The Process of Computational Science

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My approach to Computational Science is

Holistic

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Computational Science

starting with the numerics of PDEs,

and mathematics of the computation,

through the distillation into

high quality numerical libraries,

to scientific discovery through computing.

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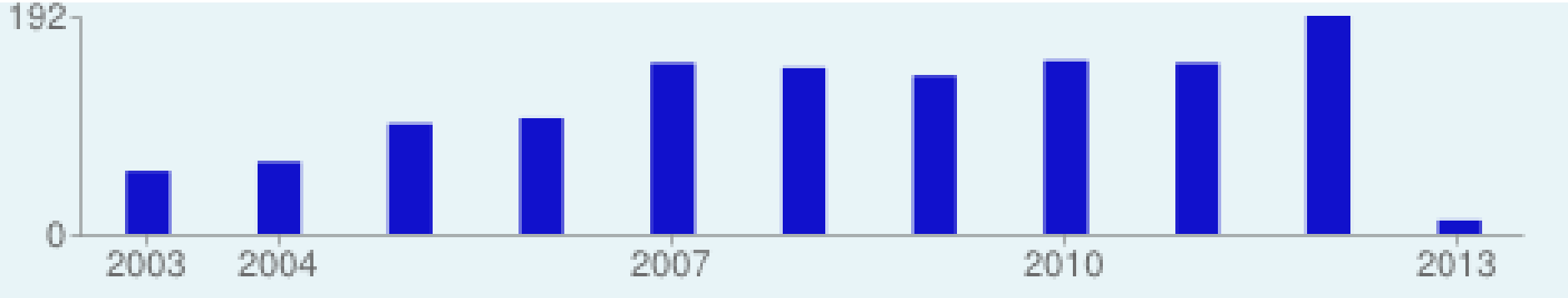
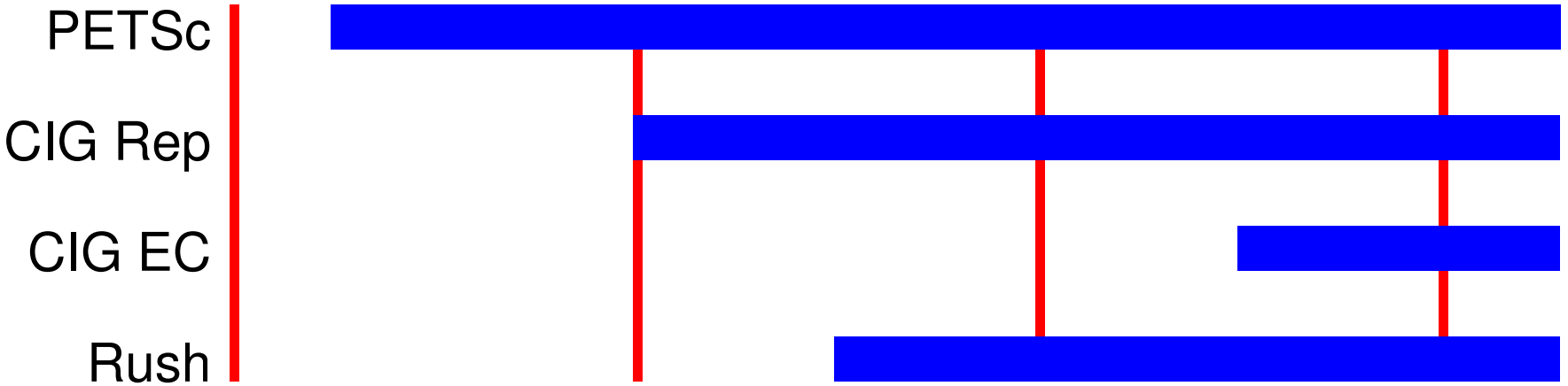
Community Involvement

PETSc Citations





Outline

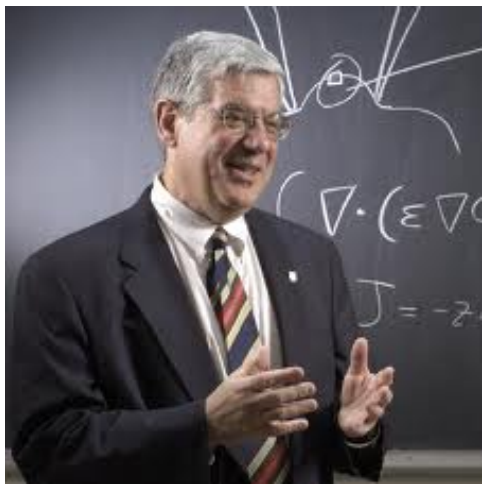
Collaborators

BIBEE Researchers

Jaydeep Bardhan

Classical DFT Researchers

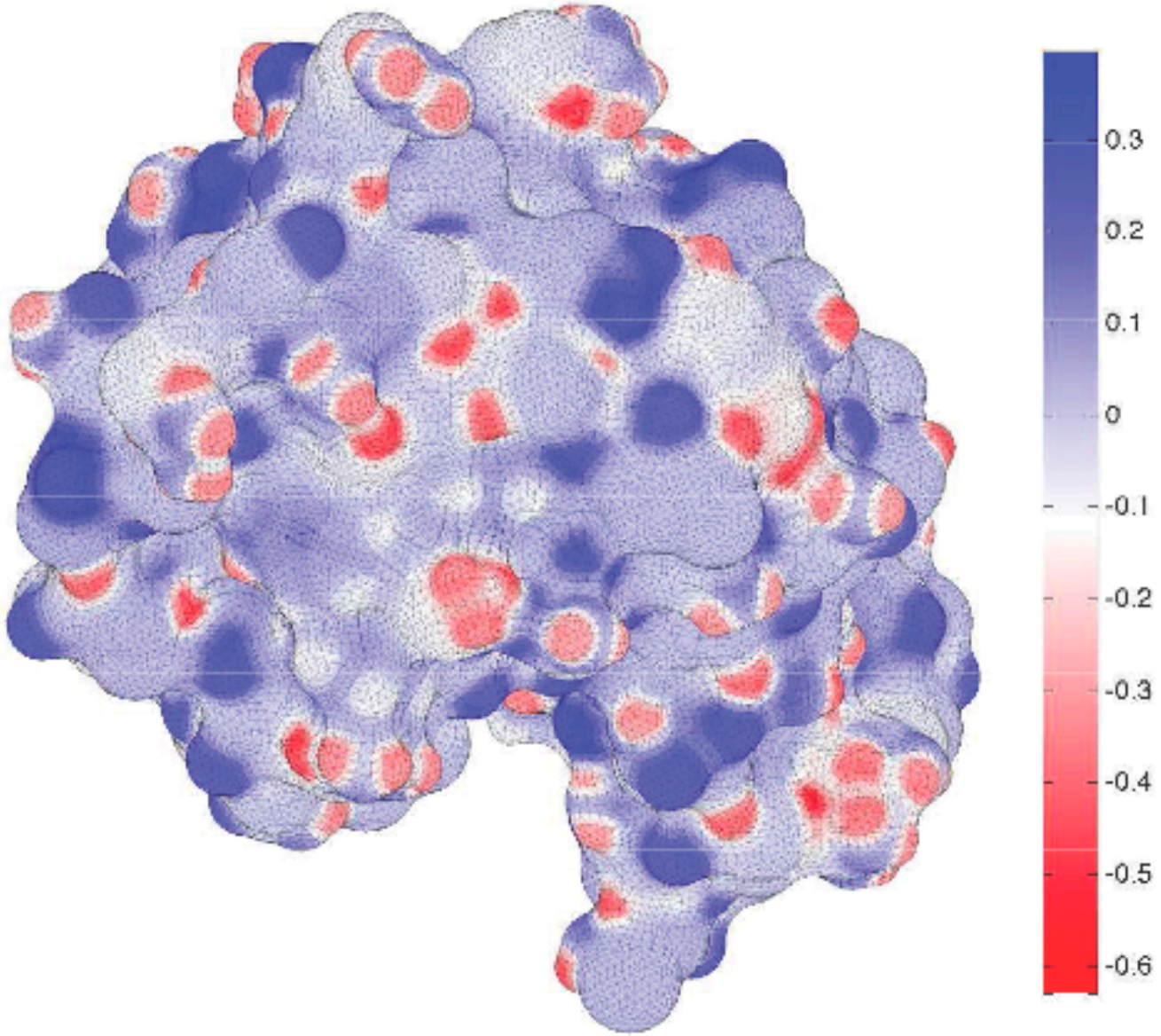
Dirk Gillespie



Bob Eisenberg

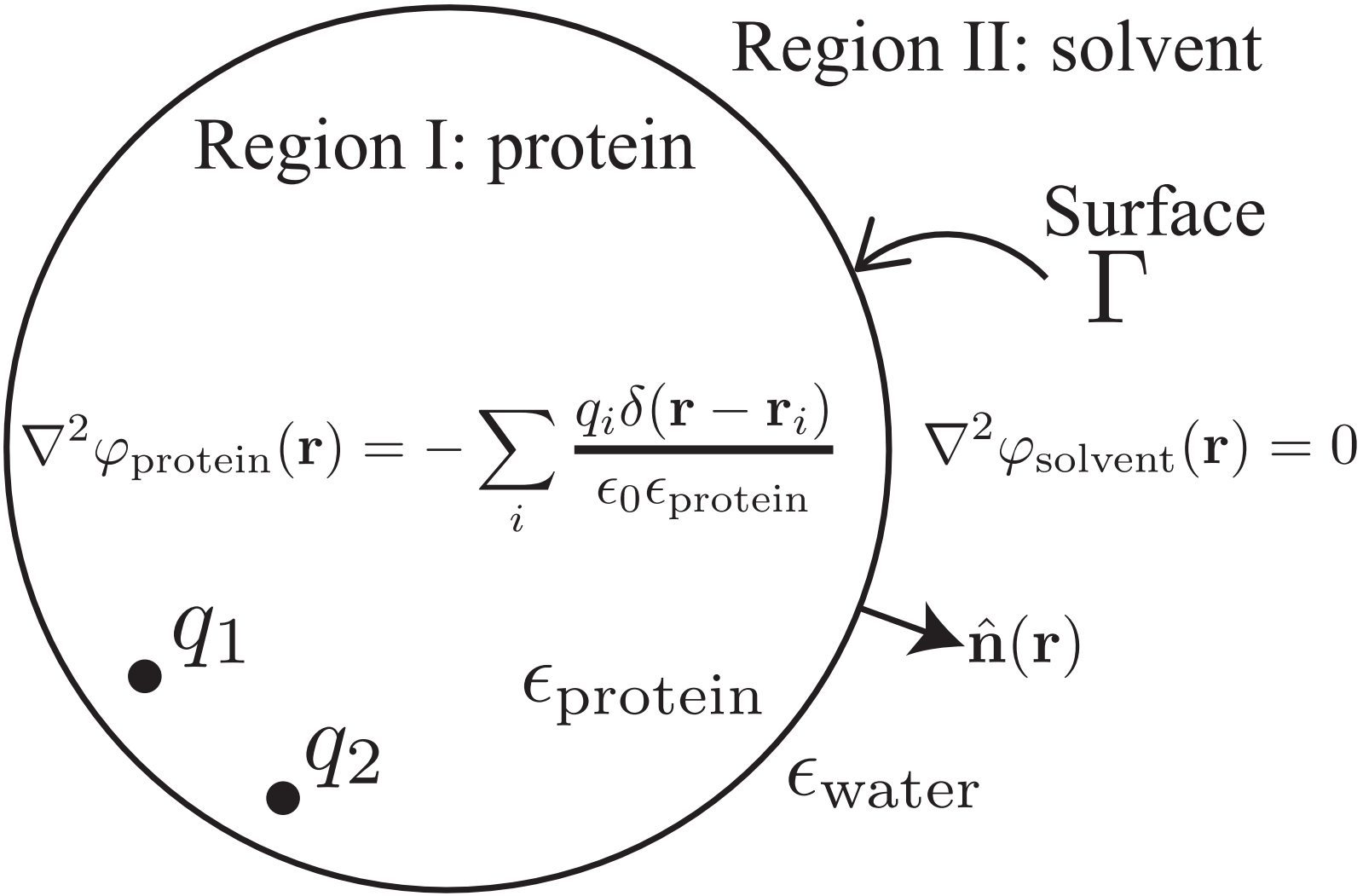
Bioelectrostatics

The Natural World



Bioelectrostatics

Physical Model



Bioelectrostatics

Mathematical Model

$$\sigma(\vec{r}) + \hat{\epsilon} \int_\Gamma \frac{\partial}{\partial n(\vec{r})} \frac{\sigma(\vec{r}')d^2\vec{r}'}{4\pi||\vec{r} - \vec{r}'||} = -\hat{\epsilon} \sum_{k=1}^{Q} \frac{\partial}{\partial n(\vec{r})} \frac{q_k}{4\pi||\vec{r} - \vec{r}_k||} \quad (1)$$

$$\left(\mathcal{I} + \hat{\epsilon}\mathcal{D}^*\right)\sigma(\vec{r}) = \quad (2)$$

where we define

$$\hat{\epsilon} = \frac{1}{2}\frac{\epsilon_1 - \epsilon_2}{\epsilon_1 + \epsilon_2} < 0$$

Bioelectrostatics

Mathematical Model

The *reaction* potential is given by

$$\phi^R(\vec{r}) = \int_\Gamma \frac{\sigma(\vec{r}')d^2\vec{r}'}{4\pi\epsilon_1||\vec{r}-\vec{r}'||}$$

which defines the electrostatic part of the solvation free energy

$$\begin{aligned}\Delta G_{es} &= \frac{1}{2}q^T\phi^R \\ &= \frac{1}{2}q^T Lq \\ &= \frac{1}{2}q^T CA^{-1}Bq\end{aligned}$$

Problem

Boundary element discretizations of the solvation problem (Eq. 1):

- can be expensive to solve, and hard to precondition
- are more accurate than required by intermediate design iterations

BIBEE

Approximate $\mathcal{D}^*$ by a diagonal operator

Boundary Integral-Based Electrostatics Estimation

Coulomb Field Approximation: uniform normal field

$$\left(1 - \frac{\hat{\epsilon}}{2}\right)\sigma_{CFA} = Bq \tag{3}$$

Preconditioning: consider only local effects

$$\sigma_P = Bq \tag{4}$$

Lower Bound: no good physical motivation

$$\left(1 + \frac{\hat{\epsilon}}{2}\right)\sigma_{LB} = Bq \tag{5}$$

Energy Bounds: First Step

Replace C with B

We will need the single layer operator $\mathcal{S}$

$$\mathcal{S}\tau(\vec{r}) = \int \frac{\tau(\vec{r}')d^2\vec{r}'}{4\pi||\vec{r} - \vec{r}'||}$$

Energy Bounds: First Step

Replace C with B

The potential at the boundary Γ given by

$$\phi^{Coulomb}(\vec{r}) = C^T q$$

can also be obtained by solving an exterior Neumann problem for τ,

$$\begin{aligned}
\phi^{Coulomb}(\vec{r}) &= \mathcal{S}\tau \\
&= \mathcal{S}(\mathcal{I} - 2\mathcal{D}^*)^{-1}(\frac{2}{\hat{\epsilon}}Bq) \\
&= \frac{2}{\hat{\epsilon}}\mathcal{S}(\mathcal{I} - 2\mathcal{D}^*)^{-1}Bq
\end{aligned}$$

so that the solvation energy is given by

$$\frac{1}{2}q^T CA^{-1}Bq = \frac{1}{\hat{\epsilon}}q^T B^T(\mathcal{I} - 2\mathcal{D}^*)^{-T}\mathcal{S}(\mathcal{I} + \hat{\epsilon}\mathcal{D}^*)^{-1}Bq$$

Energy Bounds: Second Step

Quasi-Hermiticity

It is well known that (Hsaio and Wendland)

$$\mathcal{S}\mathcal{D}^* = \mathcal{D}\mathcal{S}$$

and

$$\mathcal{S} = \mathcal{S}^{1/2}\mathcal{S}^{1/2}$$

which means that we can define a Hermitian operator H similar to $\mathcal{D}^*$

$$H = \mathcal{S}^{1/2}\mathcal{D}^*\mathcal{S}^{-1/2}$$

leading to an energy

$$\frac{1}{2}q^T CA^{-1}Bq = \frac{1}{\hat{\epsilon}}q^T B^T \mathcal{S}^{1/2}(\mathcal{I} - 2H)^{-1}(\mathcal{I} + \hat{\epsilon}H)^{-1}\mathcal{S}^{1/2}Bq$$

Energy Bounds: Third Step

Eigendecomposition

The spectrum of $\mathcal{D}^*$ is in $[-\frac{1}{2}, \frac{1}{2})$, and the energy is

$$\frac{1}{2} q^T C A^{-1} B q = \sum_i \frac{1}{\hat{\epsilon}} (1 - 2\lambda_i)^{-1} (1 + \hat{\epsilon}\lambda_i)^{-1} x_i^2$$

where

$$H = V \Lambda V^T$$

and

$$\vec{x} = V^T \mathcal{S}^{1/2} B q$$

Energy Bounds: Diagonal Approximations

The BIBEE approximations yield the following bounds

$$\frac{1}{2}q^T C A_{CFA}^{-1} B q = \sum_i \frac{1}{\hat{\epsilon}} (1 - 2\lambda_i)^{-1} \left(1 - \frac{\hat{\epsilon}}{2}\right)^{-1} x_i^2 \quad (6)$$

$$\frac{1}{2}q^T C A_{P}^{-1} B q = \sum_i \frac{1}{\hat{\epsilon}} (1 - 2\lambda_i)^{-1} x_i^2 \quad (7)$$

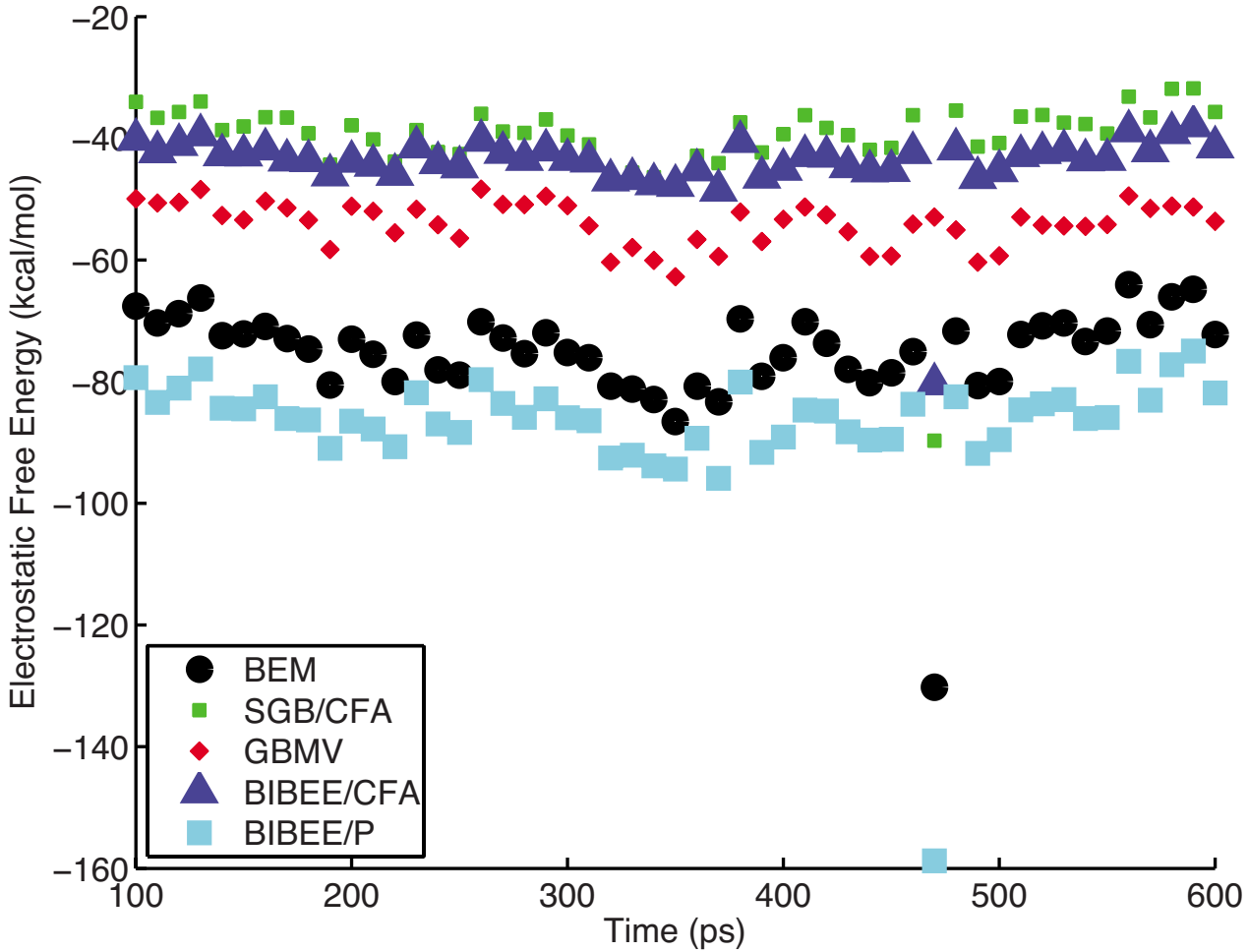
$$\frac{1}{2}q^T C A_{LB}^{-1} B q = \sum_i \frac{1}{\hat{\epsilon}} (1 - 2\lambda_i)^{-1} \left(1 + \frac{\hat{\epsilon}}{2}\right)^{-1} x_i^2 \quad (8)$$

where we note that

$$|\hat{\epsilon}| < \frac{1}{2}$$

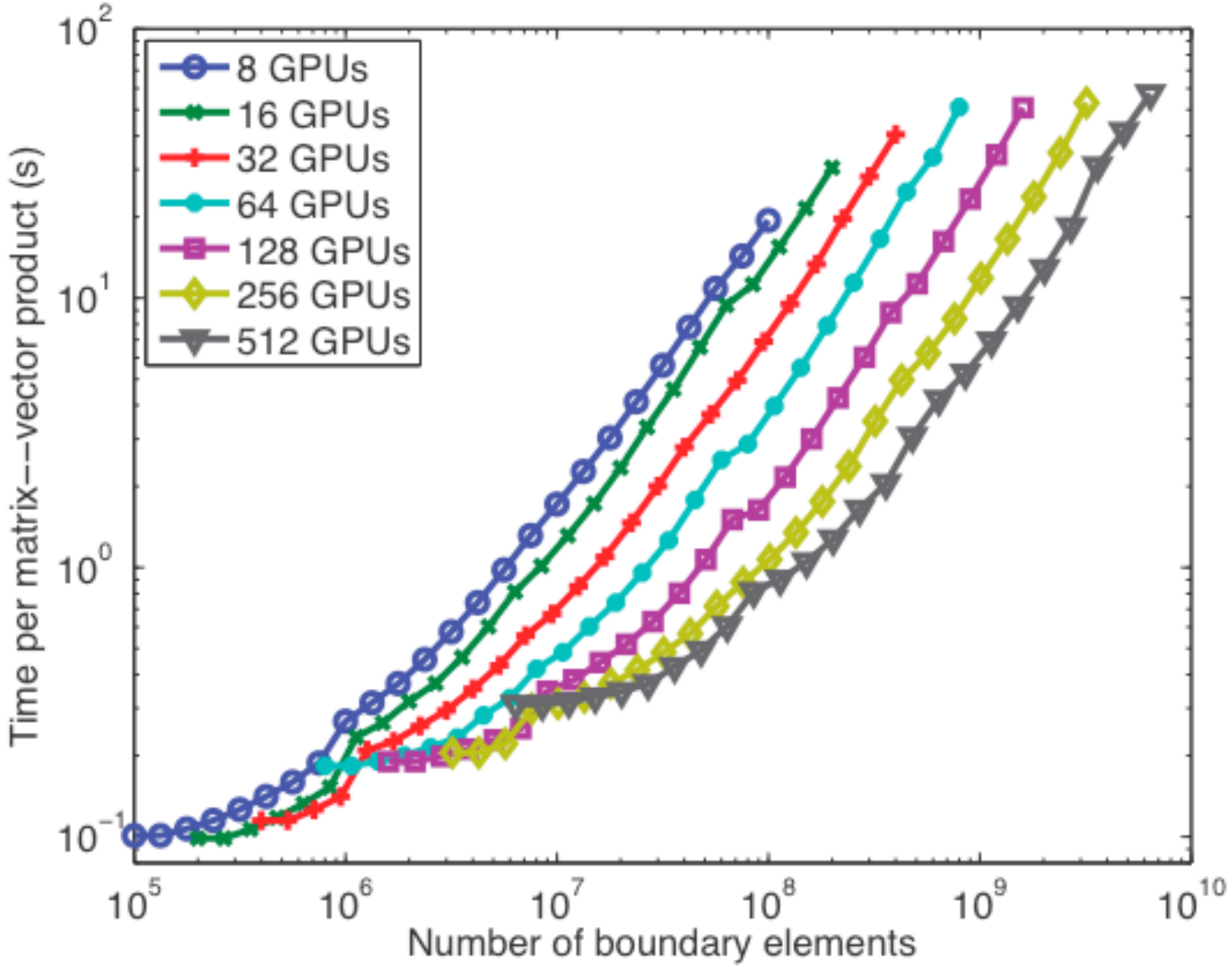
Energy Bounds: Diagonal Approximations

Electrostatic solvation free energies of met-enkephalin structures



Snapshots taken from a 500-ps MD simulation at 10-ps intervals.

BIBEE Scalabiltiy



Resolution

Boundary element discretizations of the solvation problem:

- can be expensive to solve, and hard to precondition
  - **Bounding the electrostatic free energies associated with linear continuum models of molecular solvation**, JCP, 2009
  - BIBEE-FMM (uses kifmm3d)
- are more accurate than required by intermediate design iterations
  - Accuracy is not tunable

Evolution of BIBEE

- Sharp bounds for solvation energy
- Exploration of behavior in simplified geometries
  - **Mathematical Analysis of the BIBEE Approximation for Molecular Solvation: Exact Results for Spherical Inclusions**, JCP, 2011
  - Represent BIBEE as a deformed boundary condition
  - Fully developed series solution
  - Improve accuracy by combining CFA and P approximations
- Application to protein-ligand binding
  - **Analysis of fast boundary-integral approximations for modeling electrostatic contributions of molecular binding**, Molecular-Based Mathematical Biology, 2013

Future of BIBEE

- Framework for systematic exploration
  - Both analytical and computational foundation
- Reduced-basis Method with analytic solutions
  - Tested in protein binding paper above
  - The spatial high frequency part is handled by BIBEE/P topology is not important
  - The spatial low frequency part is handled by analytic solutions insensitive to bumpiness
  - **Computational science and re-discovery: open-source implementations of ellipsoidal harmonics for problems in potential theory**, CSD, 2012.
- Extend to other kernels, e.g. Yukawa
- Extend to full multilevel method

Outline

Collaborators

PETSc Developers

Barry Smith

Jed Brown

Former UC Students

Andy Terrel

Peter Brune

Problem

Traditional PDE codes cannot:

- Compare different discretizations
  - Different orders, finite elements
  - finite volume vs. finite element
- Compare different mesh types
  - Simplicial, hexahedral, polyhedral, octree
- Run 1D, 2D, and 3D problems
- Enable an optimal solver
  - Fields, auxiliary operators

Problem

Traditional Mesh/Solver Interface is Too General:

- Solver not told about discretization data, e.g. fields
- Cannot take advantage of problem structure
  - blocking
  - saddle point structure
- Cannot use auxiliary data
  - Eigen-estimates
  - null spaces

Problem

Traditional Mesh/Solver Interface is Too Specific:

- Assembly code specialized to each discretization
  - dimension
  - cell shape
  - approximation space
- Explicit references to element type
  - getVertices(faceID), getAdjacency(edgeID, VERTEX), getAdjacency(edgeID, dim = 0)
- No interface for transitive closure
  - Awkward nested loops to handle different dimensions

Mesh Representation

We represent each mesh as a Hasse Diagram:

- Can represent any CW complex
- Can be implemented as a Directed Acyclic Graph
- Reduces mesh information to a single *covering* relation
- Can discover dimension, since meshes are ranked posets

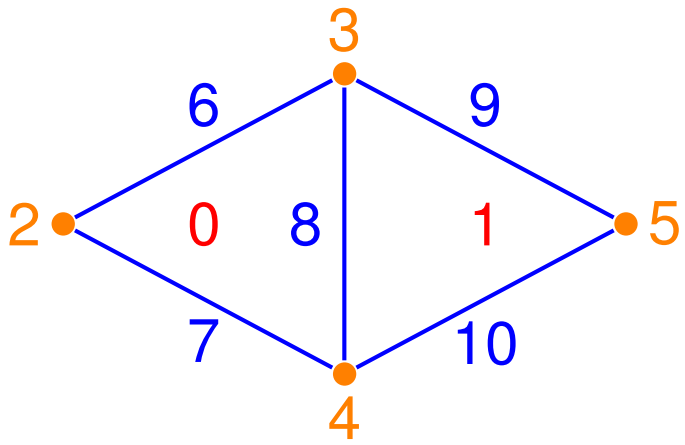
We use an abstract topological interface to organize traversals for:

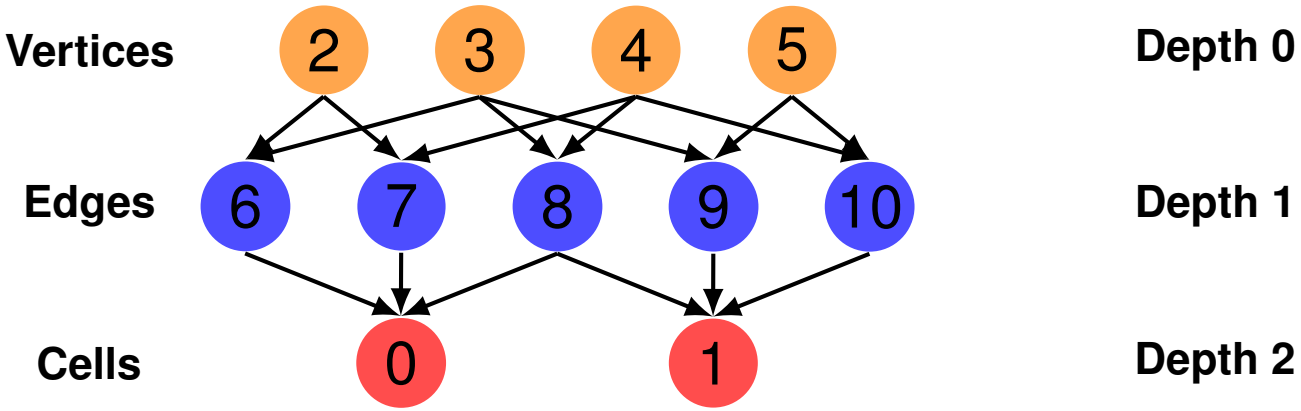
- discretization integrals
- solver size determination
- computing communication patterns

Mesh geometry is treated as just another mesh function.

Sample Meshes

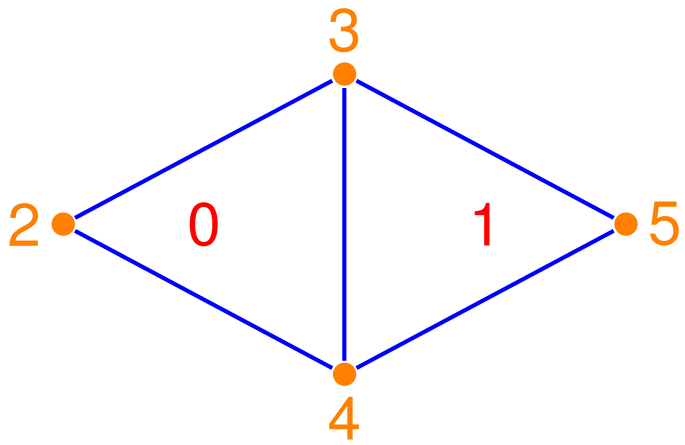
Interpolated triangular mesh

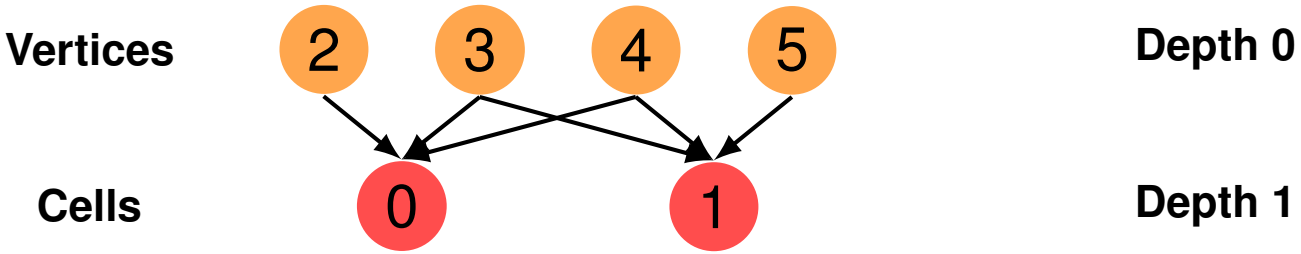




Sample Meshes

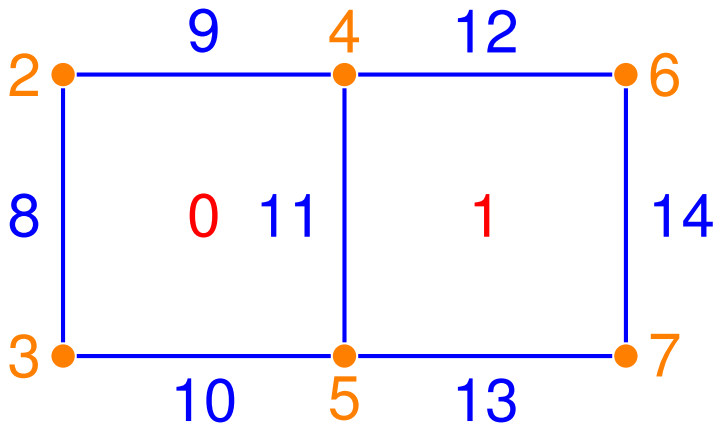
Optimized triangular mesh

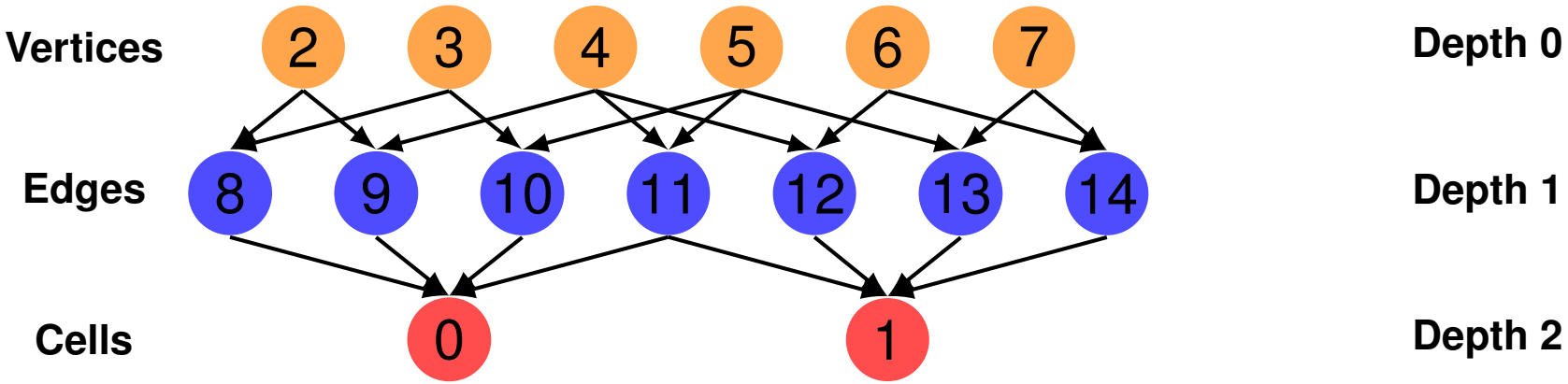




Sample Meshes

Interpolated quadrilateral mesh





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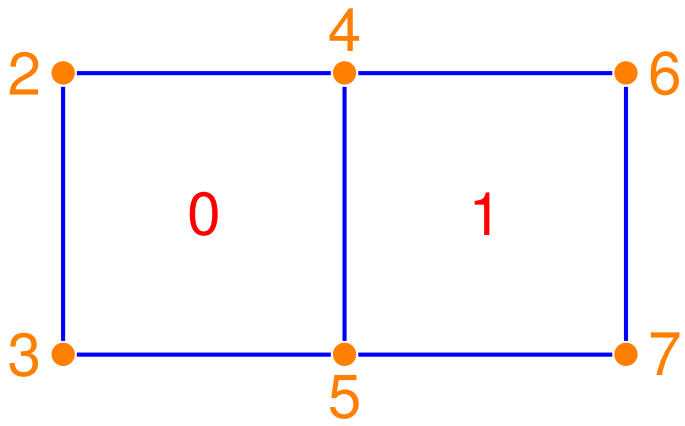
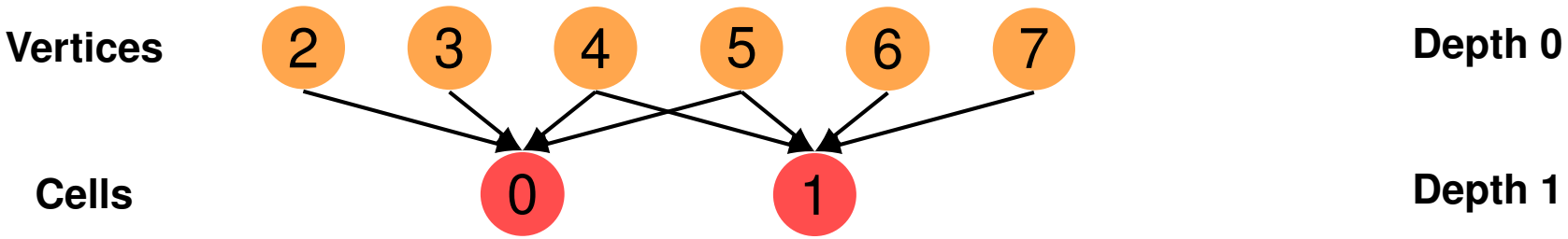
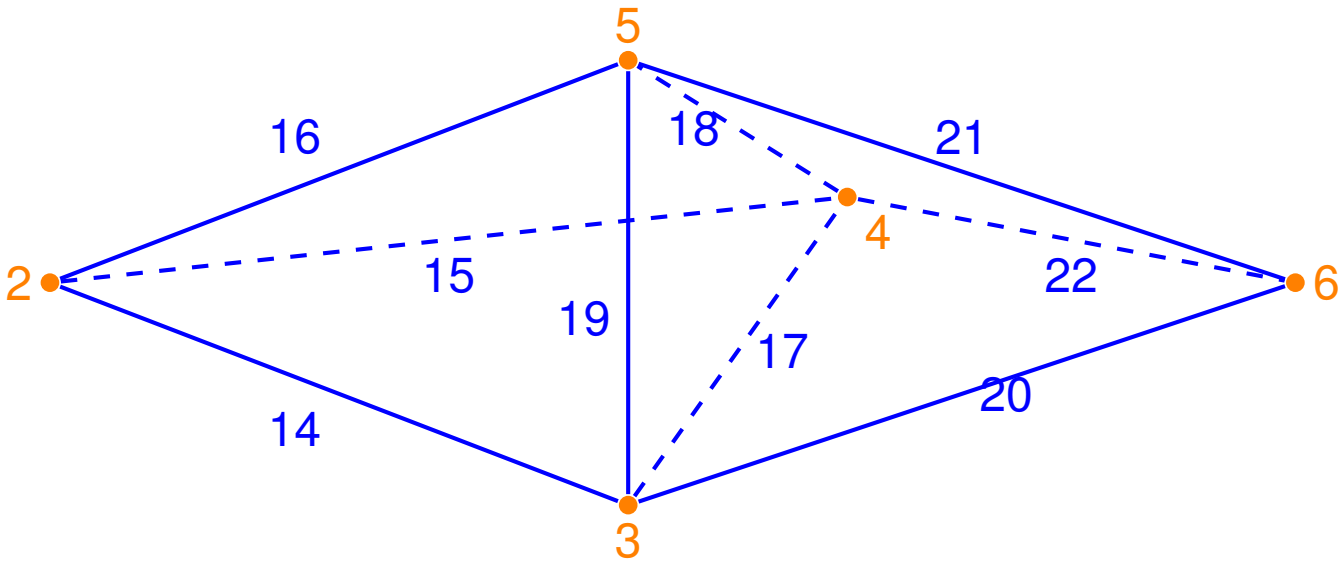
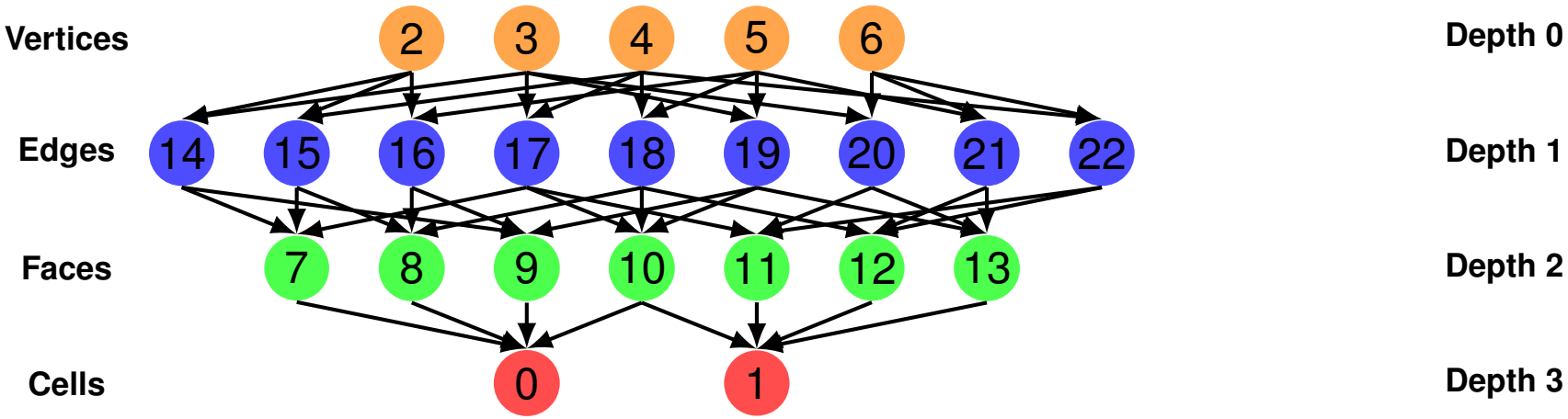




Sample Meshes

Interpolated tetrahedral mesh





Mesh Abstraction

Interface Design

By abstracting on the key topological relations, the interface can be both concise and quite general

- Single relation
- Enables dimension-independent programming
- Dual is obtained by reversing arrows
- Can associate function(al)s with DAG points
- Dual operation gives the support of the function

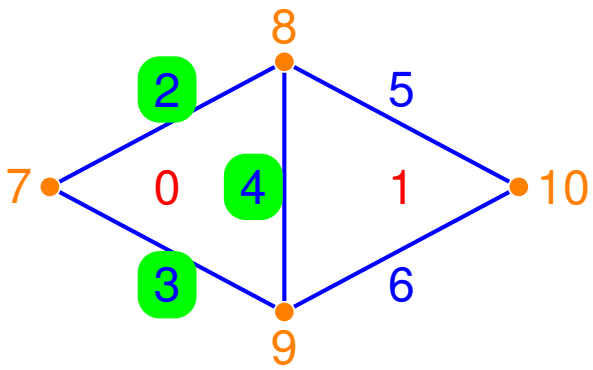
Mesh Algorithms for PDE with Sieve I: Mesh Distribution, Knepley, Karpeev, Sci. Prog., 2009.

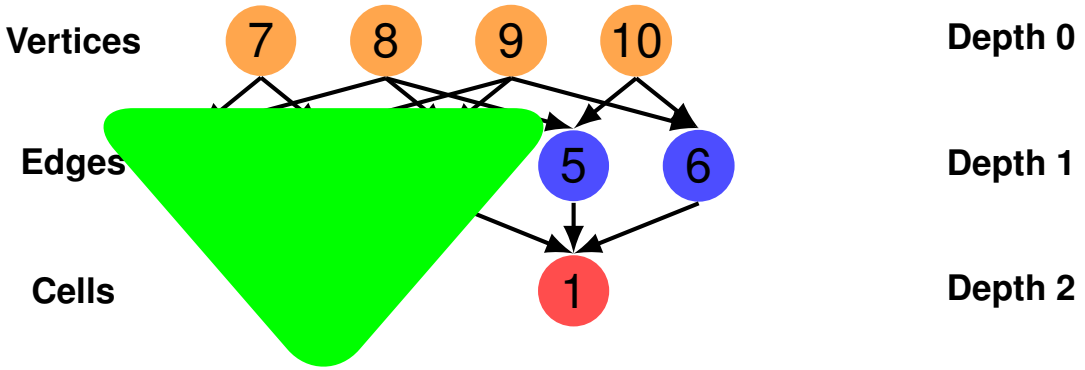
Basic Operations

Cone

We begin with the basic covering relation,

cone(0) = {2, 3, 4}



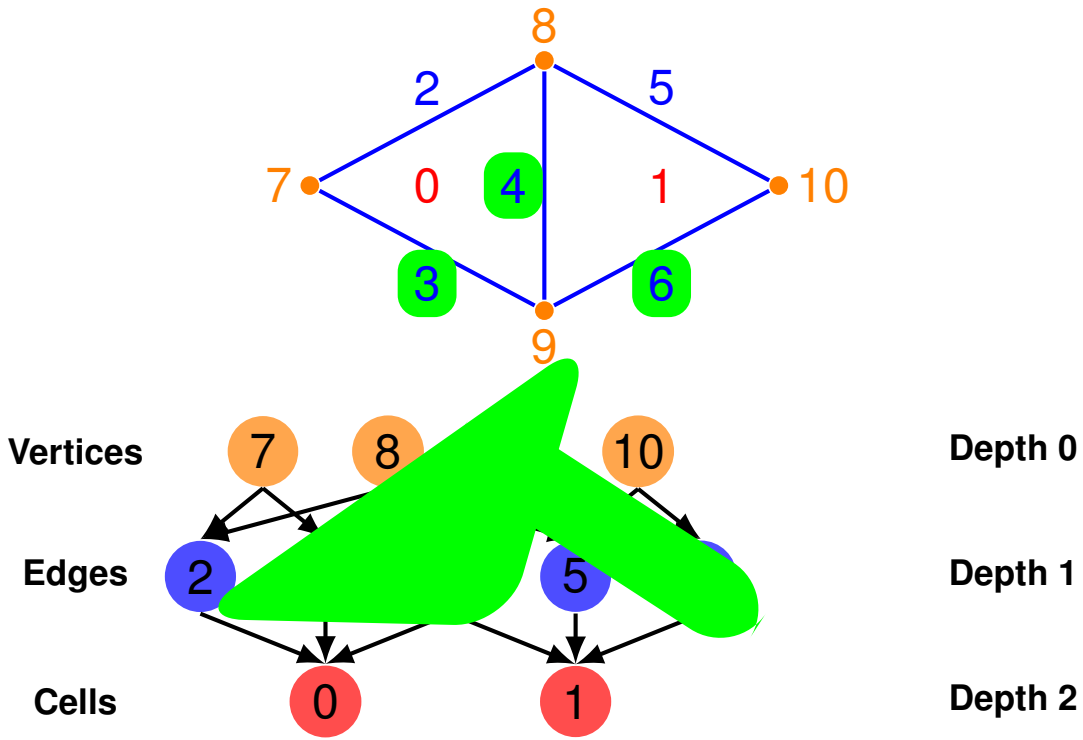


Basic Operations

Support

reverse arrows to get the dual operation,

support(9) = {3, 4, 6}

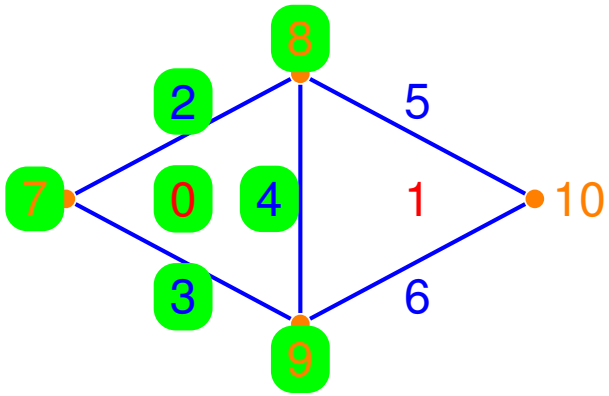


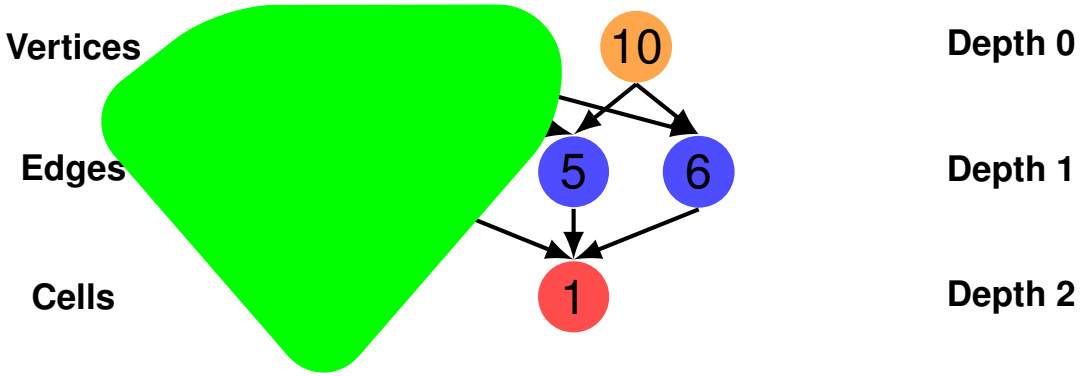
Basic Operations

Closure

add the transitive closure of the relation,

closure(0) = {0, 2, 3, 4, 7, 8, 9}



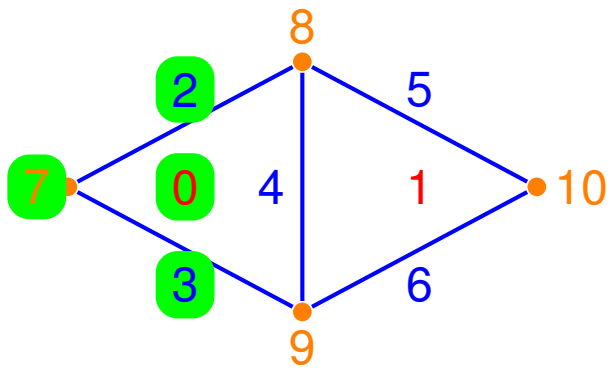


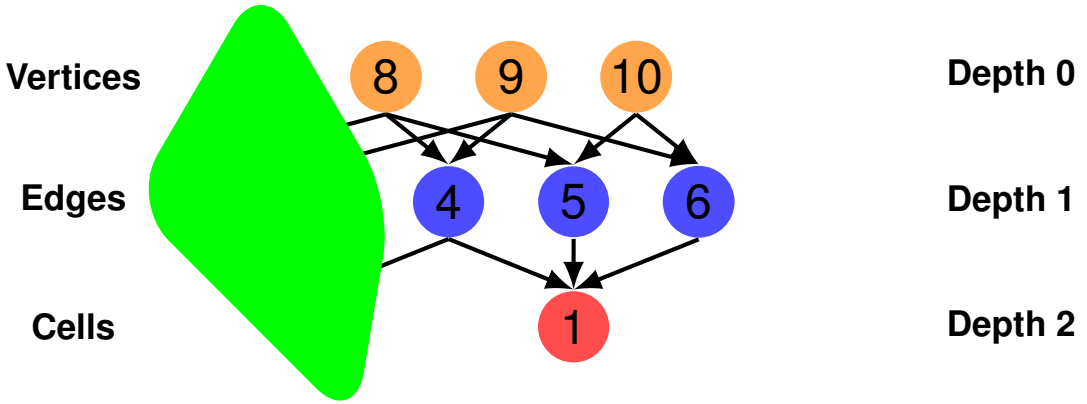
Basic Operations

Star

and the transitive closure of the dual,

star(7) = {7, 2, 3, 0}



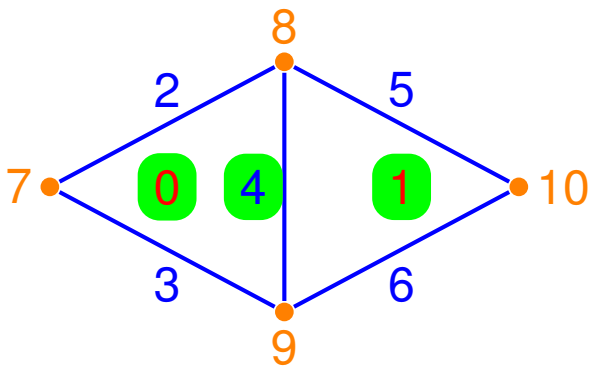


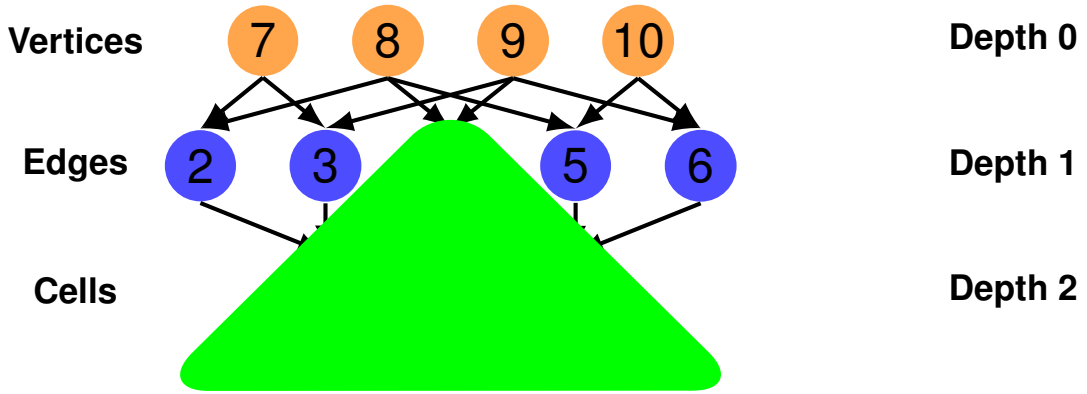
Basic Operations

Meet

and augment with lattice operations.

meet(0, 1) = {4}



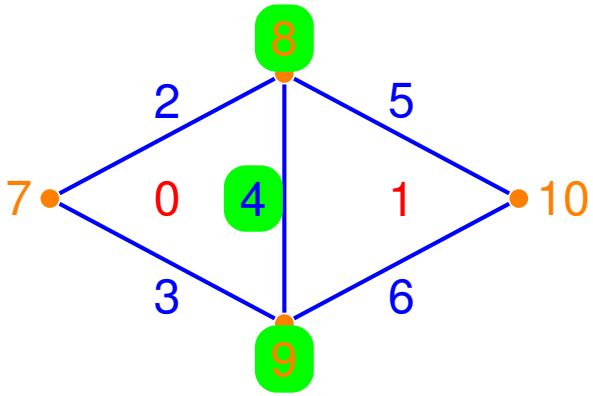


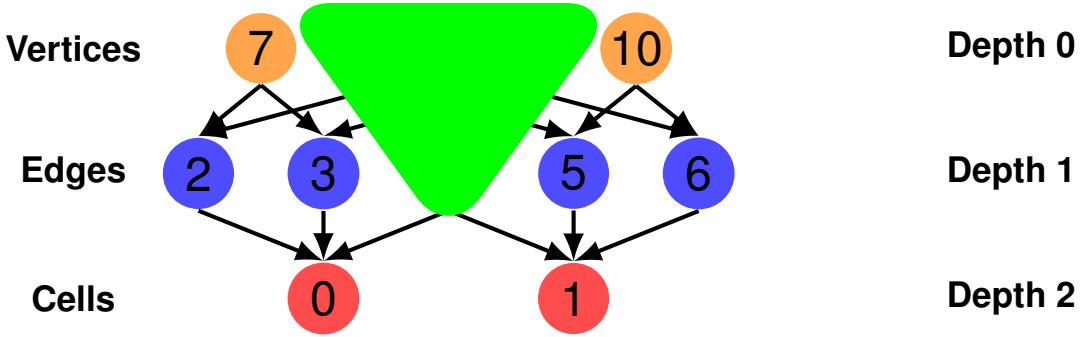
Basic Operations

Join

and augment with lattice operations.

join(8, 9) = {4}





Residual Evaluation

I developed a single residual evaluation routine independent of spatial dimension, cell geometry, and finite element:

$$F(\mathbf{u}) = 0$$

Dim	Cell Types	Discretizations
1	Simplex	Lagrange FEM
2	Tensor Product	H(div) FEM*
3	Polyhedral	H(curl) FEM*
6†	Prism	DG FEM *‡

† Peter Brune, ANL

* FEniCS Project

‡ Blaise Bourdin, LSU

We have also implemented a polyhedral FVM.

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FEM Integration Model

Proposed by Jed Brown

We consider weak forms dependent only on fields and gradients,

$$\int_\Omega \phi \cdot f_0(u, \nabla u) + \nabla\phi : \vec{f}_1(u, \nabla u) = 0. \tag{9}$$

Discretizing we have

$$\sum_e \mathcal{E}_e^T \left[B^T W^q f_0(u^q, \nabla u^q) + \sum_k D_k^T W^q \vec{f}_1^k(u^q, \nabla u^q) \right] = 0 \tag{10}$$

f_n	pointwise physics functions
u^q	field at a quad point
W^q	diagonal matrix of quad weights
B,D	basis function matrices which reduce over quad points
$\mathcal{E}$	assembly operator

Batch Integration

```
DMPlexComputeResidualFEM(dm, X, F, user)
{
  VecSet(F, 0.0);
  <Put boundary conditions into local input vector>
  <Extract coefficients and geometry for batch>
  <Integrate batch of elements>
  <Insert batch of element vectors into local vector>
  <Local to Global addition>
}
```

Batch Integration

Set boundary conditions

```
DMPlexComputeResidualFEM(dm, X, F, user)
{
  VecSet(F, 0.0);
  DMPlexProjectFunctionLocal(dm, numComponents,
    bcFuncs, INSERT_BC_VALUES, X);
  <Extract coefficients and geometry for batch>
  <Integrate batch of elements>
  <Insert batch of element vectors into local vector>
  <Local to Global addition>
}
```

Batch Integration

Extract coefficients and geometry

```
DMPlexComputeResidualFEM(dm, X, F, user)
{
  VecSet(F, 0.0);
  <Put boundary conditions into local input vector>
  DMPlexGetHeightStratum(dm, 0, &cStart, &cEnd);
  for (c = cStart; c < cEnd; ++c) {
    DMPlexComputeCellGeometry(dm, c, &v0[c*dim],
      &J[c*dim*dim], &invJ[c*dim*dim], &detJ[c]);
    DMPlexVecGetClosure(dm, NULL, X, c, NULL, &x);
    for (i = 0; i < cellDof; ++i) u[c*cellDof+i] = x[i];
    DMPlexVecRestoreClosure(dm, NULL, X, c, NULL, &x);
  }
  <Integrate batch of elements>
  <Insert batch of element vectors into local vector>
  <Local to Global addition>
}
```

Batch Integration

Integrate element batch

```
DMPlexComputeResidualFEM(dm, X, F, user)
{
  VecSet(F, 0.0);
  <Put boundary conditions into local input vector>
  <Extract coefficients and geometry for batch>
  for (field = 0; field < numFields; ++field) {
    (*mesh->integrateResidualFEM)(Ne, numFields, field,
      quad, u,
      v0, J, invJ, detJ,
      f0, f1, elemVec);
    (*mesh->integrateResidualFEM)(Nr, ...);
  }
  <Insert batch of element vectors into local vector>
  <Local to Global addition>
}
```

Batch Integration

Insert element vectors

```
DMPlexComputeResidualFEM(dm, X, F, user)
{
  VecSet(F, 0.0);
  <Put boundary conditions into local input vector>
  <Extract coefficients and geometry for batch>
  <Integrate batch of elements>
   for (c = cStart; c < cEnd; ++c) {
    DMPlexVecSetClosure(dm, NULL, F, c,
      &elemVec[c*cellDof], ADD_VALUES);
  }
  <Local to Global addition>
}
```

Batch Integration

```
DMPlexComputeResidualFEM(dm, X, F, user)
{
  VecSet(F, 0.0);
  <Put boundary conditions into local input vector>
  <Extract coefficients and geometry for batch>
  <Integrate batch of elements>
  <Insert batch of element vectors into local vector>
  <Local to Global addition>
  /* Also applies constraint matrix $I^u_c$ */
  DMLocalToGlobalBegin(dm, F, ADD_VALUES, gF);
  DMLocalToGlobalEnd(dm, F, ADD_VALUES, gF);
}
```

Element Integration

```
FEMIntegrateResidualBatch(Ne, numFields, field,
  quad[], coefficients[],
  v0s[], jacobians[], jacobianInv[], jacobianDet[],
  f0_func, f1_func)
{
  <Loop over batch of elements (e)>
    <Loop over quadrature points (q)>
      <Make x_q>
      <Make u_q and gradU_q>
      <Call f_0 and f_1>
    <Loop over element vector entries (f, fc)>
      <Add contributions from f_0 and f_1>
}
```

Element Integration

Calculate x_q

```
FEMIntegrateResidualBatch(...)
{
  <Loop over batch of elements (e)>
    <Loop over quadrature points (q)>
      for (d = 0; d < dim; ++d) {
        x[d] = v0[d];
        for (d2 = 0; d2 < dim; ++d2) {
          x[d] += J[d*dim+d2]*(quadPoints[q*dim+d2]+1);
        }
      }
      <Make u_q and gradU_q>
      <Call f_0 and f_1>
    <Loop over element vector entries (f, fc)>
      <Add contributions from f_0 and f_1>
}
```

Element Integration

Calculate u_q and ∇u_q

```
FEMIntegrateResidualBatch(...)
{
  <Loop over batch of elements (e)>
    <Loop over quadrature points (q)>
      <Make x_q>
      for (f = 0; f < numFields; ++f) {
        for (b = 0; b < Nb; ++b) {
          for (comp = 0; comp < Ncomp; ++comp) {
            u[comp] += coefficients[cidx]*basis[q+cidx];
            for (d = 0; d < dim; ++d) {
              <Transform derivative to real space>
              gradU[comp*dim+d] +=
                coefficients[cidx]*realSpaceDer[d];
            }
          }
        }
      }
      <Call f_0 and f_1>
    <Loop over element vector entries (f, fc)>
```

Element Integration

Calculate u_q and ∇u_q

```
FEMIntegrateResidualBatch(...)
{
  <Loop over batch of elements (e)>
    <Loop over quadrature points (q)>
      <Make x_q>
      for (f = 0; f < numFields; ++f) {
        for (b = 0; b < Nb; ++b) {
          for (comp = 0; comp < Ncomp; ++comp) {
            u[comp] += coefficients[cidx]*basis[q+cidx];
            for (d = 0; d < dim; ++d) {
              realSpaceDer[d] = 0.0;
              for (g = 0; g < dim; ++g) {
                realSpaceDer[d] +=
                  invJ[g*dim+d]*basisDer[(q+cidx)*dim+g];
              }
              gradU[comp*dim+d] +=
                coefficients[cidx]*realSpaceDer[d];
            }
          }
```

Element Integration

Call f_0 and f_1

```
FEMIntegrateResidualBatch(...)
{
  <Loop over batch of elements (e)>
    <Loop over quadrature points (q)>
      <Make x_q>
      <Make u_q and gradU_q>
      f0_func(u, gradU, x, &f0[q*Ncomp]);
      for (i = 0; i < Ncomp; ++i) {
        f0[q*Ncomp+i] *= detJ*quadWeights[q];
      }
      f1_func(u, gradU, x, &f1[q*Ncomp*dim]);
      for (i = 0; i < Ncomp*dim; ++i) {
        f1[q*Ncomp*dim+i] *= detJ*quadWeights[q];
      }
    <Loop over element vector entries (f, fc)>
      <Add contributions from f_0 and f_1>
}
```

Element Integration

Update element vector

```
FEMIntegrateResidualBatch(...)
{
  <Loop over batch of elements (e)>
    <Loop over quadrature points (q)>
      <Make x_q>
      <Make u_q and gradU_q>
      <Call f_0 and f_1>
    <Loop over element vector entries (f, fc)>
      for (q = 0; q < Nq; ++q) {
        elemVec[cidx] += basis[q+cidx]*f0[q+comp];
        for (d = 0; d < dim; ++d) {
          <Transform derivative to real space>
          elemVec[cidx] +=
            realSpaceDer[d]*f1[(q+comp)*dim+d];
        }
      }
}
```

GPU Integration

Porting to the GPU meant chang
only the element integration func

- Has the same flexibility as CPU versic
- Multiple threads execute each cell inte
- Achieves 100 GF/s for 2D P_1 Laplacian
- Code is available here
- Finite Element Integration on GPUs, TOMS, 2013
- **Finite Element Integration with Quadrature on the GPU**, PLC, 2013

Solver Integration: No New Code

ex62: P_2/P_1 Stokes Problem on Unstructured Mesh

Full Schur Complement

```
-ksp_type fgmres -pc_type fieldsplit -pc_fieldsplit_type schur
-pc_fieldsplit_schur_factorization_type full
  -fieldsplit_velocity_ksp_type gmres -fieldsplit_velocity_pc_type lu
  -fieldsplit_pressure_ksp_rtol 1e-10 -fieldsplit_pressure_pc_type jacobi
```

$$\begin{pmatrix} I & 0 \\ B^T A^{-1} & I \end{pmatrix} \begin{pmatrix} \hat{A} & 0 \\ 0 & \hat{S} \end{pmatrix} \begin{pmatrix} I & A^{-1}B \\ 0 & I \end{pmatrix}$$

Solver Integration: No New Code

ex62: P_2/P_1 Stokes Problem on Unstructured Mesh

SIMPLE

```
-ksp_type fgmres -pc_type fieldsplit -pc_fieldsplit_type schur
-pc_fieldsplit_schur_factorization_type full
  -fieldsplit_velocity_ksp_type gmres -fieldsplit_velocity_pc_type lu
  -fieldsplit_pressure_ksp_rtol 1e-10 -fieldsplit_pressure_pc_type jacobi
  -fieldsplit_pressure_inner_ksp_type preonly
    -fieldsplit_pressure_inner_pc_type jacobi
  -fieldsplit_pressure_upper_ksp_type preonly
    -fieldsplit_pressure_upper_pc_type jacobi
```

$$\begin{pmatrix} I & 0 \\ B^T D_A^{-1} & I \end{pmatrix} \begin{pmatrix} \hat{A} & 0 \\ 0 & \hat{S} \end{pmatrix} \begin{pmatrix} I & D_A^{-1} B \\ 0 & I \end{pmatrix}$$

Solver Integration: No New Code

ex31: P_2/P_1 Stokes Problem with Temperature on Unstructured Mesh

Additive Schwarz + Full Schur Complement

```
-ksp_type fgmres -pc_type fieldsplit -pc_fieldsplit_0_fields 0,1
-pc_fieldsplit_1_fields 2 -pc_fieldsplit_type additive
  -fieldsplit_0_ksp_type fgmres -fieldsplit_0_pc_type fieldsplit
  -fieldsplit_0_pc_fieldsplit_type schur
  -fieldsplit_0_pc_fieldsplit_schur_factorization_type full
    -fieldsplit_0_fieldsplit_velocity_ksp_type preonly
    -fieldsplit_0_fieldsplit_velocity_pc_type lu
    -fieldsplit_0_fieldsplit_pressure_ksp_rtol 1e-10
    -fieldsplit_0_fieldsplit_pressure_pc_type jacobi
  -fieldsplit_temperature_ksp_type preonly
  -fieldsplit_temperature_pc_type lu
```

$$\begin{pmatrix} \begin{pmatrix} I & 0 \\ B^T A^{-1} & I \end{pmatrix} \begin{pmatrix} A & 0 \\ 0 & S \end{pmatrix} \begin{pmatrix} I & A^{-1}B \\ 0 & I \end{pmatrix} & 0 \\ 0 & L_T \end{pmatrix}$$

Solver Integration: No New Code

ex31: P_2/P_1 Stokes Problem with Temperature on Unstructured Mesh

Least-Squares Commutator + Upper Schur Comp. + Full Schur Comp.

```
-ksp_type fgmres -pc_type fieldsplit -pc_fieldsplit_0_fields 0,1
-pc_fieldsplit_1_fields 2 -pc_fieldsplit_type schur
-pc_fieldsplit_schur_factorization_type upper
  -fieldsplit_0_ksp_type fgmres -fieldsplit_0_pc_type fieldsplit
  -fieldsplit_0_pc_fieldsplit_type schur
  -fieldsplit_0_pc_fieldsplit_schur_factorization_type full
    -fieldsplit_0_fieldsplit_velocity_ksp_type preonly
    -fieldsplit_0_fieldsplit_velocity_pc_type lu
    -fieldsplit_0_fieldsplit_pressure_ksp_rtol 1e-10
    -fieldsplit_0_fieldsplit_pressure_pc_type jacobi
  -fieldsplit_temperature_ksp_type gmres
  -fieldsplit_temperature_pc_type lsc
```

$$\begin{pmatrix} \begin{pmatrix} I & 0 \\ B^T A^{-1} & I \end{pmatrix} \begin{pmatrix} \hat{A} & 0 \\ 0 & \hat{S} \end{pmatrix} \begin{pmatrix} I & A^{-1}B \\ 0 & I \end{pmatrix} & G \\ 0 & \hat{S}_{\mathrm{LSC}} \end{pmatrix}$$

Resolution

Traditional PDE codes:

- Cannot compare different discretizations
  - **Automated FEM Discretizations for the Stokes Equation**, BIT, 2008
  - Efficient Assembly of H(div) and H(curl) Conforming Finite Elements, SISC, 2009
- Compare different mesh types
  - **A Domain Decomposition Approach to Implementing Fault Slip in Finite-Element Models of Quasi-static and Dynamic Crustal Deformation**, JGR, 2013
- Run 1D, 2D, and 3D problems
  - **Ibid.**
- Enabling an optimal solver without programming
  - **Ibid.**
  - **Composable linear solvers for multiphysics**, IPDPS, 2012
  - On the rise of strongly tilted mantle plume tails, PEPI, 2011

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Future Work

- Unify FEM and FVM residual evaulation
- Batched integration on accelerators
- Integrate auxiliary fields
- Incorporate cell problems for coefficients

Outline

PyLith

PyLith is an open source, parallel simulator for crustal deformation problems developed by myself, Brad Aagaard, and Charles Williams. PyLith employs a finite element discretization on unstructured meshes and is built on the PETSc libraries from ANL.

Brad Aagaard

Charles Williams

PyLith

- Multiple problems
  - Dynamic rupture
  - Quasi-static relaxation
- Multiple models
  - Fault constitutive models
  - Nonlinear visco-elastic-plastic
  - Finite deformation
- Multiple Meshes
  - 1D, 2D, 3D
  - Hex and tet meshes

PyLith

- Multiple problems
  - Dynamic rupture
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  - Nonlinear vi
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