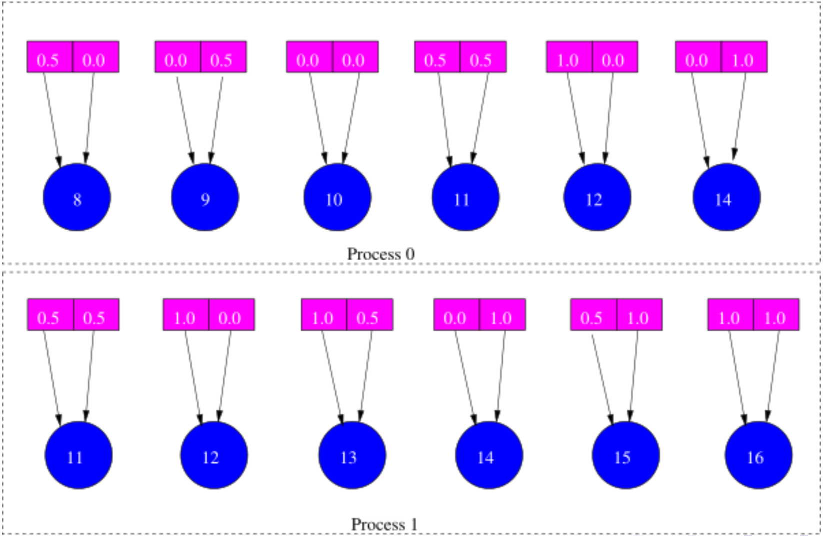
2D Example

Coordinate Section



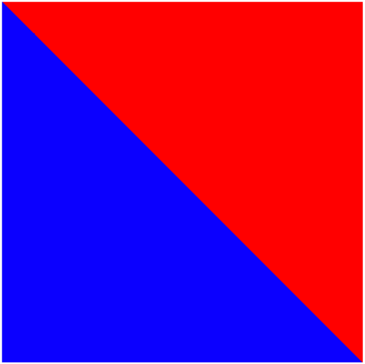
2D Example

Distributed Coordinate Section



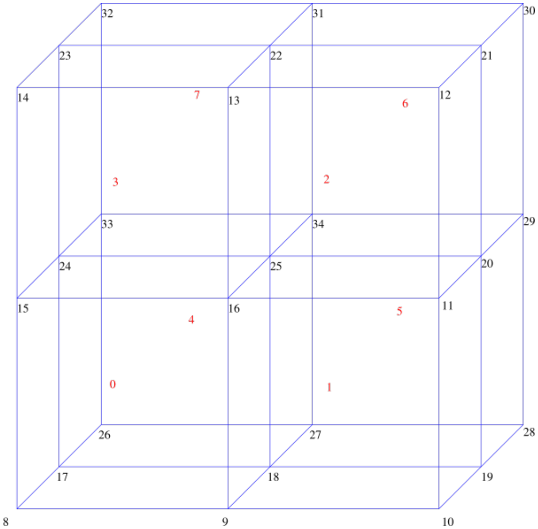
2D Example

Distributed Mesh



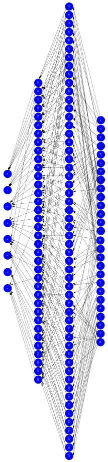
3D Example

A simple hexahedral mesh



3D Example

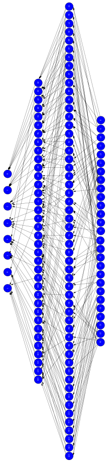
Sieve for the mesh



Its complicated!

3D Example

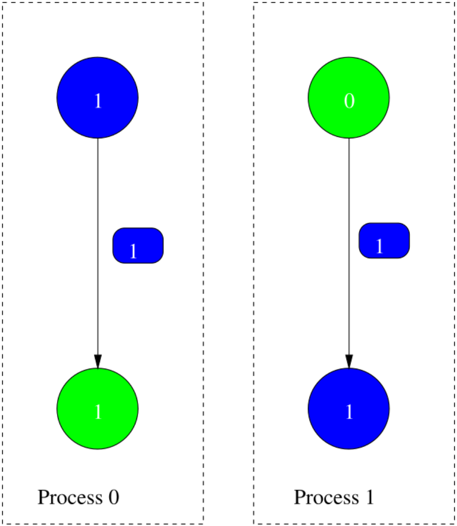
Sieve for the mesh



Its complicated!

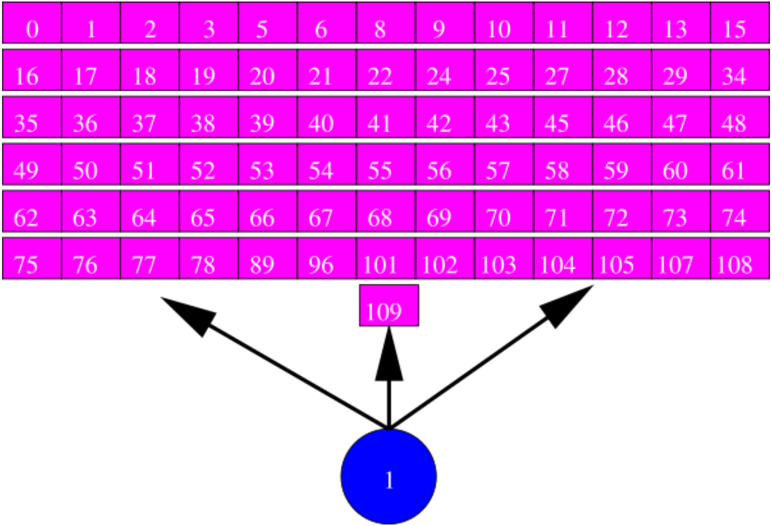
3D Example

Partition Overlap



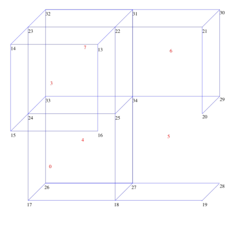
3D Example

Partition Section

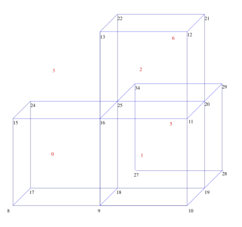


3D Example

Distributed Mesh



Process 0



Process 1

Notice cells are ghosted

Outline

3 Mesh Distribution
- Sieve
- Distribution
- Interfaces
- More on Assembly

Sieve Overview

- Hierarchy is the centerpiece
  - Strip out unneeded complexity (dimension, shape, . . .)
- Single relation, covering, handles all hierarchy
  - Rich enough for FEM
- Single operation, completion, for parallelism
  - Enforces consistency of the relation

Sieve Overview

- Hierarchy is the centerpiece
  - Strip out unneeded complexity (dimension, shape, . . .)
- Single relation, covering, handles all hierarchy
  - Rich enough for FEM
- Single operation, completion, for parallelism
  - Enforces consistency of the relation

Sieve Overview

- Hierarchy is the centerpiece
    - Strip out unneeded complexity (dimension, shape, . . .)
- Single relation, covering, handles all hierarchy
    - Rich enough for FEM
- Single operation, completion, for parallelism
    - Enforces consistency of the relation

Global and Local

Local (analytical)

- Discretization/Approximation
  - FEM integrals
  - FV fluxes
- Boundary conditions
- Largely dim dependent (e.g. quadrature)

Global (topological)

- Data management
  - Sections (local pieces)
  - Completions (assembly)
- Boundary definition
- Multiple meshes
  - Mesh hierarchies
- Largely dim independent (e.g. mesh traversal)

Global and Local

Local (analytical)

- Discretization/Approximation
  - FEM integrals
  - FV fluxes
- Boundary conditions
- Largely dim dependent (e.g. quadrature)

Global (topological)

- Data management
  - Sections (local pieces)
  - Completions (assembly)
- Boundary definition
- Multiple meshes
  - Mesh hierarchies
- Largely dim independent (e.g. mesh traversal)

Global and Local

Local (analytical)

- Discretization/Approximation
  - FEM integrals
  - FV fluxes
- Boundary conditions
- Largely dim dependent (e.g. quadrature)

Global (topological)

- Data management
  - Sections (local pieces)
  - Completions (assembly)
- Boundary definition
- Multiple meshes
  - Mesh hierarchies
- Largely dim independent (e.g. mesh traversal)

Global and Local

Local (analytical)

- Discretization/Approximation
  - FEM integrals
  - FV fluxes
- Boundary conditions
- Largely dim dependent (e.g. quadrature)

Global (topological)

- Data management
  - Sections (local pieces)
  - Completions (assembly)
- Boundary definition
- Multiple meshes
  - Mesh hierarchies
- Largely dim independent (e.g. mesh traversal)

Global and Local

Local (analytical)

- Discretization/Approximation
  - FEM integrals
  - FV fluxes
- Boundary conditions
- Largely dim dependent (e.g. quadrature)

Global (topological)

- Data management
  - Sections (local pieces)
  - Completions (assembly)
- Boundary definition
- Multiple meshes
  - Mesh hierarchies
- Largely dim independent (e.g. mesh traversal)

Hierarchical Interfaces

Global/Local Dichotomy is the Heart of DD

Software interfaces do not adequately reflect this

- PETSc DA is too specialized
  - Basically 1D methods applied to Cartesian products
- PETSc Index Sets and VecScatters are too fine
  - User “does everything”, no abstraction
- PETSc Linear Algebra (Vec & Mat) is too coarse
  - No access to the underlying connectivity structure

Unstructured Interface (before)

- Explicit references to element type
  - getVertices(edgeID), getVertices(faceID)
  - getAdjacency(edgeID, VERTEX)
  - getAdjacency(edgeID, dim = 0)
- No interface for transitive closure
  - Awkward nested loops to handle different dimensions
- Have to recode for meshes with different
  - dimension
  - shapes

Unstructured Interface (before)

- Explicit references to element type
  - getVertices(edgeID), getVertices(faceID)
  - getAdjacency(edgeID, VERTEX)
  - getAdjacency(edgeID, dim = 0)
- No interface for transitive closure
  - Awkward nested loops to handle different dimensions
- Have to recode for meshes with different
  - dimension
  - shapes

Unstructured Interface (before)

- Explicit references to element type
    - getVertices(edgeID), getVertices(faceID)
    - getAdjacency(edgeID, VERTEX)
    - getAdjacency(edgeID, dim = 0)
- No interface for transitive closure
    - Awkward nested loops to handle different dimensions
- Have to recode for meshes with different
    - dimension
    - shapes

Go Back to the Math

Combinatorial Topology gives us a framework for geometric computing.

- Abstract to a relation, covering, on sieve points
  - Points can represent any mesh element
  - Covering can be thought of as adjacency
  - Relation can be expressed in a DAG (Hasse Diagram)
- Simple query set:
  - provides a general API for geometric algorithms
  - leads to simpler implementations
  - can be more easily optimized

Go Back to the Math

Combinatorial Topology gives us a framework for geometric computing.

- Abstract to a relation, covering, on sieve points
  - Points can represent any mesh element
  - Covering can be thought of as adjacency
  - Relation can be expressed in a DAG (Hasse Diagram)
- Simple query set:
  - provides a general API for geometric algorithms
  - leads to simpler implementations
  - can be more easily optimized

Go Back to the Math

Combinatorial Topology gives us a framework for geometric computing.

- Abstract to a relation, covering, on sieve points
  - Points can represent any mesh element
  - Covering can be thought of as adjacency
  - Relation can be expressed in a DAG (Hasse Diagram)
- Simple query set:
  - provides a general API for geometric algorithms
  - leads to simpler implementations
  - can be more easily optimized

Unstructured Interface (after)

- NO explicit references to element type
  - A point may be any mesh element
  - getCone(point): adjacent (d-1)-elements
  - getSupport(point): adjacent (d+1)-elements
- Transitive closure
  - closure(cell): The computational unit for FEM
- Algorithms independent of mesh
  - dimension
  - shape (even hybrid)
  - global topology
  - data layout

Unstructured Interface (after)

- NO explicit references to element type
  - A point may be any mesh element
  - getCone(point): adjacent (d-1)-elements
  - getSupport(point): adjacent (d+1)-elements
- Transitive closure
  - closure(cell): The computational unit for FEM
- Algorithms independent of mesh
  - dimension
  - shape (even hybrid)
  - global topology
  - data layout

Unstructured Interface (after)

- NO explicit references to element type
  - A point may be any mesh element
  - getCone(point): adjacent (d-1)-elements
  - getSupport(point): adjacent (d+1)-elements
- Transitive closure
  - closure(cell): The computational unit for FEM
- Algorithms independent of mesh
  - dimension
  - shape (even hybrid)
  - global topology
  - data layout

Hierarchy Abstractions

- Generalize to a set of linear spaces
  - `Sieve` provides topology, can also model `Mat`
  - `Section` generalizes `Vec`
  - Spaces interact through an `Overlap` (just a `Sieve`)
- Basic operations
  - Restriction to finer subspaces, `restrict()/update()`
  - Assembly to the subdomain, `complete()`
- Allow reuse of geometric and multilevel algorithms

Outline

Integration

```
cells = mesh->heightStratum(0);
for(c = cells->begin(); c != cells->end(); ++c) {
  <Compute cell geometry>
  <Retrieve values from input vector>
  for(q = 0; q < numQuadPoints; ++q) {
    <Transform coordinates>
    for(f = 0; f < numBasisFuncs; ++f) {
      <Constant term>
      <Linear term>
      <Nonlinear term>
      elemVec[f] *= weight[q]*detJ;
    }
  }
  <Update output vector>
}
<Aggregate updates>
```

Integration

```
cells = mesh->heightStratum(0);
for(c = cells->begin(); c != cells->end(); ++c) {
  coords = mesh->restrict(coordinates, c);
  v0, J, invJ, detJ = computeGeometry(coords);
  <Retrieve values from input vector>
  for(q = 0; q < numQuadPoints; ++q) {
    <Transform coordinates>
    for(f = 0; f < numBasisFuncs; ++f) {
      <Constant term>
      <Linear term>
      <Nonlinear term>
      elemVec[f] *= weight[q]*detJ;
    }
  }
  <Update output vector>
}
```

Integration

```
cells = mesh->heightStratum(0);
for(c = cells->begin(); c != cells->end(); ++c) {
  <Compute cell geometry>
  <Retrieve values from input vector>
  for(q = 0; q < numQuadPoints; ++q) {
    <Transform coordinates>
    for(f = 0; f < numBasisFuncs; ++f) {
      <Constant term>
      <Linear term>
      <Nonlinear term>
      elemVec[f] *= weight[q]*detJ;
    }
  }
  <Update output vector>
}
<Aggregate updates>
```

Integration

```
cells = mesh->heightStratum(0);
for(c = cells->begin(); c != cells->end(); ++c) {
  <Compute cell geometry>
  inputVec = mesh->restrict(U, c);
  for(q = 0; q < numQuadPoints; ++q) {
    <Transform coordinates>
    for(f = 0; f < numBasisFuncs; ++f) {
      <Constant term>
      <Linear term>
      <Nonlinear term>
      elemVec[f] *= weight[q]*detJ;
    }
  }
  <Update output vector>
}
<Aggregate updates>
```

Integration

```
cells = mesh->heightStratum(0);
for(c = cells->begin(); c != cells->end(); ++c) {
  <Compute cell geometry>
  <Retrieve values from input vector>
  for(q = 0; q < numQuadPoints; ++q) {
    <Transform coordinates>
    for(f = 0; f < numBasisFuncs; ++f) {
      <Constant term>
      <Linear term>
      <Nonlinear term>
      elemVec[f] *= weight[q]*detJ;
    }
  }
  <Update output vector>
}
<Aggregate updates>
```

Integration

```
cells = mesh->heightStratum(0);
for(c = cells->begin(); c != cells->end(); ++c) {
  <Compute cell geometry>
  <Retrieve values from input vector>
  for(q = 0; q < numQuadPoints; ++q) {
    realCoords = J*refCoords[q] + v0;
    for(f = 0; f < numBasisFuncs; ++f) {
      <Constant term>
      <Linear term>
      <Nonlinear term>
      elemVec[f] *= weight[q]*detJ;
    }
  }
  <Update output vector>
}
<Aggregate updates>
```

Integration

```
cells = mesh->heightStratum(0);
for(c = cells->begin(); c != cells->end(); ++c) {
  <Compute cell geometry>
  <Retrieve values from input vector>
  for(q = 0; q < numQuadPoints; ++q) {
    <Transform coordinates>
    for(f = 0; f < numBasisFuncs; ++f) {
      <Constant term>
      <Linear term>
      <Nonlinear term>
      elemVec[f] *= weight[q]*detJ;
    }
  }
  <Update output vector>
}
<Aggregate updates>
```

Integration

```
cells = mesh->heightStratum(0);
for(c = cells->begin(); c != cells->end(); ++c) {
  <Compute cell geometry>
  <Retrieve values from input vector>
  for(q = 0; q < numQuadPoints; ++q) {
    <Transform coordinates>
    for(f = 0; f < numBasisFuncs; ++f) {
      elemVec[f] += basis[q,f]*rhsFunc(realCoords);
      <Linear term>
      <Nonlinear term>
      elemVec[f] *= weight[q]*detJ;
    }
  }
  <Update output vector>
}
<Aggregate updates>
```

Integration

```
cells = mesh->heightStratum(0);
for(c = cells->begin(); c != cells->end(); ++c) {
  <Compute cell geometry>
  <Retrieve values from input vector>
  for(q = 0; q < numQuadPoints; ++q) {
    <Transform coordinates>
    for(f = 0; f < numBasisFuncs; ++f) {
      <Constant term>
      <Linear term>
      <Nonlinear term>
      elemVec[f] *= weight[q]*detJ;
    }
  }
  <Update output vector>
}
<Aggregate updates>
```

Integration

```
cells = mesh->heightStratum(0);
for(c = cells->begin(); c != cells->end(); ++c) {
  <Compute cell geometry>
  <Retrieve values from input vector>
  for(q = 0; q < numQuadPoints; ++q) {
    <Transform coordinates>
    for(f = 0; f < numBasisFuncs; ++f) {
      <Constant term>
      for(d = 0; d < dim; ++d)
        for(e) testDerReal[d] += invJ[e,d]*basisDer[q,
      for(g = 0; g < numBasisFuncs; ++g) {
        for(d = 0; d < dim; ++d)
          for(e) basisDerReal[d] += invJ[e,d]*basisDer
          elemMat[f,g] += testDerReal[d]*basisDerReal[
        elemVec[f] += elemMat[f,g]*inputVec[g];
      }
```

Integration

```
cells = mesh->heightStratum(0);
for(c = cells->begin(); c != cells->end(); ++c) {
  <Compute cell geometry>
  <Retrieve values from input vector>
  for(q = 0; q < numQuadPoints; ++q) {
    <Transform coordinates>
    for(f = 0; f < numBasisFuncs; ++f) {
      <Constant term>
      <Linear term>
      <Nonlinear term>
      elemVec[f] *= weight[q]*detJ;
    }
  }
  <Update output vector>
}
<Aggregate updates>
```

Integration

```
cells = mesh->heightStratum(0);
for(c = cells->begin(); c != cells->end(); ++c) {
  <Compute cell geometry>
  <Retrieve values from input vector>
  for(q = 0; q < numQuadPoints; ++q) {
    <Transform coordinates>
    for(f = 0; f < numBasisFuncs; ++f) {
      <Constant term>
      <Linear term>
      elemVec[f] += basis[q,f]*lambda*exp(inputVec[f])
      elemVec[f] *= weight[q]*detJ;
    }
  }
  <Update output vector>
}
<Aggregate updates>
```

Integration

```
cells = mesh->heightStratum(0);
for(c = cells->begin(); c != cells->end(); ++c) {
  <Compute cell geometry>
  <Retrieve values from input vector>
  for(q = 0; q < numQuadPoints; ++q) {
    <Transform coordinates>
    for(f = 0; f < numBasisFuncs; ++f) {
      <Constant term>
      <Linear term>
      <Nonlinear term>
      elemVec[f] *= weight[q]*detJ;
    }
  }
  <Update output vector>
}
<Aggregate updates>
```

Integration

```
cells = mesh->heightStratum(0);
for(c = cells->begin(); c != cells->end(); ++c) {
  <Compute cell geometry>
  <Retrieve values from input vector>
  for(q = 0; q < numQuadPoints; ++q) {
    <Transform coordinates>
    for(f = 0; f < numBasisFuncs; ++f) {
      <Constant term>
      <Linear term>
      <Nonlinear term>
      elemVec[f] *= weight[q]*detJ;
    }
  }
  mesh->updateAdd(F, c, elemVec);
}
<Aggregate updates>
```

Integration

```
cells = mesh->heightStratum(0);
for(c = cells->begin(); c != cells->end(); ++c) {
  <Compute cell geometry>
  <Retrieve values from input vector>
  for(q = 0; q < numQuadPoints; ++q) {
    <Transform coordinates>
    for(f = 0; f < numBasisFuncs; ++f) {
      <Constant term>
      <Linear term>
      <Nonlinear term>
      elemVec[f] *= weight[q]*detJ;
    }
  }
  <Update output vector>
}
<Aggregate updates>
```

Integration

```
cells = mesh->heightStratum(0);
for(c = cells->begin(); c != cells->end(); ++c) {
  <Compute cell geometry>
  <Retrieve values from input vector>
  for(q = 0; q < numQuadPoints; ++q) {
    <Transform coordinates>
    for(f = 0; f < numBasisFuncs; ++f) {
      <Constant term>
      <Linear term>
      <Nonlinear term>
      elemVec[f] *= weight[q]*detJ;
    }
  }
  <Update output vector>
}
Distribution<Mesh>::completeSection(mesh, F);
```

Boundary Conditions

Dirichlet conditions may be expressed as

$$u|_\Gamma = g$$

and implemented by constraints on dofs in a Section

- The user provides a function.

Neumann conditions may be expressed as

$$\nabla u \cdot \hat{n}|_\Gamma = h$$

and implemented by explicit integration along the boundary

- The user provides a weak form.

Dirichlet Values

- Topological boundary is marked during generation
- Cells bordering boundary are marked using `markBoundaryCells()`
- To set values:
  1. Loop over boundary cells
  2. Loop over the element closure
  3. For each boundary point i, apply the functional N_i to the function g
- The functionals are generated with the quadrature information
- Section allocation applies Dirichlet conditions automatically
  - Values are stored in the Section
  - `restrict()` behaves normally, `update()` ignores constraints

Dual Basis Application

We would like the action of a dual basis vector (functional)

$$< \mathcal{N}_i, f >= \int_{\mathrm{ref}} N_i(x) f(x) dV$$

- Projection onto $\mathcal{P}$
- Code is generated from FIAT specification
  - Python code generation package inside PETSc
- Common interface for all elements

Outline

Outline

4 Further Work
- FEM
- UMG
- PyLith

FIAT

Finite Element Integrator And Tabulator by Rob Kirby

http://fenicsproject.org/

FIAT understands

- Reference element shapes (line, triangle, tetrahedron)
- Quadrature rules
- Polynomial spaces
- Functionals over polynomials (dual spaces)
- Derivatives

Can build arbitrary elements by specifying the Ciarlet triple (K, P, P')

FIAT is part of the FEniCS project

FIAT

Finite Element Integrator And Tabulator by Rob Kirby

http://fenicsproject.org/

FIAT understands

- Reference element shapes (line, triangle, tetrahedron)
- Quadrature rules
- Polynomial spaces
- Functionals over polynomials (dual spaces)
- Derivatives

Can build arbitrary elements by specifying the Ciarlet triple (K, P, P')

FIAT is part of the FEniCS project

FFC

FFC is a compiler for variational forms by Anders Logg.

Here is a mixed-form Poisson equation:

$$a((\tau, w), (\sigma, u)) = L((\tau, w)) \qquad \forall (\tau, w) \in V$$

where

$$\begin{aligned} a((\tau, w), (\sigma, u)) &= \int_\Omega \tau\sigma - \nabla \cdot \tau u + w \nabla \cdot u \, dx \\ L((\tau, w)) &= \int_\Omega wf \, dx \end{aligned}$$

FFC
Mixed Poisson

```
shape = "triangle"

BDM1 = FiniteElement("Brezzi-Douglas-Marini",shape,1)
DG0  = FiniteElement("Discontinuous Lagrange",shape,0)

element      = BDM1 + DG0
(tau, w)     = TestFunctions(element)
(sigma, u)   = TrialFunctions(element)

a = (dot(tau, sigma) - div(tau)*u + w*div(sigma))*dx

f = Function(DG0)
L = w*f*dx
```

FFC

Here is a discontinuous Galerkin formulation of the Poisson equation:

$$a(v,u) = L(v) \qquad \forall v \in V$$

where

$$\begin{aligned} a(v,u) &= \int_\Omega \nabla u \cdot \nabla v \, dx \\ &+ \sum_S \int_S - < \nabla v > \cdot [[u]]_n - [[v]]_n \cdot < \nabla u > -(\alpha/h) vu \, dS \\ &+ \int_{\partial\Omega} -\nabla v \cdot [[u]]_n - [[v]]_n \cdot \nabla u - (\gamma/h) vu \, ds \\ L(v) &= \int_\Omega vf \, dx \end{aligned}$$

FFC
DG Poisson

```
DG1 = FiniteElement("Discontinuous Lagrange",shape,1)
v = TestFunctions(DG1)
u = TrialFunctions(DG1)
f = Function(DG1)
g = Function(DG1)
n = FacetNormal("triangle")
h = MeshSize("triangle")
a = dot(grad(v), grad(u))*dx
  - dot(avg(grad(v)), jump(u, n))*dS
  - dot(jump(v, n), avg(grad(u)))*dS
  + alpha/h*dot(jump(v, n) + jump(u, n))*dS
  - dot(grad(v), jump(u, n))*ds
  - dot(jump(v, n), grad(u))*ds
  + gamma/h*v*u*ds
L = v*f*dx + v*g*ds
```

Outline

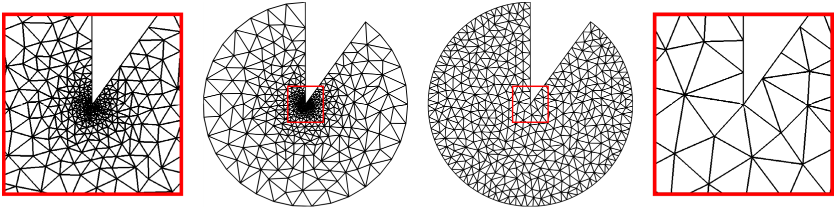
4 Further Work
- FEM
- UMG
- PyLith

A Priori refinement

For the Poisson problem, meshes with reentrant corners have a length-scale requirement in order to maintain accuracy:

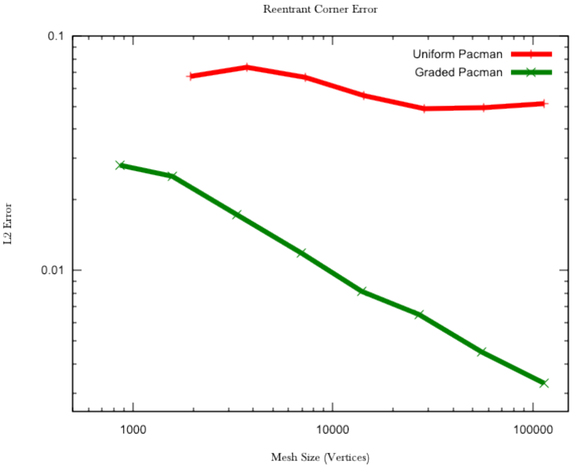
$$C_{low} r^{1-\mu} \leq h \leq C_{high} r^{1-\mu}$$

$$\mu \leq \frac{\pi}{\theta}$$



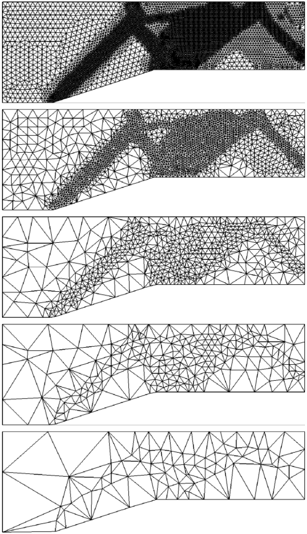
The Folly of Uniform Refinement

uniform refinement may fail to eliminate error



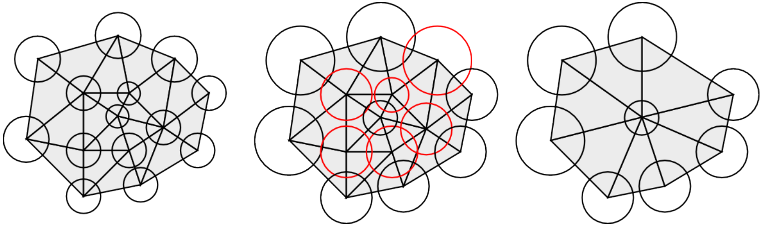
Geometric Multigrid

- We allow the user to refine for fidelity
- Coarse grids are created automatically
- Could make use of AMG interpolation schemes



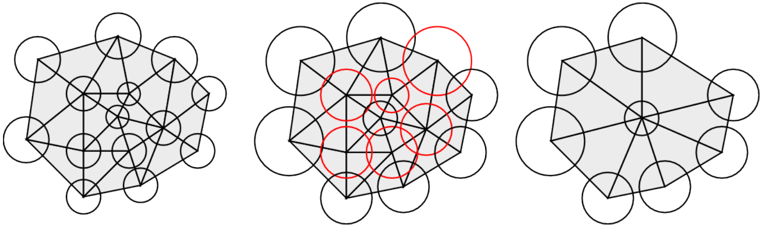
Function Based Coarsening

- (Miller, Talmor, Teng; 1997)
- triangulated planar graphs $\equiv$ disk-packings (Koebe; 1934)
- define a spacing function S() over the vertices
- obvious one: $S(v) = \frac{dist(NN(v),v)}{2}$



Function Based Coarsening

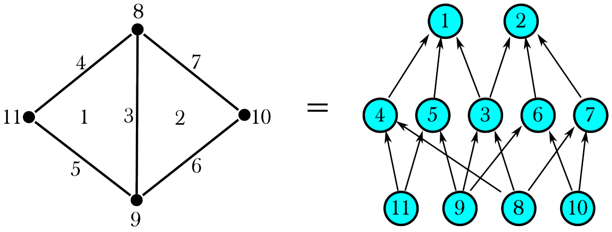
- pick a subset of the vertices such that $\beta(S(v) + S(w)) > dist(v, w)$
- for all $v, w \in M$, with $\beta > 1$
- dimension independent
- provides guarantees on the size/quality of the resulting meshes



Implementation in *Sieve*

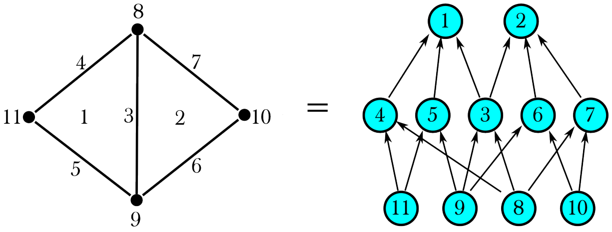
Peter Brune, 2008

- vertex neighbors: $cone(support(v)) \setminus v$
- vertex link: $closure(star(v)) \setminus star(closure(v))$
- connectivity graph induced by limiting sieve depth
- remeshing can be handled as local modifications on the sieve
- meshing operations, such as *cone construction* easy



Implementation in *Sieve*
Peter Brune, 2008

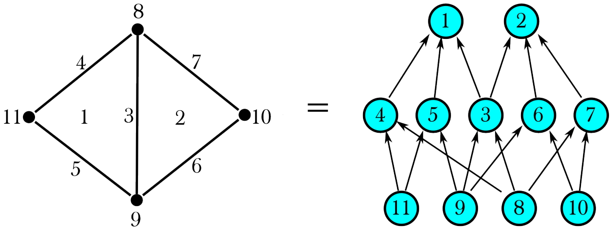
- vertex neighbors: $cone(support(v)) \setminus v$
- vertex link: $closure(star(v)) \setminus star(closure(v))$
- connectivity graph induced by limiting sieve depth
- remeshing can be handled as local modifications on the sieve
- meshing operations, such as *cone construction* easy



Implementation in *Sieve*

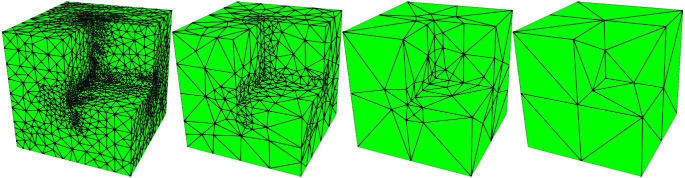
Peter Brune, 2008

- vertex neighbors: $cone(support(v)) \setminus v$
- vertex link: $closure(star(v)) \setminus star(closure(v))$
- connectivity graph induced by limiting sieve depth
- remeshing can be handled as local modifications on the sieve
- meshing operations, such as *cone construction* easy



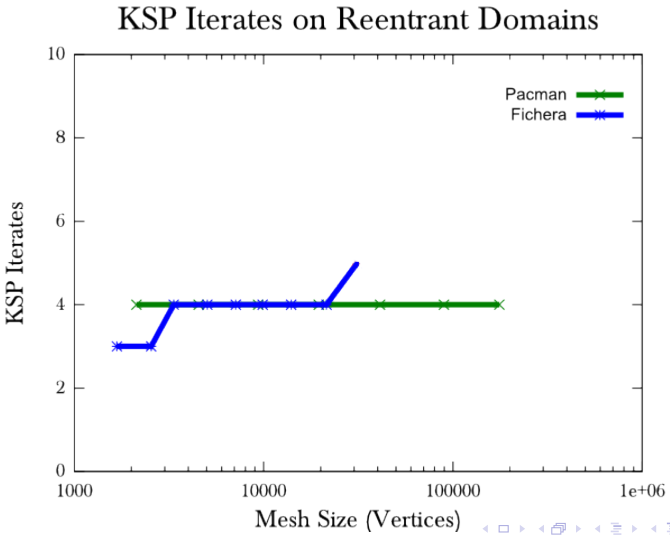
3D Test Problem

- Reentrant corner
- $-\Delta u = f$
- $f(x, y, z) = 3\sin(x + y + z)$
- Exact Solution: $u(x, y, z) = \sin(x + y + z)$



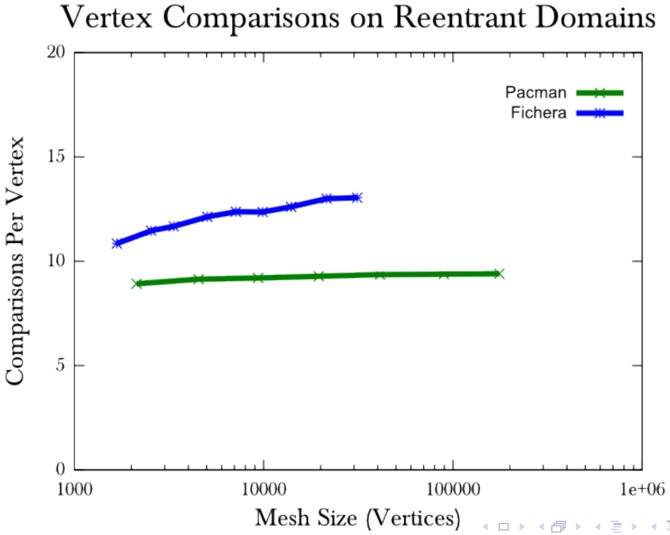
GMG Performance

Linear solver iterates are nearly as system size increases:



GMG Performance

Coarsening work is nearly constant as system size increases:



Quality Experiments

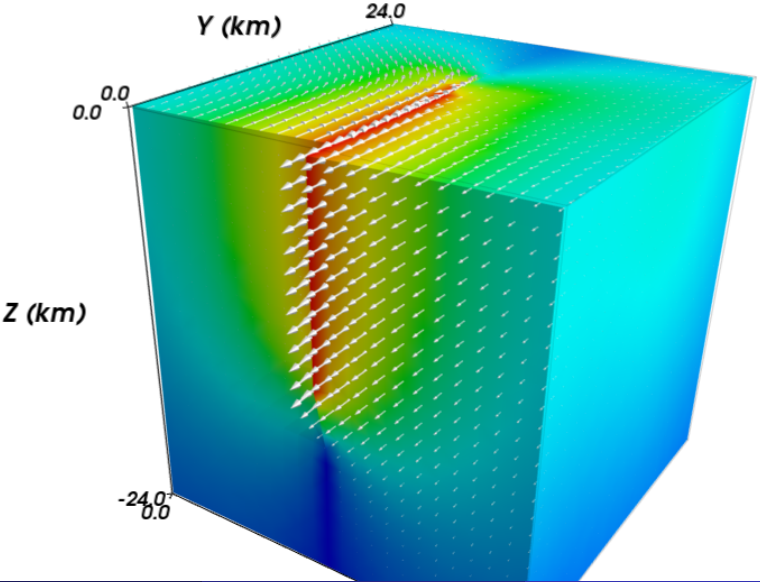
Table: Hierarchy quality metrics - 2D

Pacman Mesh, $\beta = 1.45$						
level	cells	vertices	$\frac{min(h_K)}{h_k}$	max $\frac{h_K}{\rho_K}$	min(h_K)	max. overlap
0	19927	10149	0.020451	4.134135	0.001305	-
1	5297	2731	0.016971	4.435928	0.002094	23
2	3028	1572	0.014506	4.295703	0.002603	14
3	1628	856	0.014797	5.295322	0.003339	14
4	863	464	0.011375	6.403574	0.003339	14
5	449	250	0.022317	6.330512	0.007979	13

Outline

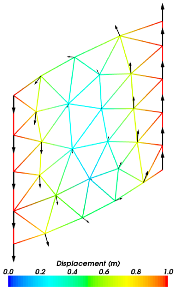
4 Further Work
- FEM
- UMG
- PyLith

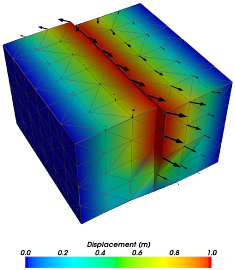
Reverse-slip Benchmark



Multiple Mesh Types

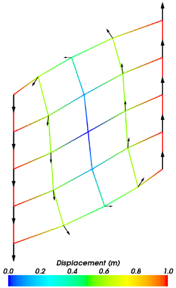
Triangular

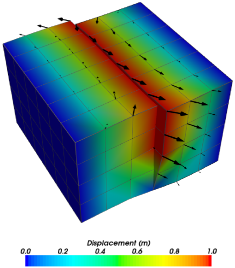




Tetrahedral

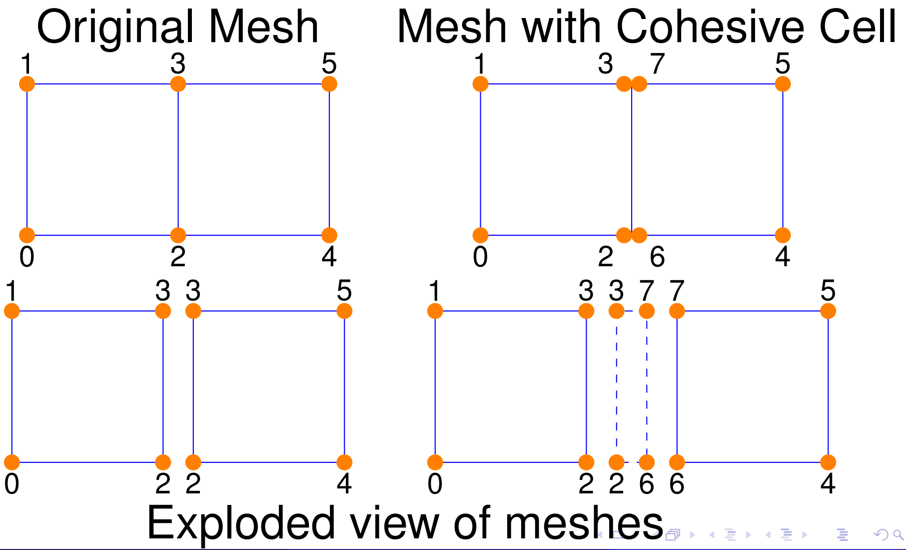
Rectangular





Hexahedral

Cohesive Cells



Cohesive Cells

Cohesive cells are used to enforce slip conditions on a fault

- Demand complex mesh manipulation
  - We allow specification of only fault vertices
  - Must "sew" together on output
- Use Lagrange multipliers to enforce constraints
  - Forces illuminate physics
- Allow different fault constitutive models
  - Simplest is enforced slip
  - Now have fault constitutive models

Conclusions

Better mathematical abstractions bring concrete benefits

- Vast reduction in complexity
  - Declarative, rather than imperative, specification
  - Dimension independent code
- Opportunites for optimization
  - Higher level operations missed by traditional compilers
  - Single communication routine to optimize
- Expansion of capabilities
  - Easy model definition
  - Arbitrary elements
  - Complex geometries and embedded boundaries