

FEniCS and Sieve Tutorial

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March 5, 2007

Workshop on Automating the Development of
Scientific Computing Software
LSU, Baton Rouge, LA

- Introduce FEniCS Automated Mathematical Modeling paradigm
- Enable students to develop new simulations with FEniCS
 - Demonstrate sample problems and typical operations
- Describe PETSc-Sieve project
 - High performance parallel infrastructure

Tutorial Goals

- Introduce FEniCS Automated Mathematical Modeling paradigm
- Enable students to develop new simulations with FEniCS
 - Demonstrate sample problems and typical operations
- Describe PETSc-Sieve project
 - High performance parallel infrastructure

- Introduce FEniCS Automated Mathematical Modeling paradigm
- Enable students to develop new simulations with FEniCS
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- Describe PETSc-Sieve project
 - High performance parallel infrastructure

Outline

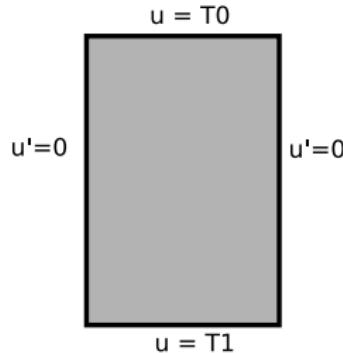
- 1 FEM Concepts
- 2 Getting Started
- 3 Poisson
- 4 Stokes
- 5 Function and Operator Abstractions
- 6 Optimal Solvers

FEM at a Glance

Strong Form

Find u on domain Ω , given f and BC

$$-\Delta u = f$$



FEM at a Glance

Weak Form

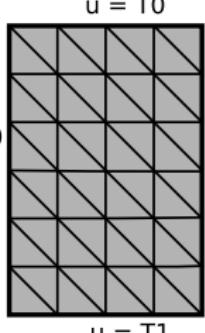
Find u on domain Ω , given f and BC,
such that for all v in the function space S

$$a(u,v) = (f,v) \quad u'=0$$


FEM at a Glance

Discretization

Find \underline{u}_h on a triangulation of domain Ω ,
given f and BC,
such that for all v in the function space S

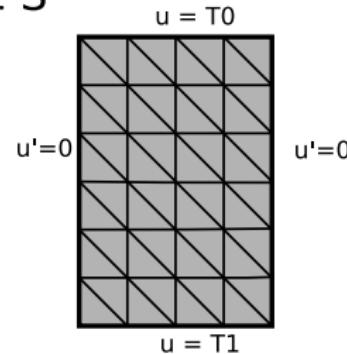
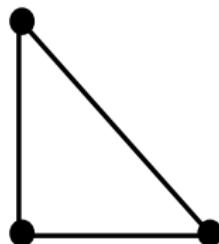
$$a(\underline{u}_h, v) = (f, v)$$


FEM at a Glance

Discretization

Find u_h on a triangulation of domain Ω ,
given f and BC,
such that for all v_h
in the function space $V \subset S$

$$a(u_h, v_h) = (f, v_h)$$



FEM at a Glance

Discrete System

$$A \begin{bmatrix} x \end{bmatrix} = b$$

Outline

1 FEM Concepts

2 Getting Started

- Quick Introduction to FEniCS
- Quick Introduction to PETSc
- Download & Install

3 Poisson

4 Stokes

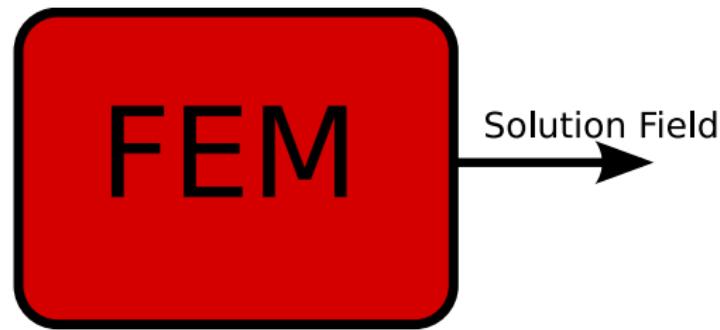
5 Function and Operator Abstractions

6 Optimal Solvers

The FEniCS Project

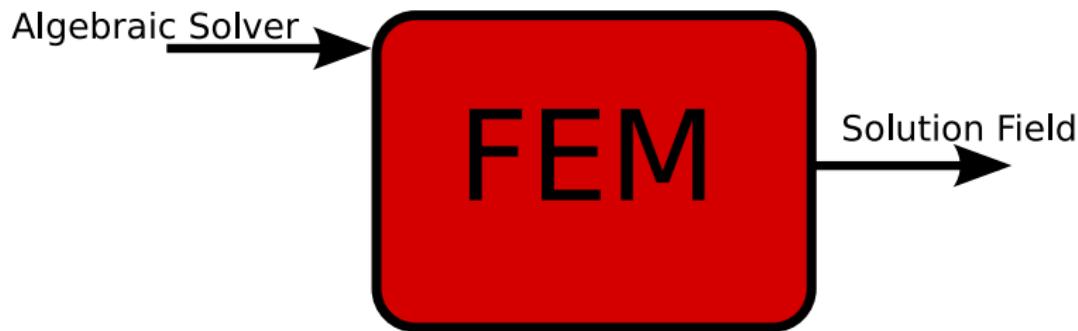
- Started in 2003 as a collaboration between
 - Chalmers
 - University of Chicago
- Now spans
 - Chalmers and KTH
 - University of Oslo and Simula Research
 - University of Chicago and Argonne National Laboratory
 - Cambridge University
 - TU Delft
- Focused on Automated Mathematical Modelling
- Allows researchers to easily and rapidly develop simulations

The FEniCS Project



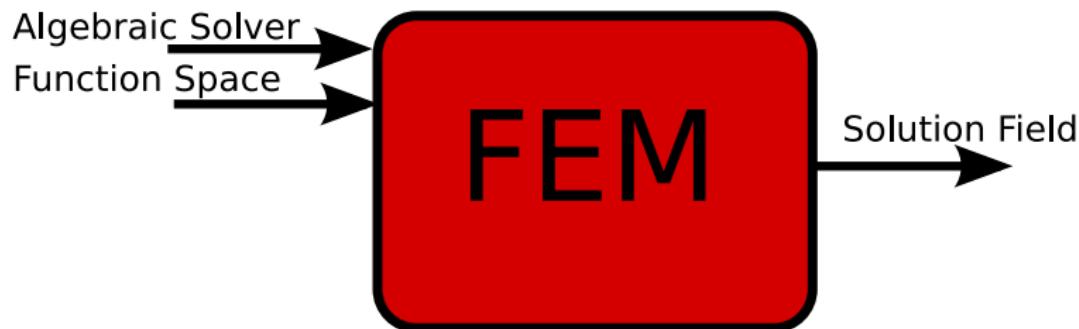
DOLFIN: The simulation engine which pulls all the pieces together.

The FEniCS Project



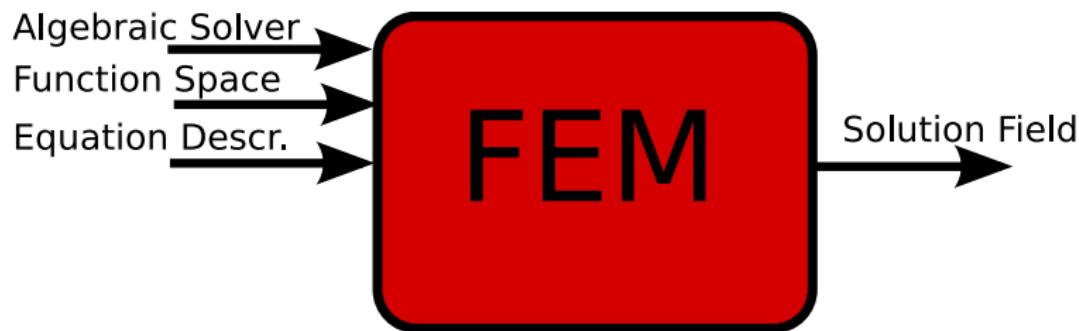
PETSc, uBlas, UMFPACK (separate projects outside FEniCS)

The FEniCS Project



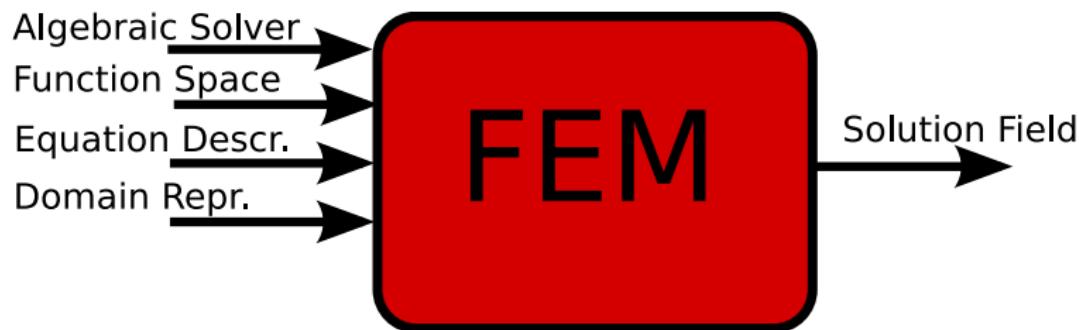
FIAT: Finite element Integrator And Tabulator
SyFi: SYmbolic FInite elements

The FEniCS Project



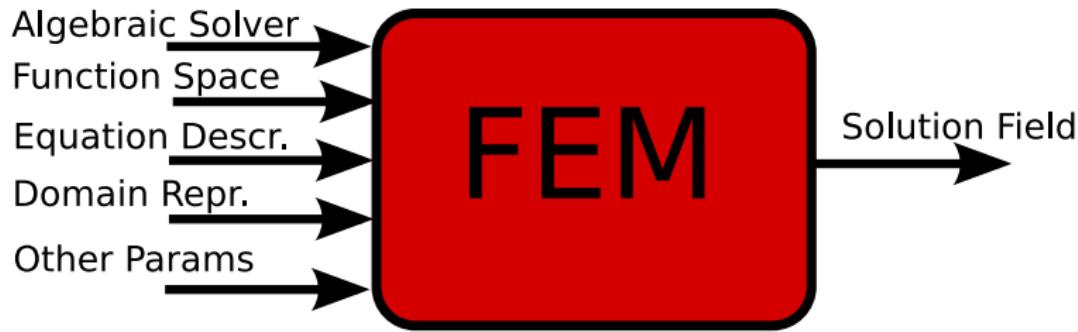
FFC: Fenics Form Compiler, or SyFi

The FEniCS Project



DOLFIN Mesh Library

The FEniCS Project



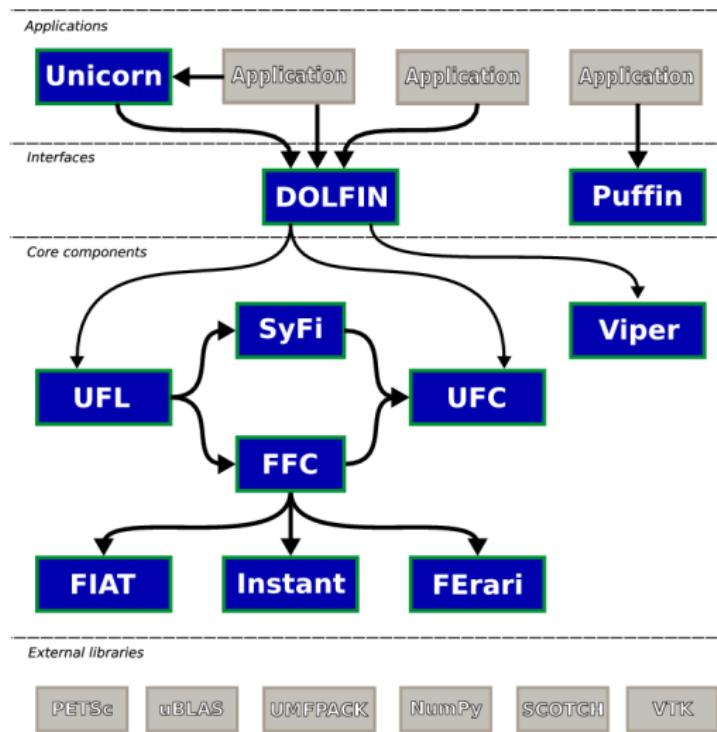
UNICORN: a unified continuum mechanics solver

The FEniCS Project

Other projects

Project	Description
UFC	Links equation discretization to algebraic solver
Viper	Uses pyvtk to produce quick plots
Instant	JIT C compiler for inline functions in python
Puffin	Educational project
FErari	Optimizations for evaluation of variational forms
Sieve	Abstractions for parallel mesh and function representation

The FEniCS Project



What is PETSc?

A freely available and supported research code

- Download from <http://www.mcs.anl.gov/petsc>
- Free for everyone, including industrial users
- Hyperlinked manual, examples, and manual pages for all routines
- Hundreds of tutorial-style examples
- Support via email: petsc-maint@mcs.anl.gov
- Usable from C, C++, Fortran 77/90, and Python

What is PETSc?

- Portable to any parallel system supporting MPI, including:
 - Tightly coupled systems
 - Cray T3E, SGI Origin, IBM SP, HP 9000, Sub Enterprise
 - Loosely coupled systems, such as networks of workstations
 - Compaq, HP, IBM, SGI, Sun, PCs running Linux or Windows
- PETSc History
 - Begun September 1991
 - Over 20,000 downloads since 1995 (version 2), currently 300 per month
- PETSc Funding and Support
 - Department of Energy
 - SciDAC, MICS Program, INL Reactor Program
 - National Science Foundation
 - CIG, CISE, Multidisciplinary Challenge Program

What Can We Handle?

- PETSc has run problems with over **500 million** unknowns
 - <http://www.scconference.org/sc2004/schedule/pdfs/pap111.pdf>
- PETSc has run on over **6,000** processors efficiently
 - ftp://info.mcs.anl.gov/pub/tech_reports/reports/P776.ps.Z
- PETSc applications have run at **2 Teraflops**
 - LANL PFLOTRAN code

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Download and Install

Debian Packages

- **UFC:**

```
apt-get install ufc
```

- **FIAT:**

```
apt-get install fiat
```

- **FFC:**

```
apt-get install ffc
```

- **DOLFIN:**

```
apt-get install dolfin
```

- **Viper:**

```
apt-get install dolfin
```

You also need

```
deb http://www.fenics.org/debian/ unstable main  
deb-src http://www.fenics.org/debian/ unstable main  
in your /etc/apt/source.list, and the key  
wget http://www.fenics.org/debian/pubring.gpg -O- | sudo apt-key add -
```

Download and Install

Source Tarballs

- **UFC:**

<http://www.fenics.org/pub/software/ufc/v1.0/ufc-1.1.tar.gz>

- **FIAT:**

<http://www.fenics.org/pub/software/fiat/FIAT-0.3.4.tar.gz>

- **FFC:**

<http://www.fenics.org/pub/software/ffc/v0.4/ffc-0.4.4.tar.gz>

- **DOLFIN:**

<http://www.fenics.org/pub/software/dolfin/v0.7/dolfin-0.7.2.tar.gz>

- **Viper:**

<http://www.fenics.org/pub/software/viper/v0.2/viper-0.2.0.tgz>

Download and Install

Mercurial Repositories

- **UFC:**

```
hg clone http://www.fenics.org/hg/ufc  
python setup.py install
```

- **FIAT:**

```
hg clone http://www.fenics.org/hg/fiat  
python setup.py install
```

- **FFC:**

```
hg clone http://www.fenics.org/hg/ffc  
python setup.py install
```

- **DOLFIN:**

```
hg clone http://www.fenics.org/hg/dolfin  
See http://www.fenics.org/wiki/DOLFIN
```

- **Viper:**

```
hg clone http://www.fenics.org/hg/viper  
python setup.py install
```

Cloning PETSc

- The full development repository is open to the public
 - <http://petsc.cs.iit.edu/petsc/petsc-dev>
 - <http://petsc.cs.iit.edu/petsc/BuildSystem>
- Why is this better?
 - You can clone to any release (or any specific ChangeSet)
 - You can easily rollback changes (or releases)
 - You can get fixes from us the same day
- We also make release repositories available
 - <http://petsc.cs.iit.edu/petsc-release-2.3.3>

Automatic Downloads

- Starting in 2.2.1, some packages are automatically
 - Downloaded
 - Configured and Built (in \$PETSC_DIR/externalpackages)
 - Installed in PETSc
- Currently works for
 - PETSc documentation utilities (Sowing, Igrend, c2html)
 - BLAS, LAPACK, BLACS, ScaLAPACK, PLAPACK
 - MPICH, MPE, LAM
 - ParMetis, Chaco, Jostle, Party, Scotch, Zoltan
 - MUMPS, Spooles, SuperLU, SuperLU_Dist, UMFPack, pARMS
 - BLOPEX, FFTW, SPRNG
 - Prometheus, HYPRE, ML, SPAI
 - Sundials
 - Triangle, TetGen
 - FIAT, FFC, Generator
 - Boost

Outline

1 FEM Concepts

2 Getting Started

3 Poisson

- Problem Statement
- Higher Order Elements
- Discontinuous Galerkin Methods
- Error Checking

4 Stokes

5 Function and Operator Abstractions

6 Optimal Solvers

Simple Example: Poisson

Poisson

$$-\Delta u = f \quad \text{on} \quad \Omega = [0, 1] \times [0, 1]$$

- Define our Form and compile (FIAT + FFC)
- Define our Simulation (DOLFIN)
 - Define our mesh
 - Assemble and solve
 - Post process (visualize, error, ...)

Simple Example: Poisson

Defining the form

```
element = FiniteElement("Lagrange", "triangle", 1)

v = TestFunction(element)
u = TrialFunction(element)
f = Function(element)
g = Function(element)

a = dot(grad(v), grad(u))*dx
L = v*f*dx
a = dot(grad(v), grad(u))*dx
L = v*f*dx + v*g*ds
```

see `ffc/src/demo/Poisson.form`, and compile with

```
$ ffc Poisson.form
```

Simple Example: Poisson

Writing the Simulation: Define our mesh

```
UnitSquare mesh(32, 32);
```

- Need to give boundary conditions
- Could use other meshing tools and convert to Dolfin xml format

Simple Example: Poisson

Writing the Simulation: Assemble and solve

```
// Create user defined functions
Source f(mesh); Flux g(mesh);
// Create boundary condition
Function u0(mesh, 0.0);
DirichletBoundary boundary;
DirichletBC bc(u0, mesh, boundary);
// Define PDE
PoissonBilinearForm a;
PoissonLinearForm L(f, g);
LinearPDE pde(a, L, mesh, bc);
// Solve PDE
Function u;
pde.solve(u);
```

Simple Example: Poisson

Writing the Simulation: Post process

```
// Plot solution
plot(u);
// Save solution to file
File file("poisson.pvd");
file << u;
```

Simple Example: Poisson

Now let's define our source term as:

$$f(x, y) = 500 * \exp\left(-\frac{(x - 0.5)^2 + (y - 0.5)^2}{0.02}\right)$$

```
class Source : public Function {
    Source(Mesh& mesh) : Function(mesh) {};
    real eval(const real* x) const {
        real dx = x[0] - 0.5;
        real dy = x[1] - 0.5;
        return 500.0*exp(-(dx*dx + dy*dy)/0.02);
    }
};
```

Simple Example: Poisson

Boundary conditions given by

$$\begin{aligned} u(x,y) &= 0 && \text{for } x = 0 \\ du/dn(x,y) &= 25 \sin(5\pi y) && \text{for } x = 1 \\ du/dn(x,y) &= 0 && \text{otherwise} \end{aligned}$$

```

class DirichletBoundary : public SubDomain {
    bool inside(const real* x, bool on_boundary) const {
        return x[0] < DOLFIN_EPS && on_boundary;}
};

class Flux : public Function {
    Flux(Mesh& mesh) : Function(mesh) {};
    real eval(const real* x) const {
        if (x[0] > DOLFIN_EPS)
            return 25.0*sin(5.0*DOLFIN_PI*x[1]);
        else return 0.0;}
};

```

Simple Example: Poisson

Include headers and your done¹

```
#include <dolfin.h>
#include "Poisson.h"
using namespace dolfin;
```

¹See [dolfin/src/demo/pde/poisson/cpp](#)

Simple Example: Poisson

Simulate!

Example: High Order Poisson

Poisson

This time use higher order Lagrangian elements

$$-\Delta u = f \quad \text{on} \quad \Omega = [0, 1] \times [0, 1]$$

- Define our Form and compile (FIAT + FFC)
- Define our Simulation (DOLFIN)
 - Define our mesh
 - Assemble and solve
 - Post process (visualize, error, ...)

Example: High Order Poisson

Defining the form

```
element = FiniteElement("Lagrange", "triangle", p)

v = TestFunction(element)
u = TrialFunction(element)
f = Function(element)
g = Function(element)

a = dot(grad(v), grad(u))*dx
L = v*f*dx
a = dot(grad(v), grad(u))*dx
L = v*f*dx + v*g*ds
```

Compile with

```
$ ffc HOPoisson.form
```

Example: High Order Poisson

Use the same DOLFIN code.

Simulate!

Example: Discontinuous Galerkin Poisson Poisson

$$-\Delta u = f \quad \text{on} \quad \Omega = [0, 1] \times [0, 1]$$

Using a discontinuous Galerkin formulation (interior penalty method).

- Define our Form and compile (FIAT + FFC)
- Define our Simulation (DOLFIN)
 - Define our mesh
 - Assemble and solve
 - Post process (visualize, error, ...)

Example: Discontinuous Galerkin Poisson

Defining the form

```
element = FiniteElement("Discontinuous Lagrange",
                        "triangle", 1)

...
n = FacetNormal("triangle")
h = MeshSize("triangle")
alpha = 4.0; gamma = 8.0
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), mult(u, n))*ds
    - dot(mult(v, n), grad(u))*ds + gamma/h*v*u*ds
```

see ffc/src/demo/PoissonDG.form, and compile with

```
$ ffc PoissonDG.form
```

Example: Discontinuous Galerkin Poisson

Writing the Simulation: Assemble and solve

```
// Create user defined functions
Source f(mesh); Flux g(mesh);
FacetNormal n(mesh);
AvgMeshSize h(mesh);
// Define PDE
PoissonBilinearForm a;
PoissonLinearForm L(f, g);
LinearPDE pde(a, L, mesh, bc);
// Solve PDE
Function u;
pde.solve(u);
```

Example: Discontinuous Galerkin Poisson

Simulate!

Example: L2 Error Check

L2 Error:

$$\|u - u_h\|_{L^2(\Omega)}$$

- Define our Form and compile (FIAT + FFC)
- Add to our Simulation (DOLFIN)
 - Post process (visualize, error, ...)

Example: L2 Error Check

Defining the form

```
P0 = FiniteElement("Discontinuous Lagrange", "triangle", 0)
Element1 = FiniteElement("Lagrange", "triangle", 1)

U = Function(Element1)
u = Function(Element1)
v = BasisFunction(P0)

e = U - u

L = v*dot(e,e)*dx

$ ffc L2Error.form
```

Example: L2 Error Check

Writing the Simulation: Post process

```
ExactSolution U_ex;
Vector tmp;
L2Error::LinearForm L2Error(U,u);
FEM::assemble(L2Error, tmp, mesh);
real error = sqrt(fabs(tmp.sum()));
```

Outline

1 FEM Concepts

2 Getting Started

3 Poisson

4 Stokes

- Mixed Methods
- Iterated Penalty Methods

5 Function and Operator Abstractions

6 Optimal Solvers

Stokes Equations: Basic Fluids Modeling

Function Space Matters

Stokes Equation

- Taylor-Hood
- Crouzeix-Raviart
- Iterated Penalty

$$\begin{aligned}-\Delta \mathbf{u} + \nabla p &= f \\ \nabla \cdot \mathbf{u} &= 0\end{aligned}$$

Stokes Equations: Basic Fluids Modeling

Function Space Matters

$$\frac{du}{dt} + u \cdot \nabla u = -\frac{\nabla p}{\rho} + \nu \Delta u$$

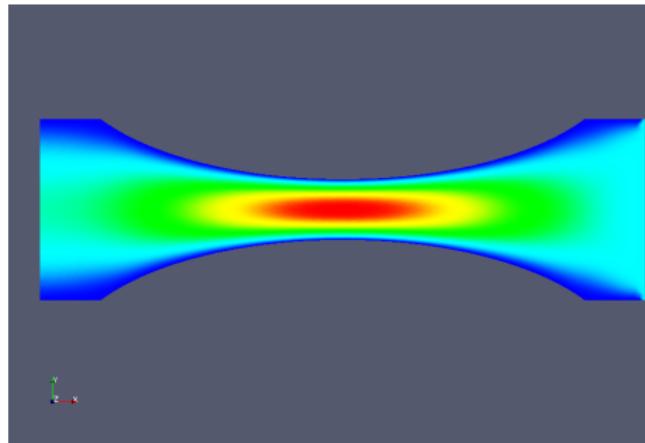
Stokes Equation
Taylor-Hood
Crouzeix-Raviart
Iterated Penalty

Navier-Stokes

- Stokes Solver
- Nonlinear Solver
- Time Stepping

Stokes Equations: Basic Fluids Modeling

Function Space Matters



Stokes Equation
Taylor-Hood
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Iterated Penalty

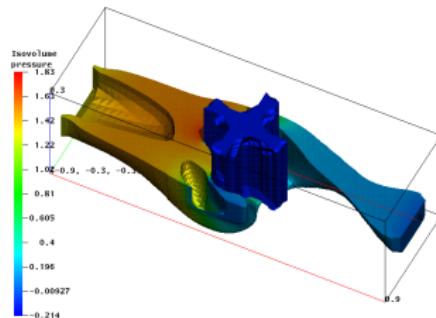
Navier-Stokes
Stokes Solver
Nonlinear Solver
Time Stepping

Non-Newtonian
Flow

- Oldroyd-B
- Grade 2

Stokes Equations: Basic Fluids Modeling

Function Space Matters



Navier-Stokes
Stokes Solver
Nonlinear Solver
Time Stepping

Stokes Equation
Taylor-Hood
Crouzeix-Raviart
Iterated Penalty

Non-Newtonian
Odroyd-B
Grade 2

...

Fluid Solid Interfaces

- Free Boundary Problems
- Couple to legacy Codes

Stokes Mixed Methods

Stokes: Mixed Method Formulation

Let $V = H^1(\Omega)^n$ and $\Pi = \{q \in L^2(\Omega) : \int_{\Omega} q dx = 0\}$. Given $F \in V'$, find functions $\mathbf{u} \in V$ and $p \in \Pi$ such that

$$\begin{aligned} a(\mathbf{u}, \mathbf{v}) + b(\mathbf{v}, p) &= F(\mathbf{v}) \quad \forall \mathbf{v} \in V \\ b(\mathbf{u}, q) &= 0 \quad \forall q \in \Pi \end{aligned}$$

Where,

$$\begin{aligned} a(\mathbf{u}, \mathbf{v}) &:= \int_{\Omega} \nabla \mathbf{u} \cdot \nabla \mathbf{v} dx, \\ b(\mathbf{v}, q) &:= \int_{\Omega} (\nabla \cdot \mathbf{v}) q dx \end{aligned}$$

Stokes Mixed Method

Defining the form

```
P2 = VectorElement("Lagrange", "triangle", 2)
P1 = FiniteElement("Lagrange", "triangle", 1)
TH = P2 + P1

(v, q) = TestFunctions(TH)
(u, p) = TrialFunctions(TH)

f = Function(P2)

a = (dot(grad(v), grad(u)) - div(v)*p + q*div(u))*dx
L = dot(v, f)*dx
```

see dolfin/src/demo/pde/stokes/taylor-hood/cpp/Stokes.form,
and compile with

```
$ ffc Stokes.form
```

Stokes Mixed Method

Define our mesh

Use a predefined mesh, can be made with Triangle, Gmsh, ... and converted to DOLFIN mesh form with dolfin-convert
Use a MeshFunction to mark up different dof on boundary

```
// Read mesh and sub domain markers
Mesh mesh("dolfin-2.xml.gz");
MeshFunction<unsigned int> sub_domains(mesh,
                                         "subdomains.xml.gz");
```

Stokes Mixed Method

New Boundary Conditions

```
// Create functions for boundary conditions
Noslip noslip(mesh); Inflow inflow(mesh);
Function zero(mesh, 0.0);

// Define sub systems for boundary conditions
SubSystem velocity(0);
SubSystem pressure(1);

// BC's per field
DirichletBC bc0(noslip, sub_domains, 0, velocity);
DirichletBC bc1(inflow, sub_domains, 1, velocity);
DirichletBC bc2(zero, sub_domains, 2, pressure);
Array <BoundaryCondition*> bcs(&bc0, &bc1, &bc2);
```

Stokes Mixed Method

Assemble and solve

```
// Set up PDE
Function f(mesh, 0.0);
StokesBilinearForm a;
StokesLinearForm L(f);
LinearPDE pde(a, L, mesh, bcs);

// Solve PDE
Function u;
Function p;
pde.set("PDE linear solver", "direct");
pde.solve(u, p);
```

Stokes Mixed Method

Writing the Simulation: Post process

```
// Plot solution
plot(u);
plot(p);
// Save solution to file
File file("velocity.pvd");
file << u;
File file("pressure.pvd");
file << p;
```

Stokes Mixed Method

```
// Functions for boundary condition for velocity
class Noslip : public Function {
public:
    Noslip(Mesh& mesh) : Function(mesh) {}
    void eval(real* values, const real* x) const {
        values[0] = 0.0;
        values[1] = 0.0;
    }
};

class Inflow : public Function {
public:
    Inflow(Mesh& mesh) : Function(mesh) {}
    void eval(real* values, const real* x) const {
        values[0] = -1.0;
        values[1] = 0.0; }
};
```

Stokes Mixed Method

Simulate!

Iterated Penalty

Stokes: Iterated Penalty Formulation

Let $r \in \mathbb{R}$ and $\rho > 0$ define u^n and $p = w^n$ by

$$\begin{aligned} a(\mathbf{u}^n, \mathbf{v}) + r(\nabla \cdot \mathbf{u}^n, \nabla \cdot \mathbf{v}) &= F(\mathbf{v}) - (\nabla \cdot \mathbf{v}, \nabla \cdot \mathbf{w}^n) \\ \mathbf{w}^{n+1} &= \mathbf{w}^n + \rho \mathbf{u}^n \end{aligned}$$

Stokes IP Method

Defining the form

```
Element = FiniteElement("Vector Lagrange", "triangle", 4)

U = TrialFunction(Element)
v = TestFunction(Element)
f = Function(Element)
w = Function(Element)
c = Constant()

a = (dot(grad(v), grad(U)) - c * div(U) * (div(v)))*dx
L = dot(v, f) * dx + dot(div(v), div(w))*dx

$ ffc Stokes.form
```

Stokes IP Method

Assemble and solve

Setup is relatively the same.

```
Function f(mesh, 0.0), w, u;  
real rho, r, div_u_error;  
Stokes::BilinearForm a(rho);  
rho = r = 1.0e3;  
w.init(mesh, a.trial());
```

Stokes IP Method

Assemble and solve

But we iterate our solution based on L2Error.

```
for(int j; j<MAX_ITERS; j++)
{
    Stokes::LinearForm L(f,w);
    PDE pde(a, L, mesh, bcs);
    // Compute solution
    pde.solve(U);
    Vector tmp = w.vector() + r * (U.vector());
    w = Function(tmp);
    L2div::LinearForm div_u(U);
    FEM::assemble(div_u, tmp, mesh);
    div_u_error = sqrt(fabs(tmp.sum()));
    if (div_u_error < 5.0e-7) break;
}
```

Stokes IP Method

Simulate!

Questions

Fenics Webpage:
<http://www.fenics.org/>

Join the mailing lists!

Outline

- 1 FEM Concepts
- 2 Getting Started
- 3 Poisson
- 4 Stokes
- 5 Function and Operator Abstractions
 - Linear Algebra & Iterative Solvers
 - Rethinking the Mesh
 - Parallelism
 - FEM
- 6 Optimal Solvers

Linear Algebra Abstractions

- Need clear interfaces to ALL levels in the conceptual hierarchy
- Abstractions allow reuse of iterative solvers (Krylov methods)
 - Vec and Mat objects
 - KSP uses only the action of Mat on Vec, MatMult()
- PETSc provides a range of data types
 - MPIAIJ, MPIAIJPERM, SuperLU, ...
 - Arbitrary user code accommodated using MATSHELL objects

Solver Choice

- Can choose solver at runtime
 - `-ksp_type bicgstab`
- Can customize solver
 - `-ksp_gmres_restart 500`
 - Inapplicable options are ignored (same with API calls)
- Monitoring
 - `-ksp_monitor -ksp_view`

Hierarchy Abstractions

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

Unstructured Interface (before)

- Explicit references to element type
 - `getVertices(edgeID)`, `getVertices(faceID)`
 - `getAdjaceny(edgeID, VERTEX)`
 - `getAdjaceny(edgeID, dim = 0)`
- No interface for transitive closure
 - Awkward nested loops to handle different dimensions
- Have to recode for meshes with different
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Go Back to the Math

Combinatorial Topology gives us a framework for geometric computing.

- Abstract to a relation, *covering*, on *points*
 - Points can represent any mesh element
 - Covering can be thought of as adjacency
 - Relation can be expressed in a DAG (for cell complexes)
- Simple query set:
 - provides a general API for geometric algorithms
 - leads to simpler implementations
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- NO explicit references to element type
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 - `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

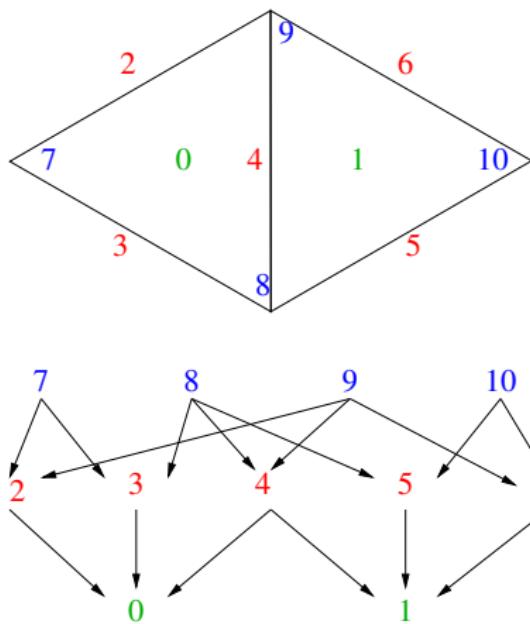
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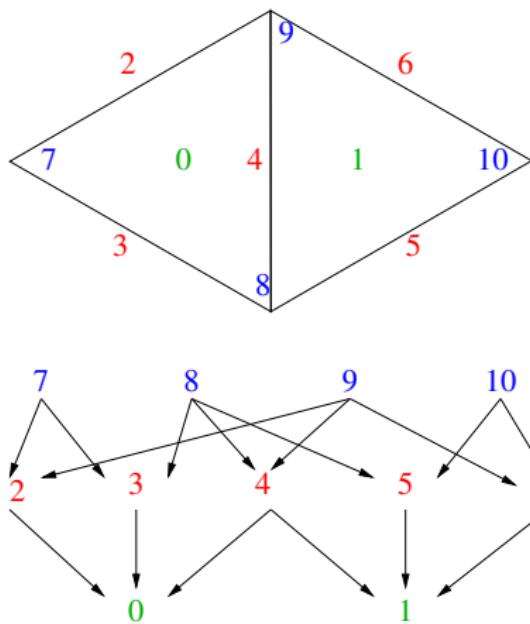
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Doublet Mesh



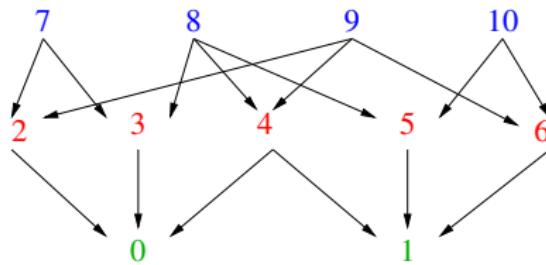
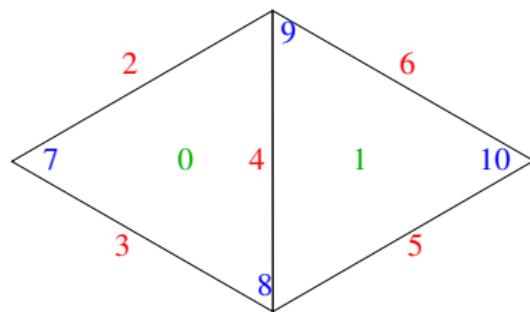
- Incidence/covering arrows
- $\text{cone}(0) = \{2, 3, 4\}$
- $\text{support}(7) = \{2, 3\}$

Doublet Mesh



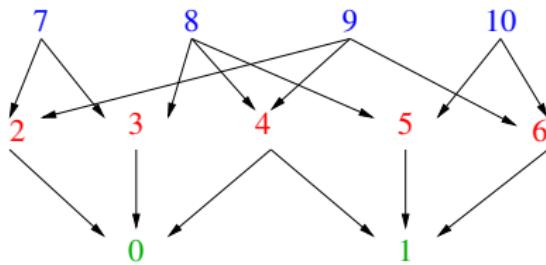
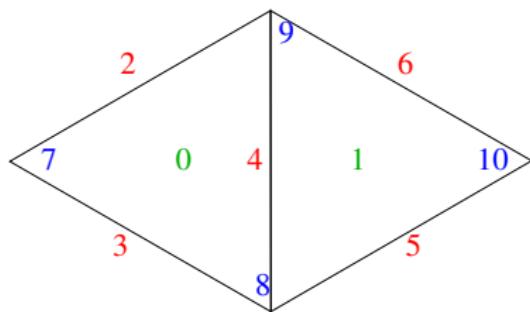
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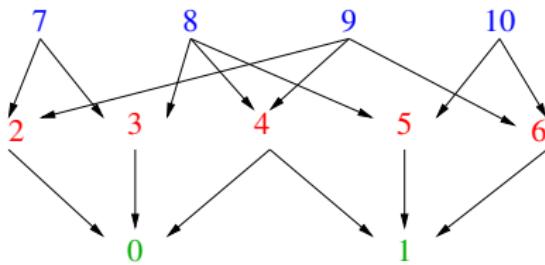
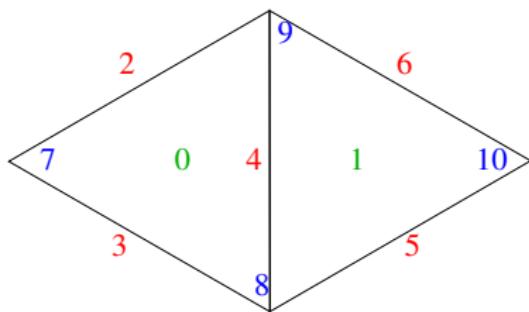
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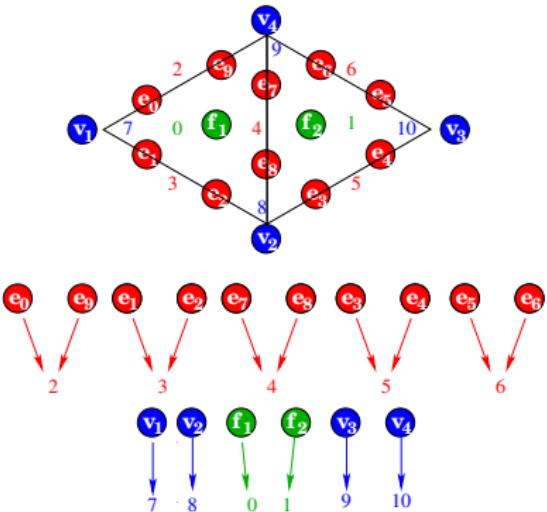
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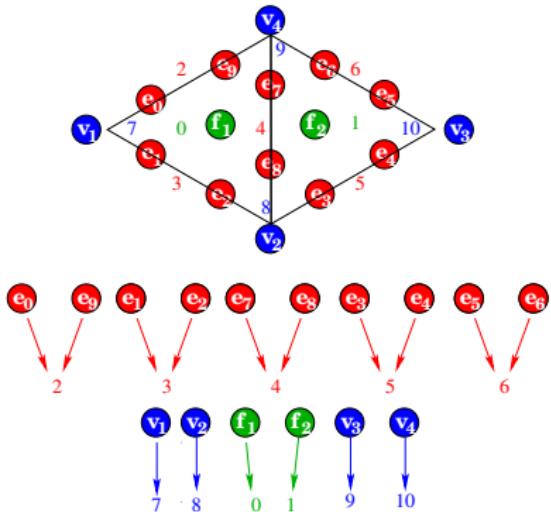
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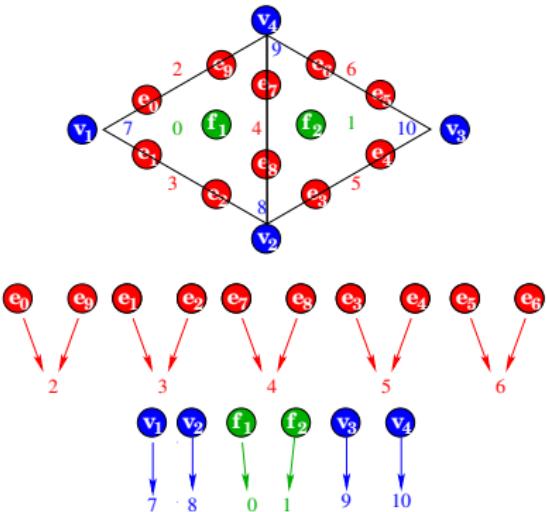
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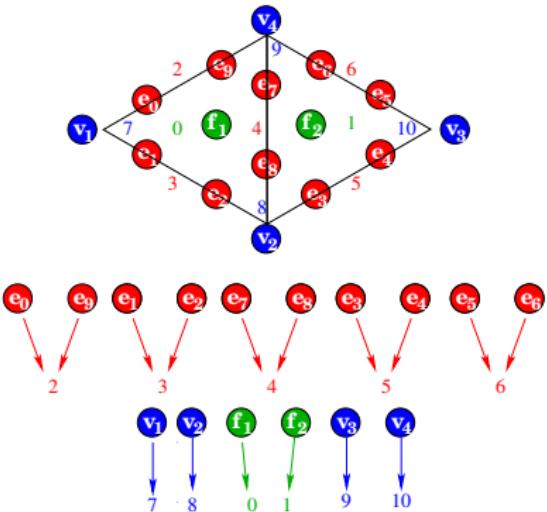
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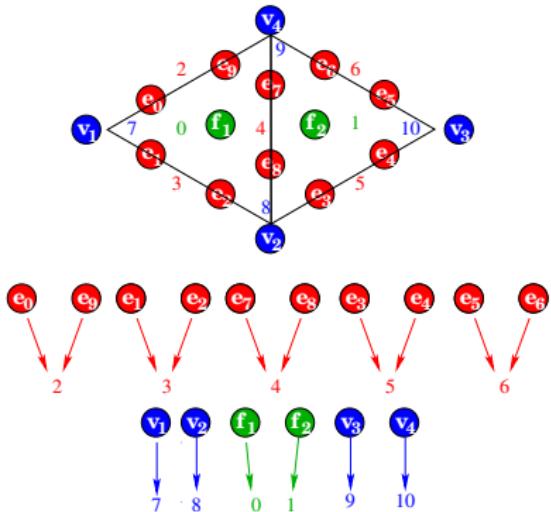
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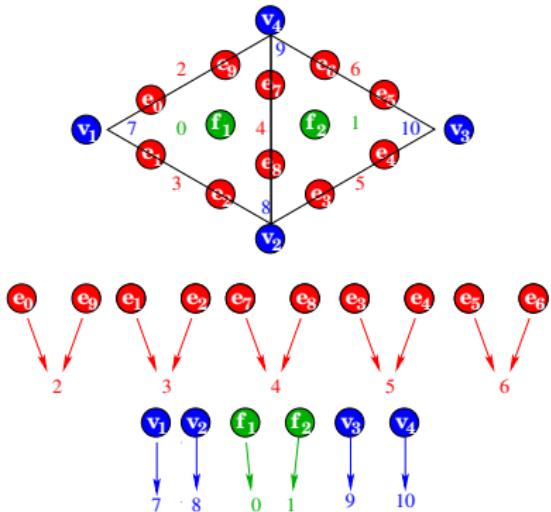
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- Topological traversals: follow connectivity

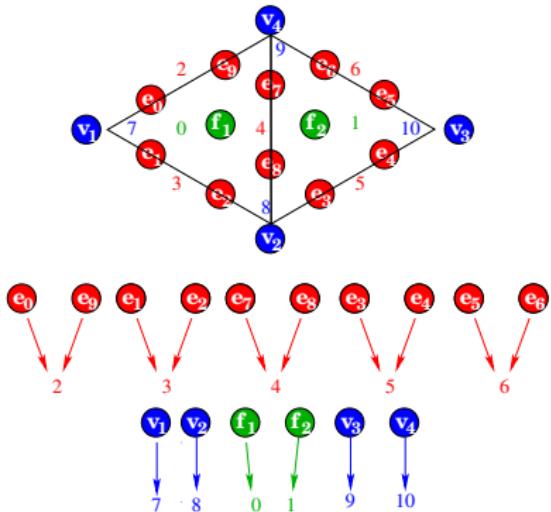
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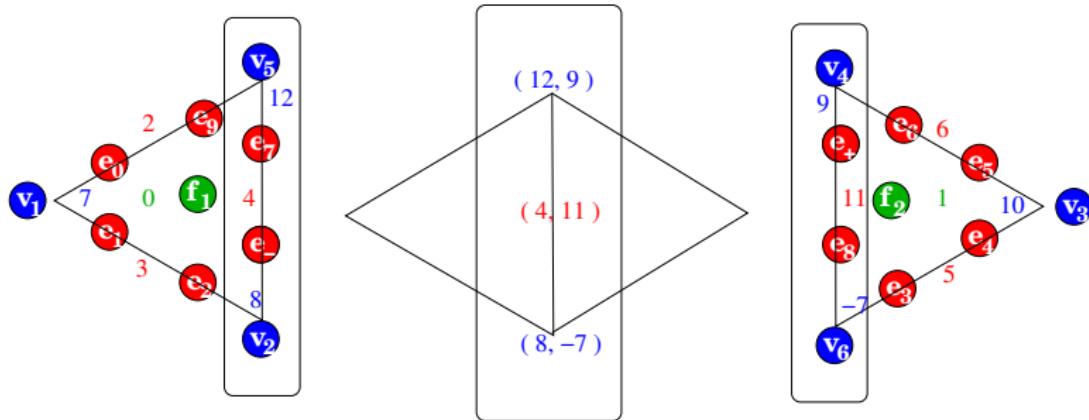
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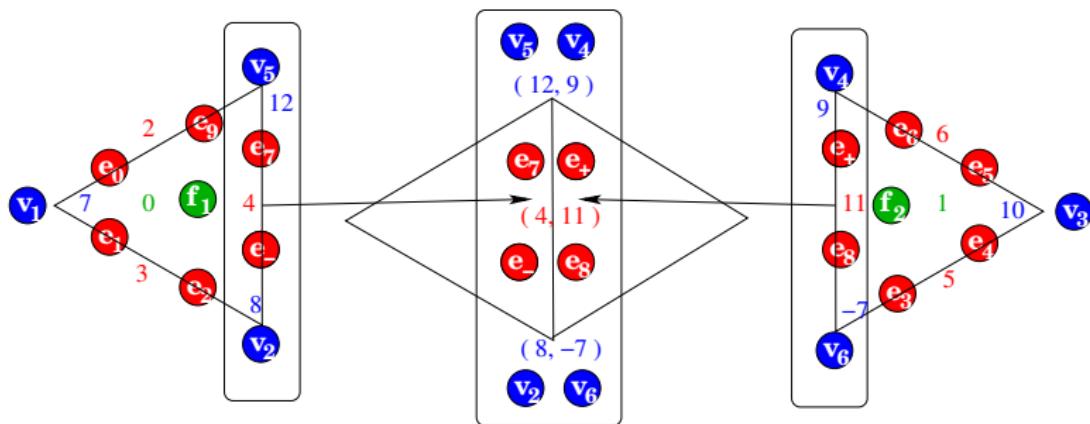
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Restriction



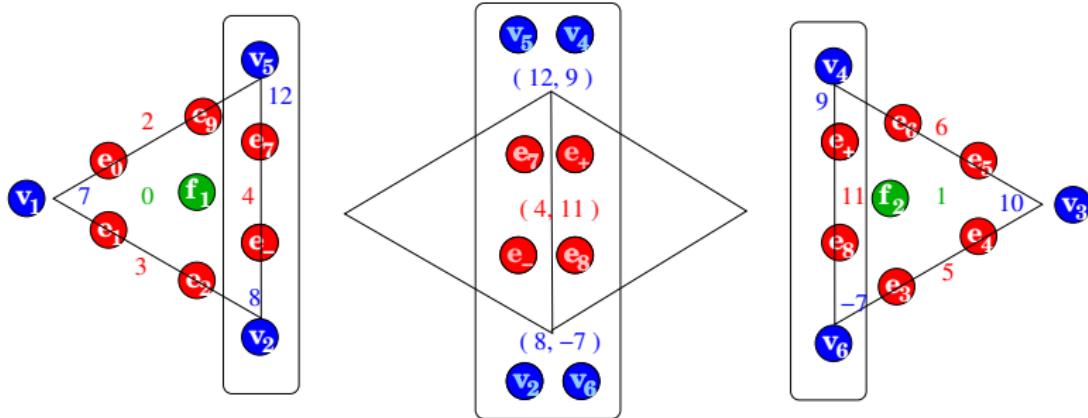
- Localization
 - Restrict to patches (here an edge closure)
 - Compute locally

Delta



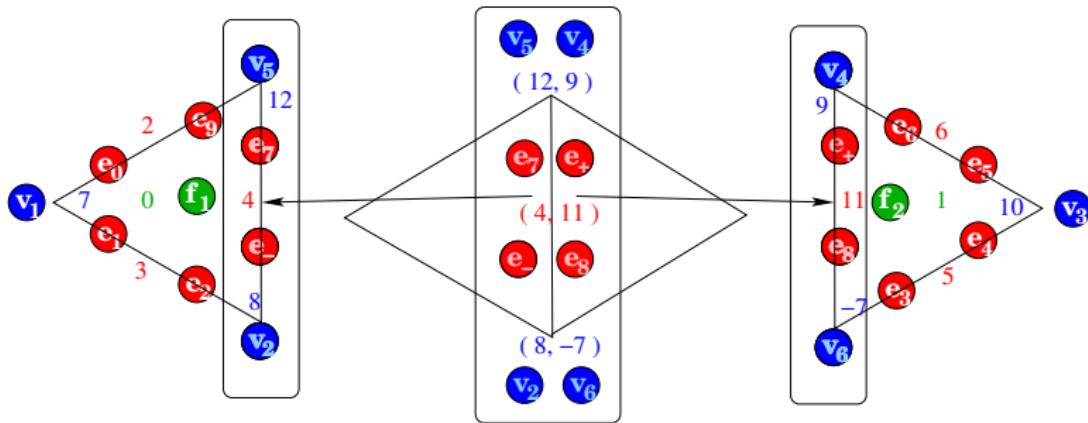
- Delta
 - Restrict further to the overlap
 - Overlap now carries twice the data

Fusion



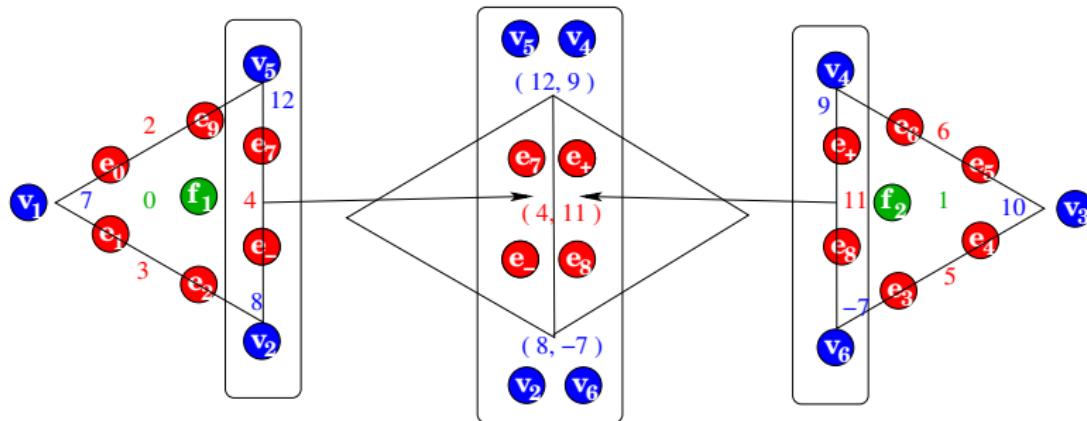
- Merge/reconcile data on the overlap
 - Addition (FEM)
 - Replacement (FD)
 - Coordinate transform (Sphere)
 - Linear transform (MG)

Update



- Update
 - Update local patch data
 - Completion = restrict → fuse → update, *in parallel*

Completion



- A ubiquitous *parallel* form of *restrict* —→ *fuse* —→ *update*
- Operates on Sections
 - Sieves can be "downcast" to Sections
- Based on two operations
 - Data exchange through overlap
 - Fusion of shared data

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
- accumulating matvec for a partially assembled matrix

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Distributing a mesh means

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

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

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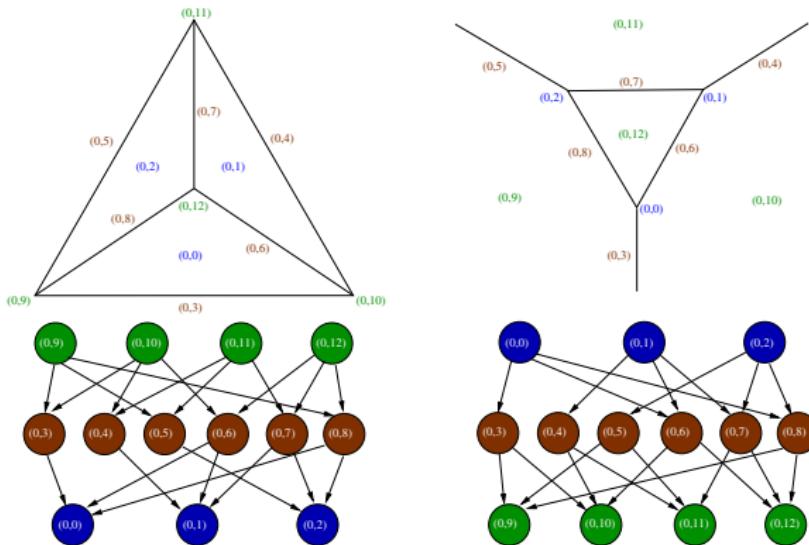
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The Mesh Dual



Construct mesh dual by

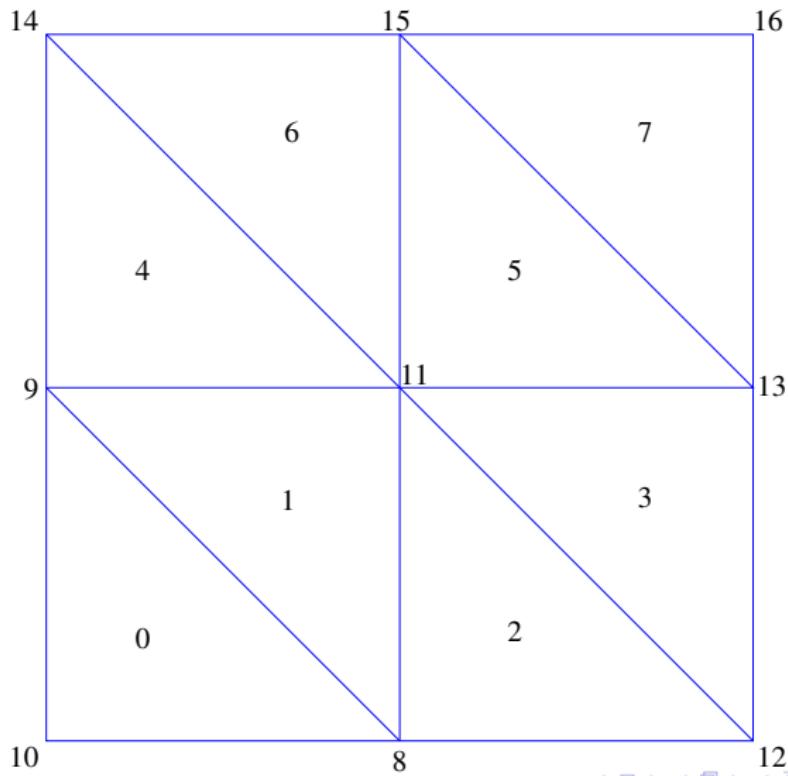
- reversing sieve arrows
- taking the `support()` of each face
- taking the `meet()` of each cell pair

Mesh Partition

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

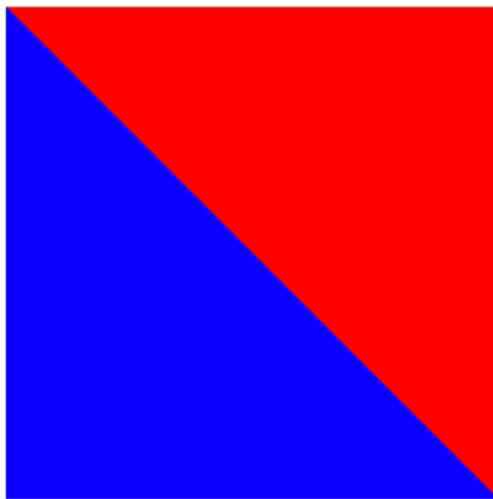
2D Example

A simple triangular mesh



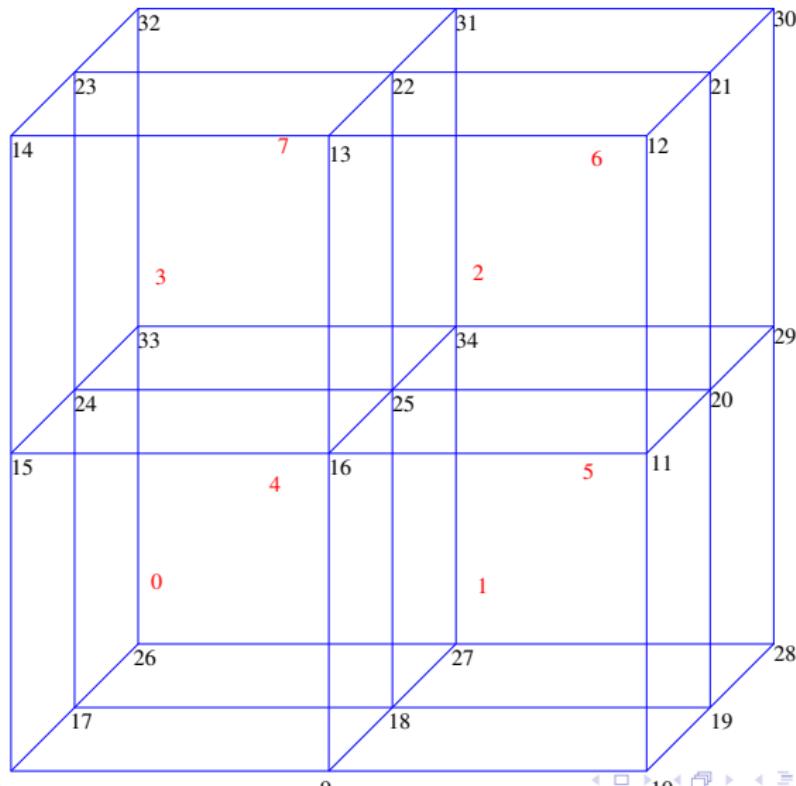
2D Example

Distributed Mesh



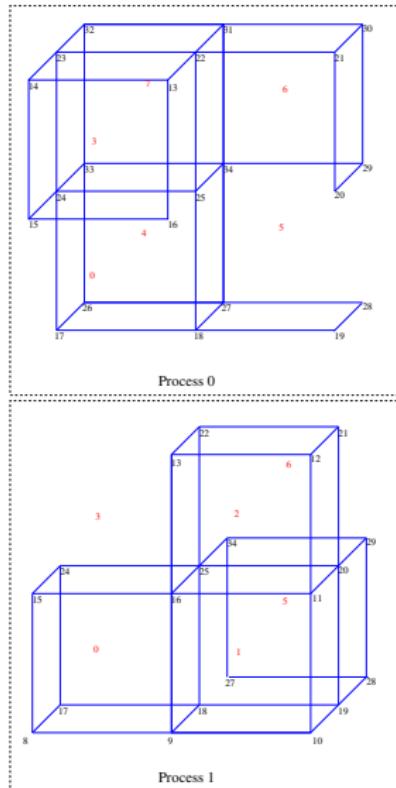
3D Example

A simple hexahedral mesh



3D Example

Distributed Mesh



FEM Components

- Section definition
- Integration
- Boundary conditions

Finite Element Integrator And Tabulator by Rob Kirby

<http://www.fenics.org/fiat>

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, as is the PETSc Sieve module

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FIAT Integration

The quadrature.fiat file contains:

- An element (usually a family and degree) defined by FIAT
- A quadrature rule

It is run

- automatically by make, or
- independently by the user

It can take arguments

- --element_family and --element_order, or
- make takes variables ELEMENT and ORDER

Then make produces quadrature.h with:

- Quadrature points and weights
- Basis function and derivative evaluations at the quadrature points
- Integration against dual basis functions over the cell
- Local dofs for Section allocation

Section Allocation

We only need the fiber dimensions of each point

- Determined by discretization
 - By symmetry, only depend on point depth
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 - Decouples storage and parallelism from discretization

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Kinds of Unknowns

We must map local unknowns to the global basis

- FIAT reports the *kind* of unknown
- Scalars are invariant
 - Lagrange
- Vectors transform as J^{-T}
 - Hermite
- Normal vectors require Piola transform and a choice of orientation
 - Raviart-Thomas
- Moments transform as $|J^{-1}|$
 - Nedelec
- May involve a transformation over the entire closure
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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>
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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) {
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            <Linear term>
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    <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) {
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Integration

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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,f,e];
            for(g = 0; g < numBasisFuncs; ++g) {
                for(d = 0; d < dim; ++d)
                    for(e) basisDerReal[d] += invJ[e,d]*basisDer[q,g,e]
                elemMat[f,g] += testDerReal[d]*basisDerReal[d]
                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) {
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            <Linear term>
            <Nonlinear term>
            elemVec[f] *= weight[q]*detJ;
        }
    }
    <Update output vector>
}
<Aggregate updates>
```

Integration

```
cells = mesh->heightStratum(0);
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    <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>
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    for(q = 0; q < numQuadPoints; ++q) {
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            <Nonlinear term>
            elemVec[f] *= weight[q]*detJ;
        }
    }
    <Update output vector>
}
<Aggregate updates>
```

Integration

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for(c = cells->begin(); c != cells->end(); ++c) {
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    <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>
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            elemVec[f] *= weight[q]*detJ;
        }
    }
    <Update output vector>
}
Distribution<Mesh>::completeSection(mesh, F);
```

Boundary Conditions

Dirichlet conditions may be expressed as

Neumann conditions may be expressed as

Boundary Conditions

Dirichlet conditions may be expressed as

$$u|_{\Gamma} = g$$

Neumann conditions may be expressed as

Boundary Conditions

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and implemented by constraints on dofs in a Section

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

and implemented by explicit integration along the boundary

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)

$$\langle \mathcal{N}_i, f \rangle = \int_{\text{ref}} N_i(x) f(x) dV$$

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

Outline

- 1 FEM Concepts
- 2 Getting Started
- 3 Poisson
- 4 Stokes
- 5 Function and Operator Abstractions
- 6 Optimal Solvers
 - Multigrid for Structured Meshes
 - Multigrid for Unstructured Meshes

What Is Optimal?

I will define *optimal* as an $\mathcal{O}(N)$ solution algorithm

These are generally hierarchical, so we need

- hierarchy generation
- assembly on subdomains
- restriction and prolongation

Payoff

Why should I care?

- ① Current algorithms do not efficiently utilize modern machines
- ② Processor flops are increasing much faster than bandwidth
- ③ Multicore processors are the future
- ④ Optimal multilevel solvers are necessary

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Why Optimal Algorithms?

- The more powerful the computer,
the **greater** the importance of optimality
- Example:
 - Suppose Alg_1 solves a problem in time CN^2 , N is the input size
 - Suppose Alg_2 solves the same problem in time CN
 - Suppose Alg_1 and Alg_2 are able to use 10,000 processors
- In constant time compared to serial,
 - Alg_1 can run a problem 100X larger
 - Alg_2 can run a problem **10,000X** larger
- Alternatively, filling the machine's memory,
 - Alg_1 requires 100X time
 - Alg_2 runs in **constant** time

Multigrid

Multigrid is *optimal* in that it does $\mathcal{O}(N)$ work for $\|r\| < \epsilon$

- Brandt, Briggs, Chan & Smith
- Constant work per level
 - Sufficiently strong solver
 - Need a constant factor decrease in the residual
- Constant factor decrease in dof
 - Log number of levels

Linear Convergence

Convergence to $\|r\| < 10^{-9}\|b\|$ using GMRES(30)/ILU

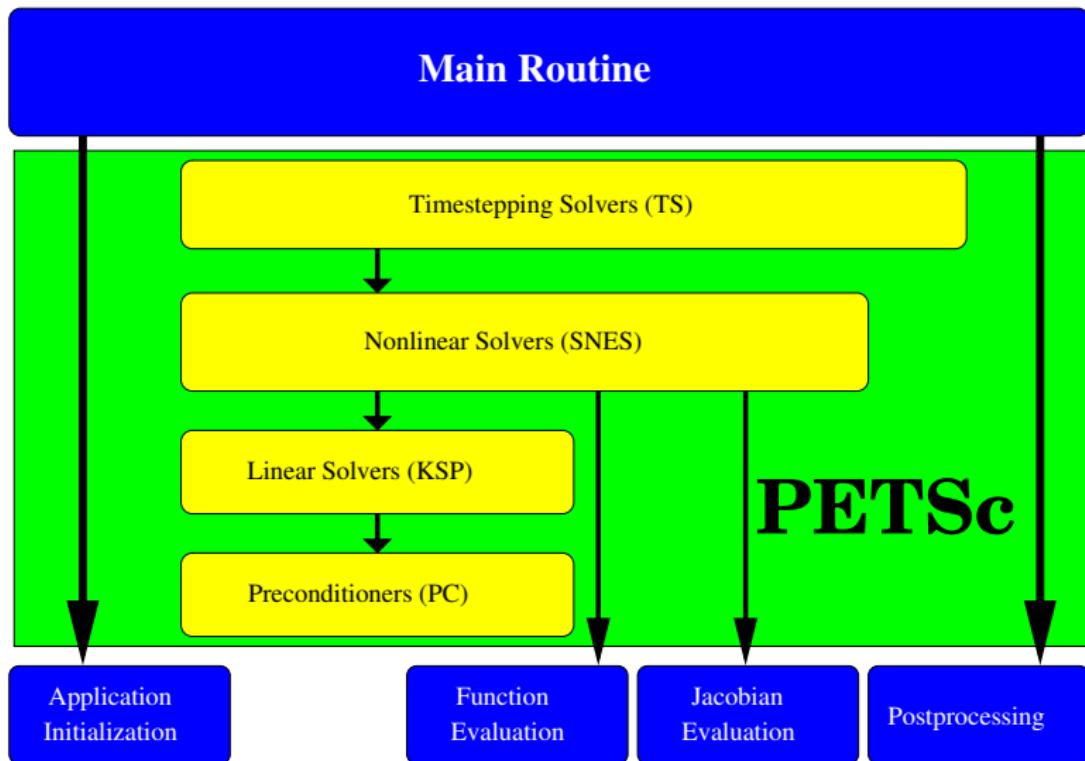
Elements	Iterations
128	10
256	17
512	24
1024	34
2048	67
4096	116
8192	167
16384	329
32768	558
65536	920
131072	1730

Linear Convergence

Convergence to $\|r\| < 10^{-9}\|b\|$ using GMRES(30)/MG

Elements	Iterations
128	5
256	7
512	6
1024	7
2048	6
4096	7
8192	6
16384	7
32768	6
65536	7
131072	6

Flow Control for a PETSc Application



SNESCallbacks

The SNES interface is based upon callback functions

- SNESSetFunction()
- SNESSetJacobian()

When PETSc needs to evaluate the nonlinear residual $F(x)$, the solver calls the **user's** function inside the application.

The user function get application state through the `ctx` variable. PETSc never sees application data.

Higher Level Abstractions

The PETSc DA class is a topology and discretization interface.

- Structured grid interface
 - Fixed simple topology
- Supports stencils, communication, reordering
 - Limited idea of operators
- Nice for simple finite differences

The PETSc Mesh class is a topology interface.

- Unstructured grid interface
 - Arbitrary topology and element shape
- Supports partitioning, distribution, and global orders

Higher Level Abstractions

The PETSc DM class is a hierarchy interface.

- Supports multigrid
 - DMMG combines it with the MG preconditioner
- Abstracts the logic of multilevel methods

The PETSc Section class is a function interface.

- Functions over unstructured grids
 - Arbitrary layout of degrees of freedom
- Support distribution and assembly

A DA is more than a Mesh

A DA contains **topology**, **geometry**, and an implicit Q1 **discretization**.

It is used as a template to create

- Vectors (functions)
- Matrices (linear operators)

Structured Meshes

The DMMG allows multigrid which some simple options

- `-dmmg_nlevels`, `-dmmg_view`
- `-pc_mg_type`, `-pc_mg_cycle_type`
- `-mg_levels_1_ksp_type`, `-dmmg_levels_1_pc_type`
- `-mg_coarse_ksp_type`, `-mg_coarse_pc_type`

Creating a DA

```
DACreate2d(comm, wrap, type, M, N, m, n, dof, s, lm[],  
ln[], DA *da)
```

wrap: Specifies periodicity

- DA_NONPERIODIC, DA_XPERIODIC, DA_YPERIODIC, or DA_XYPERIODIC

type: Specifies stencil

- DA_STENCIL_BOX or DA_STENCIL_STAR

M/N: Number of grid points in x/y-direction

m/n: Number of processes in x/y-direction

dof: Degrees of freedom per node

s: The stencil width

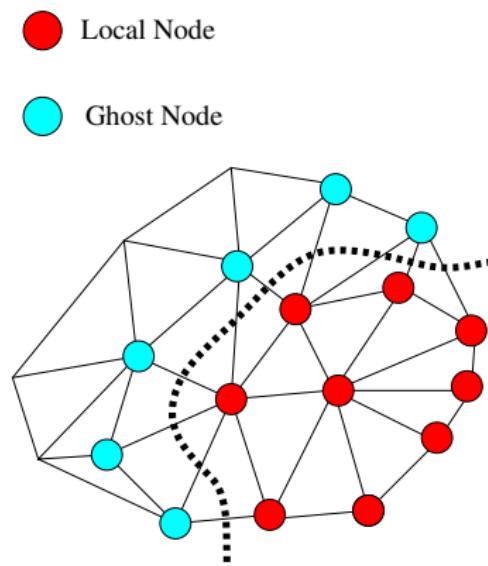
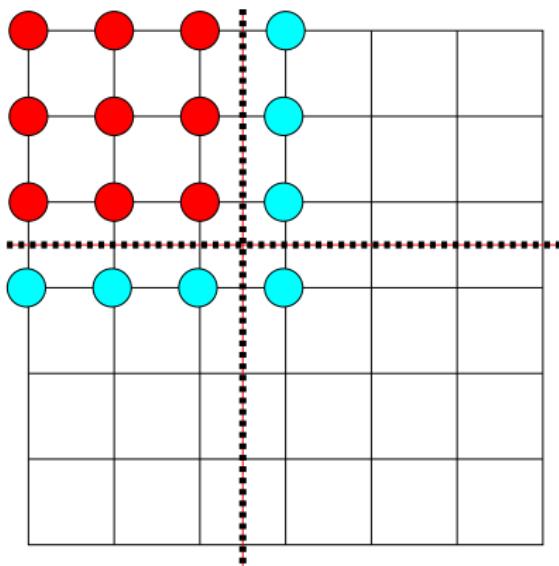
lm/n: Alternative array of local sizes

- Use PETSC_NULL for the default

Ghost Values

To evaluate a local function $f(x)$, each process requires

- its local portion of the vector x
 - its **ghost values**, bordering portions of x owned by neighboring processes



DA Global Numberings

Proc 2			Proc 3	
25	26	27	28	29
20	21	22	23	24
15	16	17	18	19
10	11	12	13	14
5	6	7	8	9
0	1	2	3	4
Proc 0		Proc 1		

Natural numbering

Proc 2			Proc 3	
21	22	23	28	29
18	19	20	26	27
15	16	17	24	25
6	7	8	13	14
3	4	5	11	12
0	1	2	9	10
Proc 0		Proc 1		

PETSc numbering

DA Global vs. Local Numbering

- **Global:** Each vertex belongs to a unique process and has a unique id
- **Local:** Numbering includes **ghost** vertices from neighboring processes

Proc 2			Proc 3	
X	X	X	X	X
12	13	14	15	X
8	9	10	11	X
4	5	6	7	X
0	1	2	3	X
Proc 0		Proc 1		

Local numbering

Proc 2			Proc 3	
21	22	23	28	29
18	19	20	26	27
15	16	17	24	25
6	7	8	13	14
3	4	5	11	12
0	1	2	9	10
Proc 0			Proc 1	

Global numbering

DA Vectors

- The DA object contains only layout (topology) information
 - All field data is contained in PETSc Vecs
- Global vectors are parallel
 - Each process stores a unique local portion
 - `DACreateGlobalVector(DA da, Vec *gvec)`
- Local vectors are sequential (and usually temporary)
 - Each process stores its local portion plus ghost values
 - `DACreateLocalVector(DA da, Vec *lvec)`
 - includes ghost values!

DA Local Function

The user provided function which calculates the nonlinear residual in 2D has signature

```
PetscErrorCode (*lfunc)(DALocalInfo *info, PetscScalar **x,  
                      PetscScalar **r, void *ctx)
```

info: All layout and numbering information

x: The current solution

- Notice that it is a multidimensional array

r: The residual

ctx: The user context passed to DASetLocalFunction()

The local DA function is activated by calling

```
SNESSetFunction(snes, r, SNESDAFormFunction, ctx)
```

Bratu Residual Evaluation

$$\Delta u + \lambda e^u = 0$$

```
BratuResidualLocal(DALocalInfo *info,Field **x,Field **f)
{
    /* Not Shown: Handle boundaries */
    /* Compute over the interior points */
    for(j = info->ys; j < info->xs+info->ym; j++) {
        for(i = info->xs; i < info->ys+info->xm; i++) {
            u          = x[j][i];
            u_xx      = (2.0*u - x[j][i-1] - x[j][i+1])*hydhx;
            u_yy      = (2.0*u - x[j-1][i] - x[j+1][i])*hxdhy;
            f[j][i]   = u_xx + u_yy - hx*hy*lambda*exp(u);
        }
    }
}
```

\$PETCS_DIR/src/snes/examples/tutorials/ex5.c

DA Local Jacobian

The user provided function which calculates the Jacobian in 2D has signature

```
PetscErrorCode (*lfunc)(DALocalInfo *info, PetscScalar **x,  
                      Mat J, void *ctx)
```

`info`: All layout and numbering information

`x`: The current solution

`J`: The Jacobian

`ctx`: The user context passed to `DASetLocalFunction()`

The local DA function is activated by calling

```
SNESSetJacobian(snes, J, J, SNESDAComputeJacobian, ctx)
```

Updating Ghosts

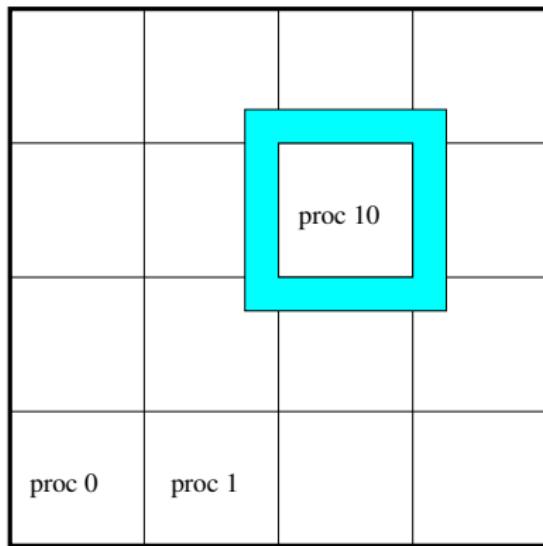
Two-step process enables overlapping computation and communication

- `DAGlobalToLocalBegin(da, gvec, mode, lvec)`
 - `gvec` provides the data
 - `mode` is either `INSERT_VALUES` or `ADD_VALUES`
 - `lvec` holds the local and ghost values
- `DAGlobalToLocalEnd(da, gvec, mode, lvec)`
 - Finishes the communication

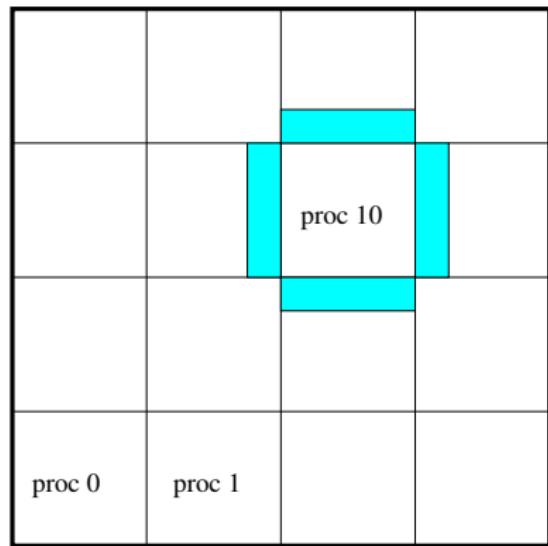
The process can be reversed with `DALocalToGlobal()`.

DA Stencils

Both the **box stencil** and **star stencil** are available.



Box Stencil



Star Stencil

Setting Values on Regular Grids

PETSc provides

```
MatSetValuesStencil(Mat A, m, MatStencil idxm[], n,
                    MatStencil idxn[], values[], mode)
```

- Each row or column is actually a MatStencil
 - This specifies grid coordinates and a component if necessary
 - Can imagine for unstructured grids, they are *vertices*
- The values are the same logically dense block in rows and columns

DMMG Integration with SNES

- DMMG supplies global residual and Jacobian to SNES
 - User supplies local version to DMMG
 - The `Rhs_*`() and `Jac_*`() functions in the example
- Allows automatic parallelism
- Allows grid hierarchy
 - Enables multigrid once interpolation/restriction is defined
- Paradigm is developed in unstructured work
 - Notice we have to scatter into contiguous global vectors (initial guess)
- Handle Neumann BC using `DMMGSetNullSpace()`

The Bratu Problem

$$\Delta u + \lambda e^u = f \quad \text{in} \quad \Omega \quad (1)$$

$$u = g \quad \text{on} \quad \partial\Omega \quad (2)$$

- Nonlinearly perturbed Poisson
- Can be treated as a nonlinear eigenvalue problem
- Has two solution branches until $\lambda \cong 6.28$

A 2D Problem

Problem has:

- 1,329,409 unknowns (on the fine level)
- 11,950,849 nonzeros

Executable	Options	Explanation
./bratu	<pre>-da_grid_x 10 -da_grid_y 10 -ksp_rtol 1.0e-9 -dmmg_nlevels 8 -mg_levels_4_pc_type sor -mg_levels_5_pc_type sor -mg_levels_6_pc_type sor -mg_levels_7_pc_type sor -snes_view</pre>	<p>Coarse grid is 10x10</p> <p>Solver tolerance</p> <p>8 levels of refinement</p> <p>Memory savings</p> <p>Describe solver</p>

A 3D Problem

Problem has:

- 912,673 unknowns (on the fine level)
- 24,137,569 nonzeros

Executable	Options	Explanation
./bratu	-dim 3	-da_grid_x 7
	-da_grid_y 7	-da_grid_z 7
	-ksp_rtol 1.0e-9	Solver tolerance
	-dmmg_nlevels 5	5 levels of refinement
	-mg_levels_3_pc_type sor	Memory savings
	-mg_levels_4_pc_type sor	
	-snes_view	Describe solver

Sections

Sections associate data to submeshes

- Name comes from section of a fiber bundle
 - Generalizes linear algebra paradigm
- Define `restrict()`,`update()`
- Define `complete()`
- Assembly routines take a Sieve and several Sections
 - This is called a Bundle

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)

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Why not use AMG?

- Of course we will try AMG
 - BoomerAMG, ML, SAMG, ASA
- Problems with vector character
- Geometric aspects to the problem
 - Material property variation
 - Faults

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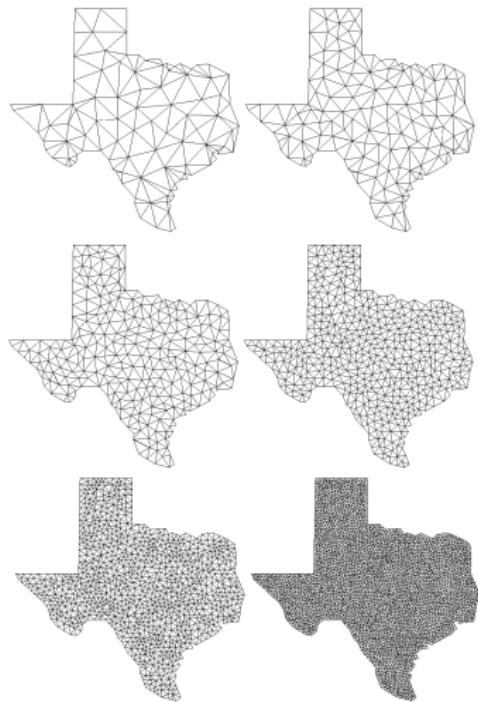
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Unstructured Meshes

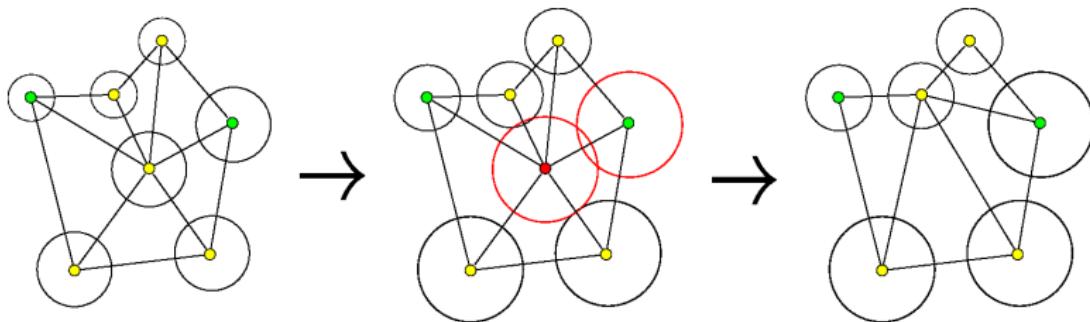
- Same DMMG options as the structured case
- Mesh refinement
 - Ruppert algorithm in Triangle and TetGen
- Mesh coarsening
 - Talmor-Miller algorithm in PETSc
- More advanced options
 - `-dmmg_refine`
 - `-dmmg_hierarchy`
- Current version only works for linear elements

Coarsening



- Users want to control the mesh
- Developed efficient, topological coarsening
 - Miller, Talmor, Teng algorithm
- Provably well-shaped hierarchy

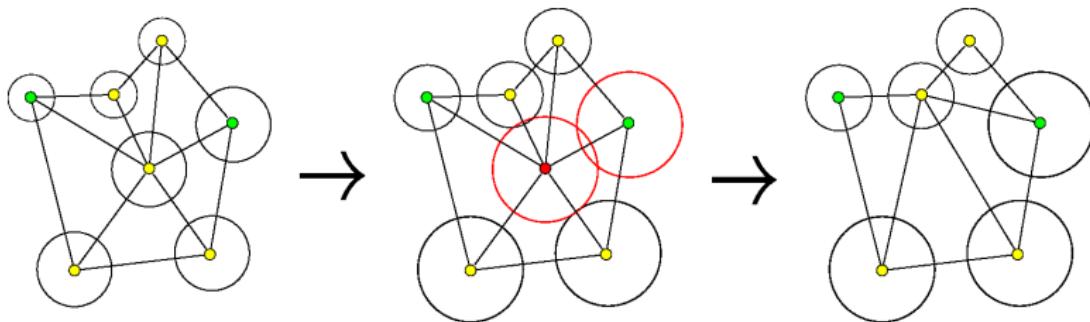
Miller-Talmor-Teng Algorithm



Simple Coarsening

- ① Compute a **spacing function** f for the mesh (Koebe)
- ② Scale f by a factor $C > 1$
- ③ Choose a maximal independent set of vertices for new f
- ④ Retriangulate

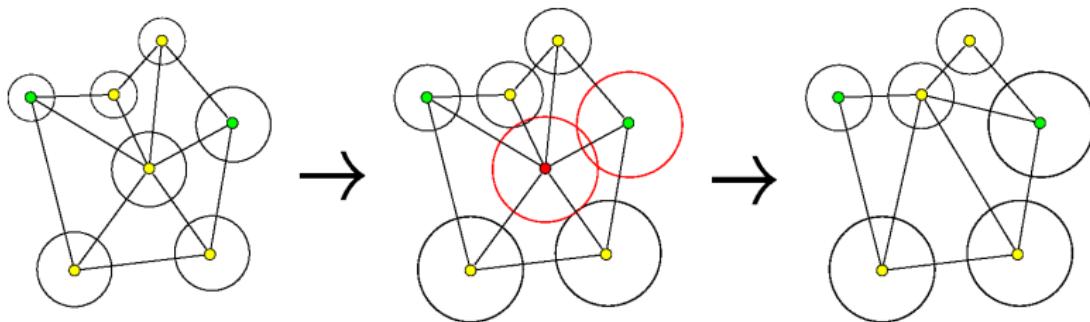
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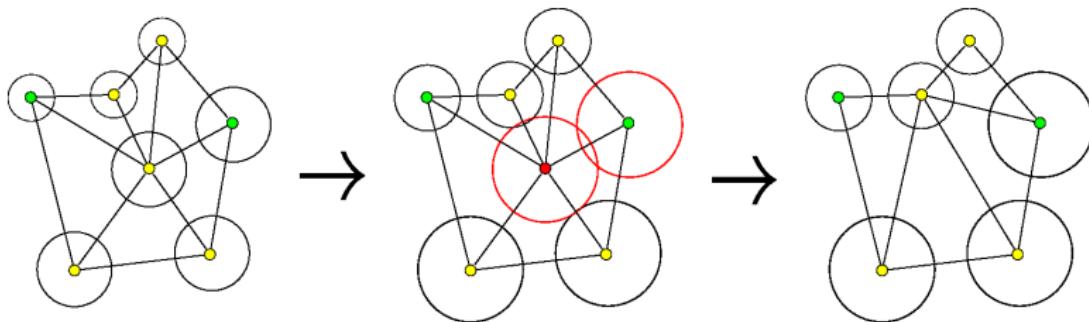
Miller-Talmor-Teng Algorithm



Simple Coarsening

- ① Compute a **spacing function** f for the mesh (Koebe)
- ② Scale f by a factor $C > 1$
- ③ Choose a maximal independent set of vertices for new f
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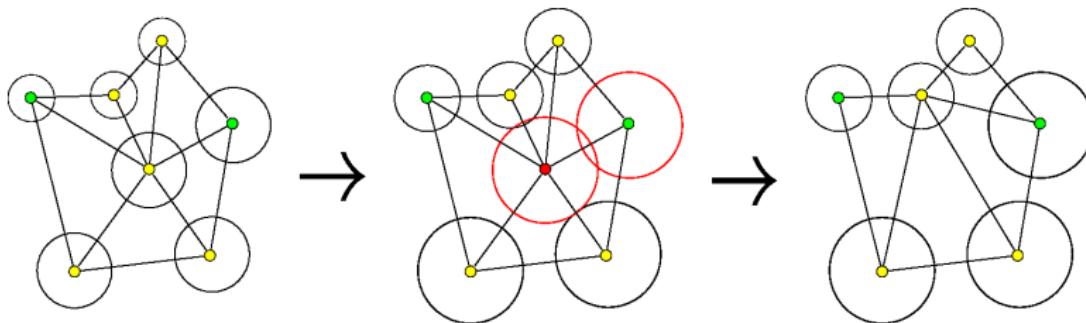
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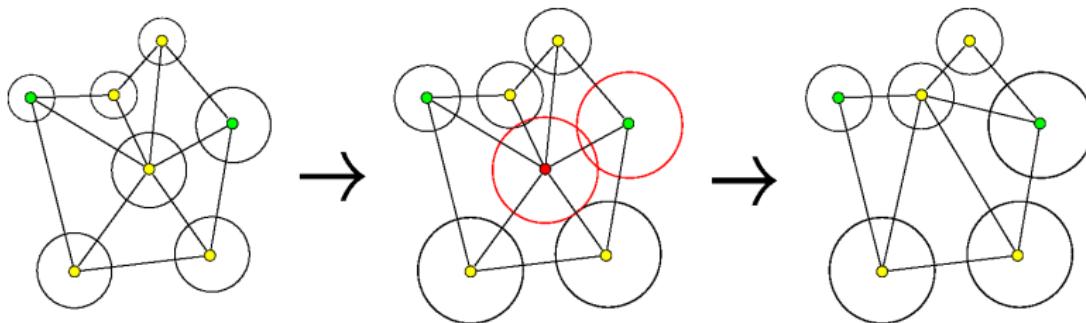
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Caveats

- ① Must generate coarsest grid in hierarchy first
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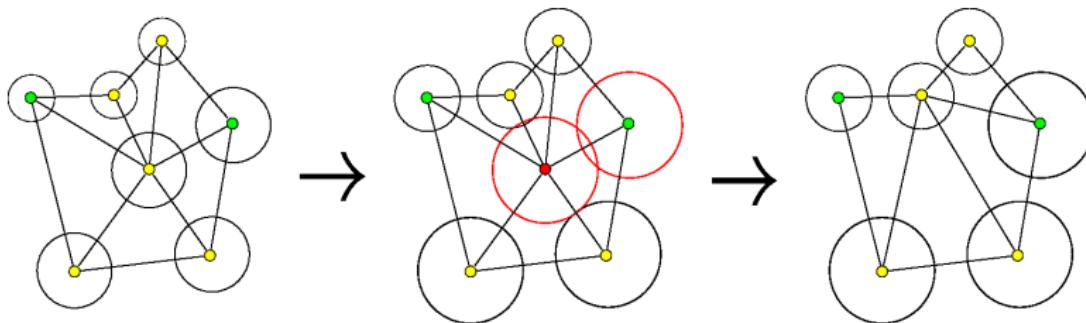
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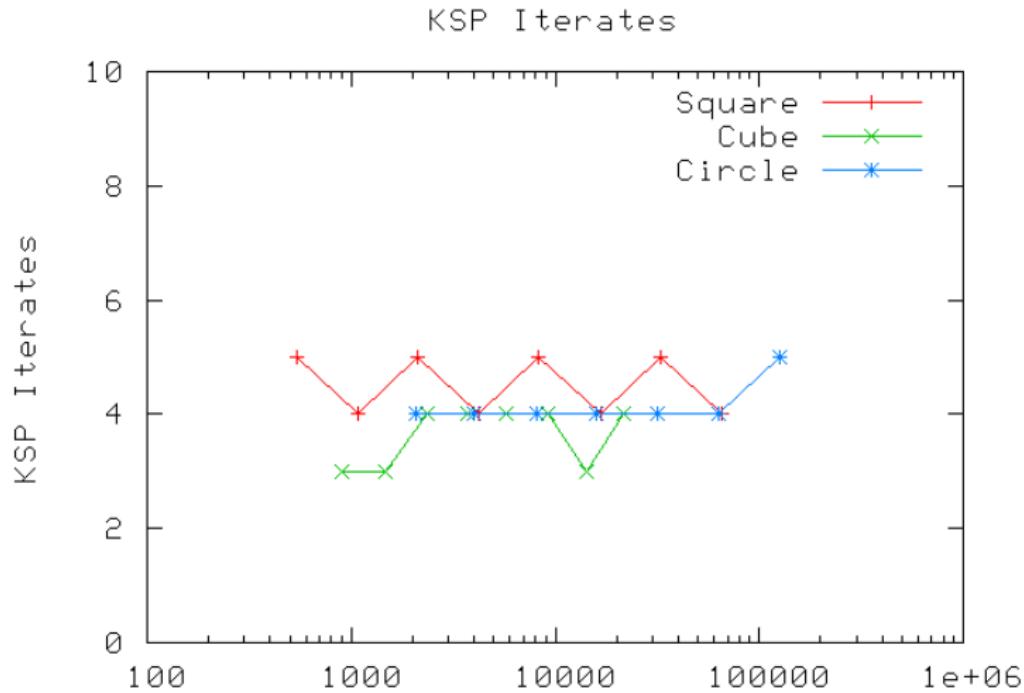
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GMG Performance

For simple domains, everything works as expected:

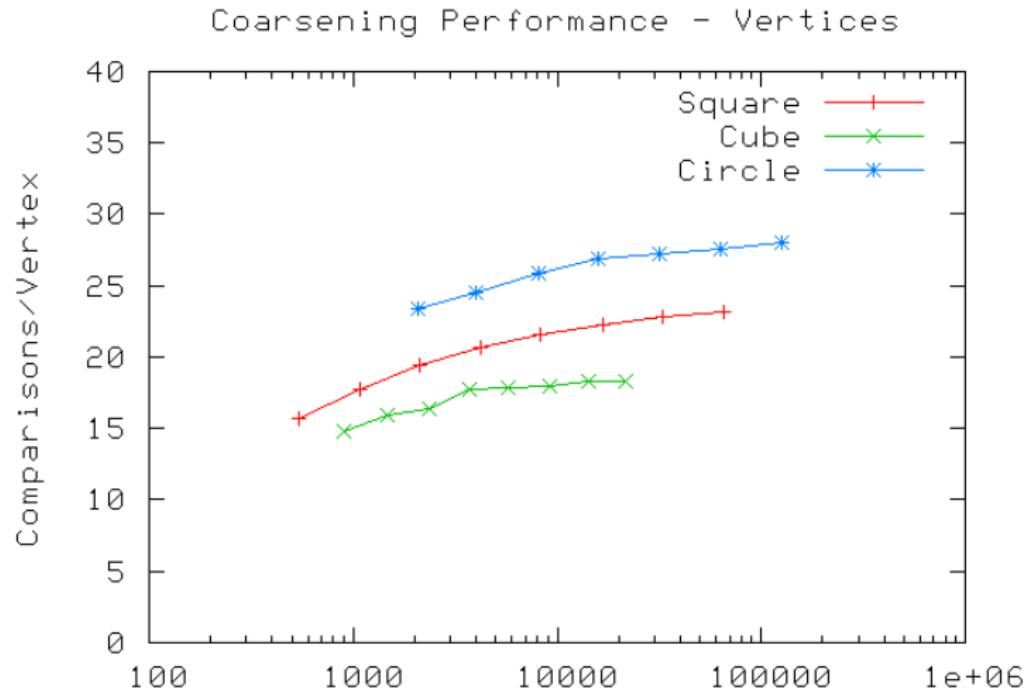
Linear solver iterates are constant as system size increases:



GMG Performance

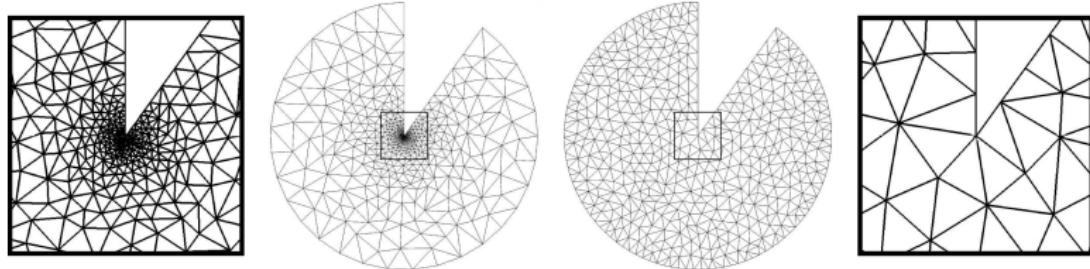
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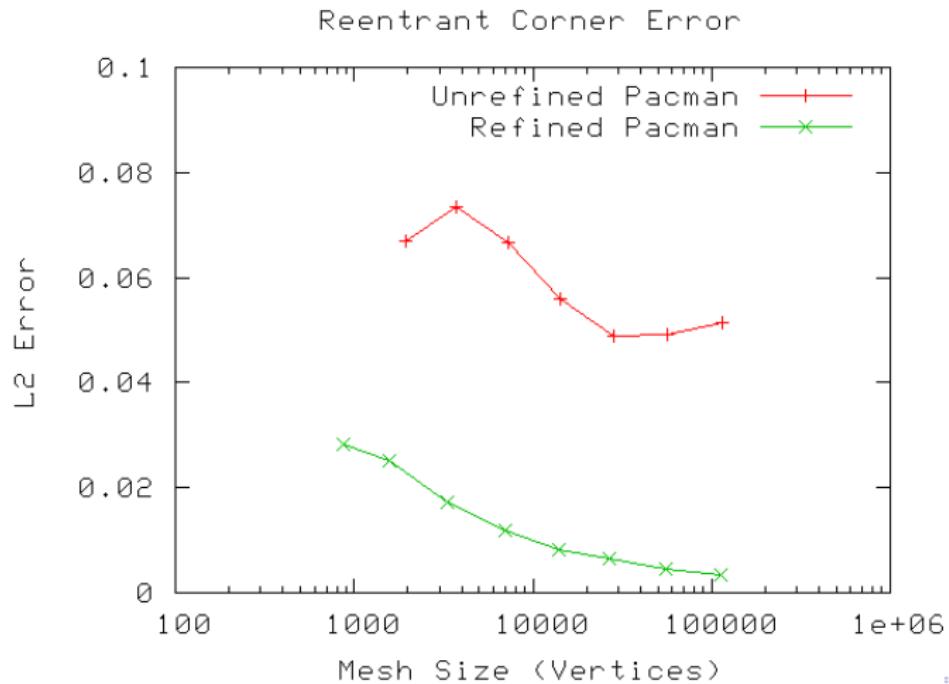
Reentrant Problems

- Reentrant corners need nonuniform refinement to maintain accuracy
- Coarsening preserves accuracy in MG without user intervention



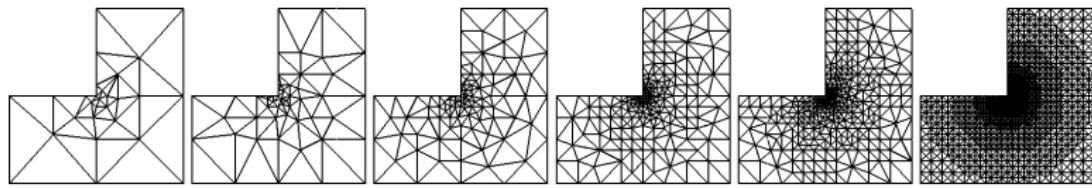
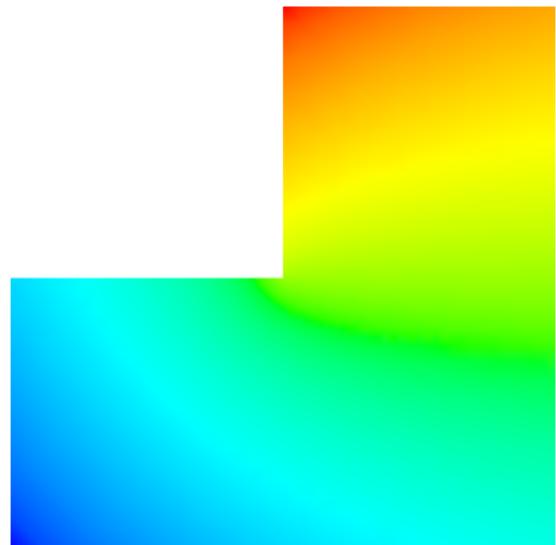
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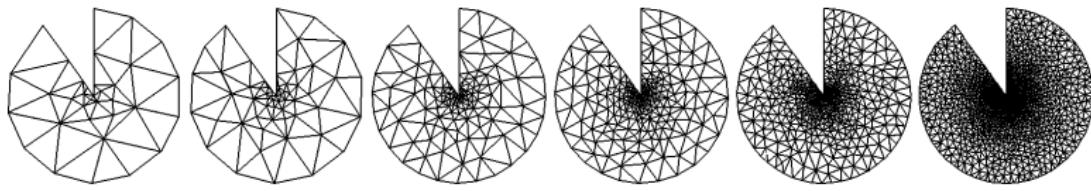
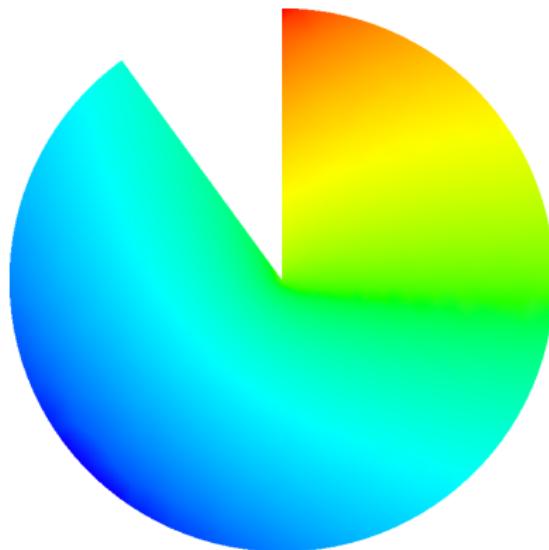
Reentrant Problems

Exact Solution for reentrant problem: $u(x, y) = r^{\frac{2}{3}} \sin(\frac{2}{3}\theta)$



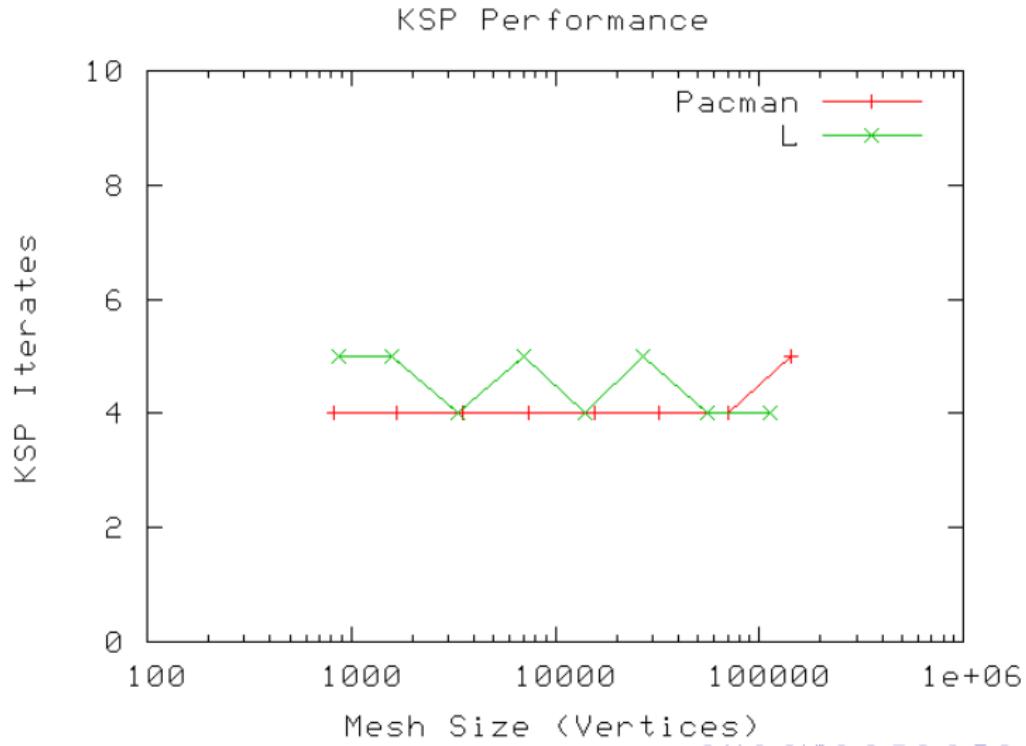
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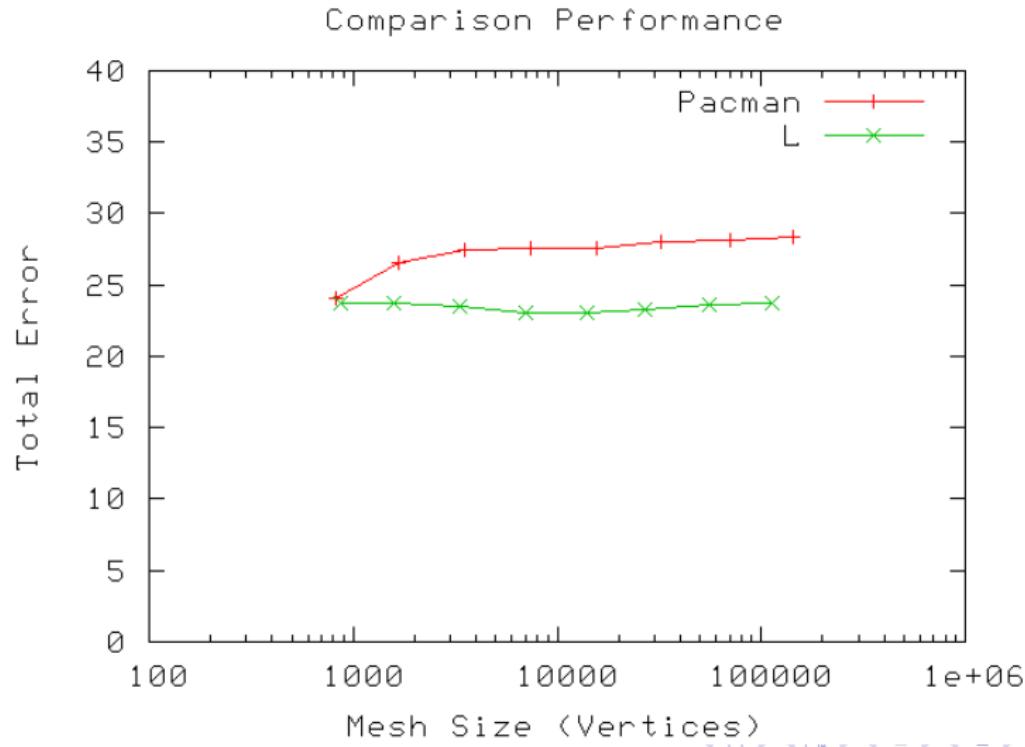
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Conclusions

Better mathematical abstractions bring concrete benefits

- Vast reduction in complexity
 - Operate directly at the equation and discretization level
 - Automatic generation of integration/assembly routines
 - Dimension independent code
- Expansion of capabilities
 - Parametric models
 - Optimized implementations of integration
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References

- **FEniCS Documentation:**

http://www.fenics.org/wiki/FEniCS_Project

- Project documentation
- Users manuals
- Repositories, bug tracking
- Image gallery

- **Publications:**

http://www.fenics.org/wiki/Related_presentations_and_publications

- Research and publications that make use of FEniCS

- **PETSc Documentation:**

<http://www.mcs.anl.gov/petsc/docs>

- PETSc Users manual
- Manual pages
- Many hyperlinked examples
- FAQ, Troubleshooting info, installation info, etc.
- Publication using PETSc

Experimentation is Essential!

Proof is not currently enough to examine solvers

- N. M. Nachtigal, S. C. Reddy, and L. N. Trefethen, *How fast are nonsymmetric matrix iterations?*, SIAM J. Matrix Anal. Appl., **13**, pp.778–795, 1992.
- Anne Greenbaum, Vlastimil Ptak, and Zdenek Strakos, *Any Nonincreasing Convergence Curve is Possible for GMRES*, SIAM J. Matrix Anal. Appl., **17** (3), pp.465–469, 1996.