

Geodynamic Simulator Building

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SIAM Parallel Processing,
Tokyo, Kantō JP March 10, 2018



A Simulator is more Useful
when the Researcher
Builds it Themselves

Outline

- 1 Flexible Meshing
 - PyLith
 - DMNetwork
- 2 Interaction of Discretizations and Solvers

Main Question

How do I handle
many different mesh types
simply and efficiently?

Current Practice

Most packages handle one kind of mesh,
or have completely separate code paths
for different meshes

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This strategy means there is
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PETSc Strategy

The `Plex` abstraction allows us to write code for

- parallel distribution and load balancing,
- traversal for function/operator assembly,
- coarsening and refinement,
- generation of missing edges/faces,
- and surface extraction,

PETSc Strategy

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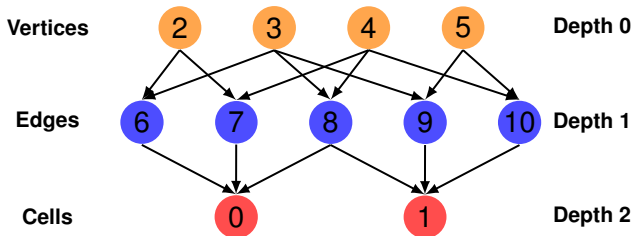
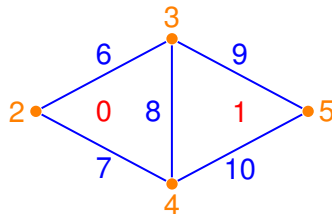
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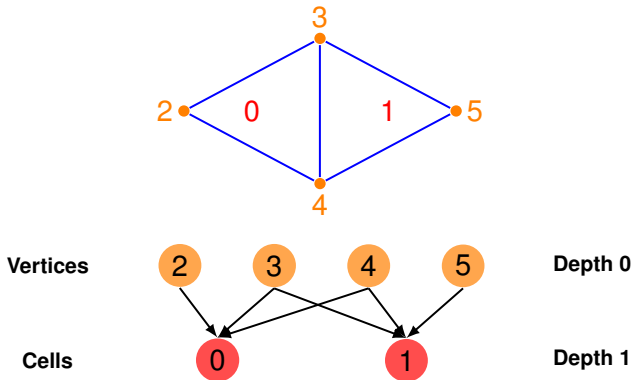
Sample Meshes

Interpolated triangular mesh



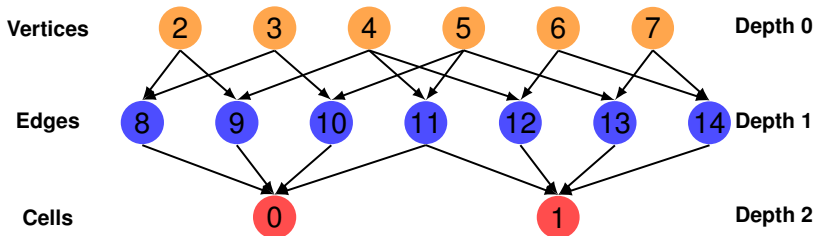
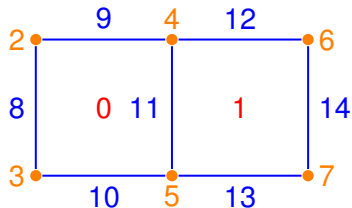
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Optimized triangular mesh



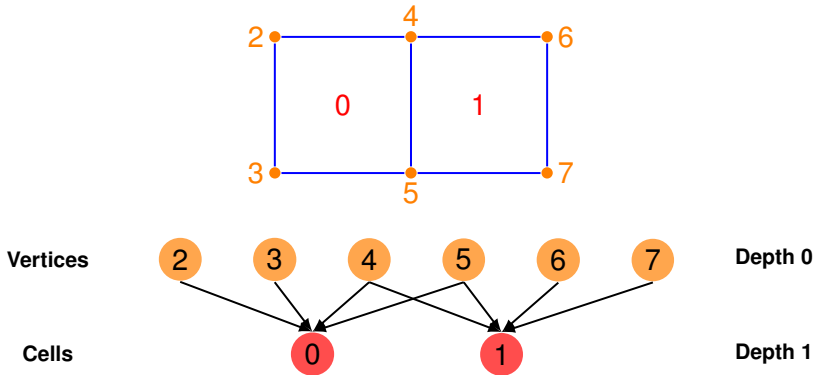
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Interpolated quadrilateral mesh



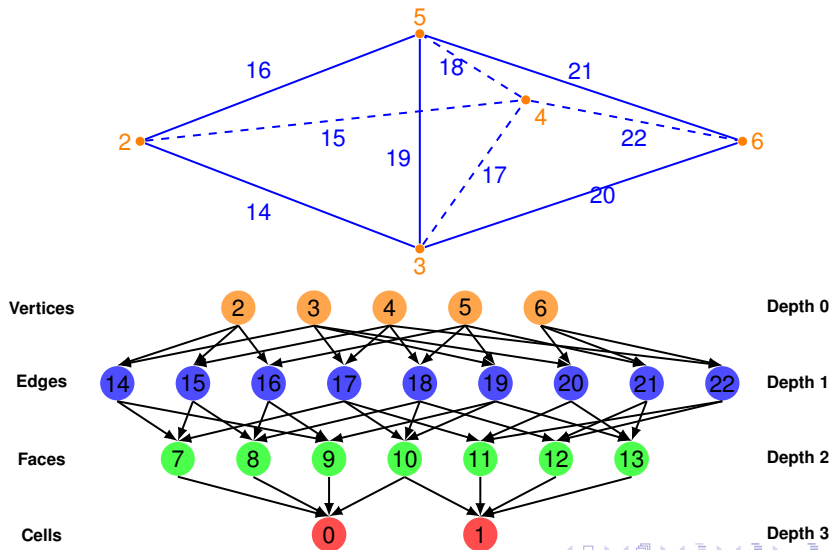
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Optimized quadrilateral mesh



Sample Meshes

Interpolated tetrahedral mesh

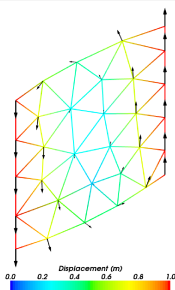


Outline

1 Flexible Meshing

- PyLith
- DMNetwork

Example: PyLith



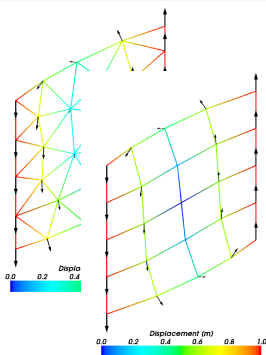
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Surface
extraction

Hybrid
meshes

Aagaard, Knepley, Williams, J. of Geophysical Research, 2013.

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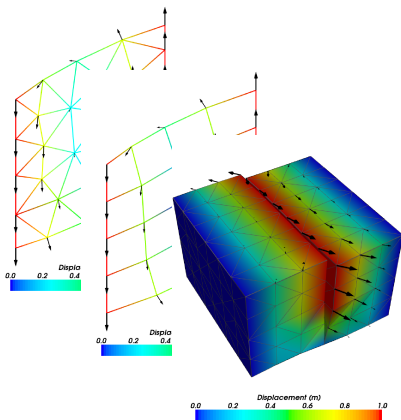
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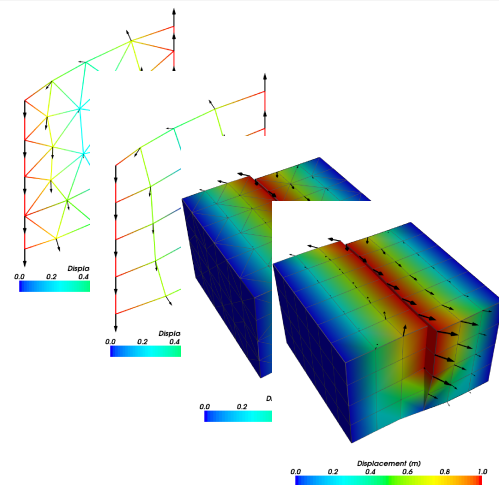
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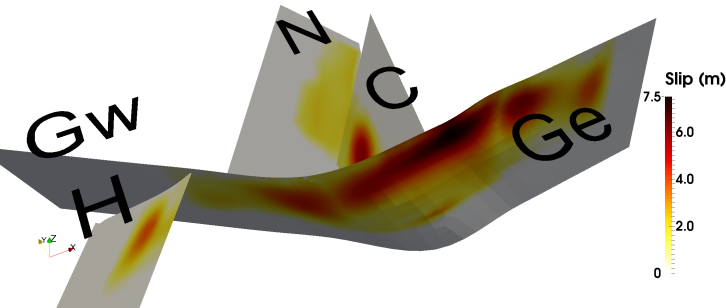
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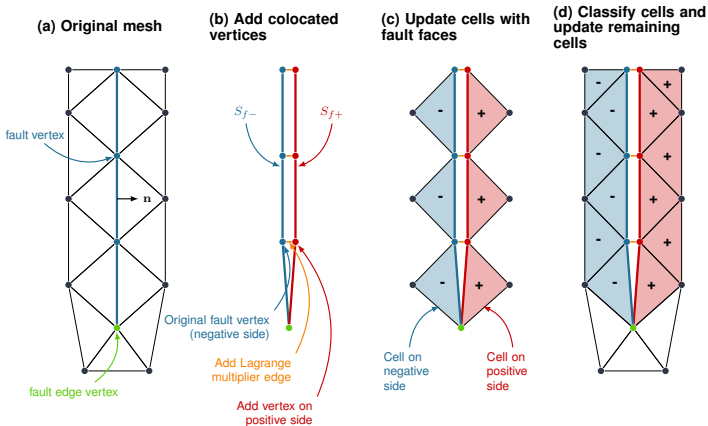
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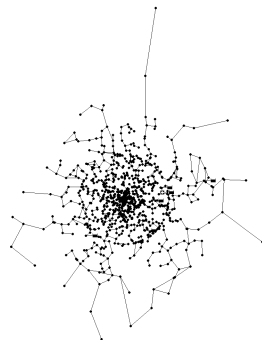
- DMNetwork

Example: DMNetwork

Plex on 30K cores of Edison
for a finite volume
hydraulic flow application.

Table IV. Execution Time of Transient State on Edison

No. of Cores	Variables (in millions)	Maximum Variables per Core (in thousands)	Linear Preconditioner		
			Block Jacobi	ASM ov. 1	ASM ov. 2
240	16	106	9.9 (48)	7.3 (25)	6.4 (20)
960	63	106	10.6 (55)	7.0 (24)	6.2 (20)
3,840	253	106	10.4 (53)	7.3 (24)	6.7 (20)
15,360	1,012	104	11.9 (53)	11.4 (26)	9.9 (20)
30,720	2,023	117	20.0 (53)	17.6 (26)	17.2 (20)



Maldonado, Abhyankar, Smith, Zhang, ACM TOMS, 2017

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- 2 Interaction of Discretizations and Solvers
 - PCTelescope
 - GMG with coefficients
 - Comparison of Discretizations

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How do I handle
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Most packages handle one discretization,
FEniCS/Firedrake is a notable exception,
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PETSc Strategy

The `Section abstraction` allows us to write code for

- parallel data layout,
- block/field decompositions,
- (variable) point-block decompositions,
- removing Dirichlet conditions,
- (nonlinear) hierarchical rediscretization,
- and partial assembly (BDDC/FETI),

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Section

A `Section` is a map

mesh point \implies (size, offset)

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Data Layout

mesh point \implies # dofs

Boundary conditions

mesh point \implies # constrained dofs

Fields

mesh point \implies # field dofs

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Decouples Mesh, Discretization, and Solver

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Decouples `Mesh`, `Discretization`, and Solver

Assembly gets dofs on each point and mesh traversal,
no need for discretization spaces

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A `Section` is a map

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Decouples `Mesh`, Discretization, and `Solver`

Solver gets data layout and ordering,
no need for mesh traversal

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Decouples Mesh, [Discretization](#), and [Solver](#)

Solver gets field and point blocking,
no need for discretization spaces

Section

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mesh point \implies (size, offset)

Decouples Mesh, Discretization, and Solver

Provides interface layer between PETSc and discretization packages Firedrake and LibMesh

Outline

2 Interaction of Discretizations and Solvers

- PCTelescope
- GMG with coefficients
- Comparison of Discretizations

Example: PCTelescope

PCTelescope abstracts the parallel distribution of a linear system, so that

May, Sanan, Rupp, Knepley, Smith, PASC, 2016. [slides](#)

Example: PCTelescope

PCTelescope abstracts the parallel distribution of a linear system, so that

a user can bring their coarse level onto a single process for a direct solve,

```
-pc_type mg
  -pc_mg_levels N
  -mg_coarse_pc_type telescope
    -mg_coarse_pc_telescope_reduction_factor nc
    -mg_coarse_telescope_pc_type lu
```

May, Sanan, Rupp, Knepley, Smith, PASC, 2016. [slides](#)

Example: PCTelescope

PCTelescope abstracts the parallel distribution of a linear system, so that

or recreate the solver from the
Gordon Bell Prize Winner 2015.

```
-pc_type mg
  -pc_mg_levels NR
  -mg_coarse_pc_type telescope
    -mg_coarse_pc_telescope_reduction_factor r
    -mg_coarse_telescope_pc_type mg
    -mg_coarse_telescope_pc_mg_levels NG
    -mg_coarse_telescope_pc_mg_galerkin
      -mg_coarse_telescope_mg_coarse_pc_type gamg
```

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The paper shows scaling up to 32^3 processors on Piz Daint.

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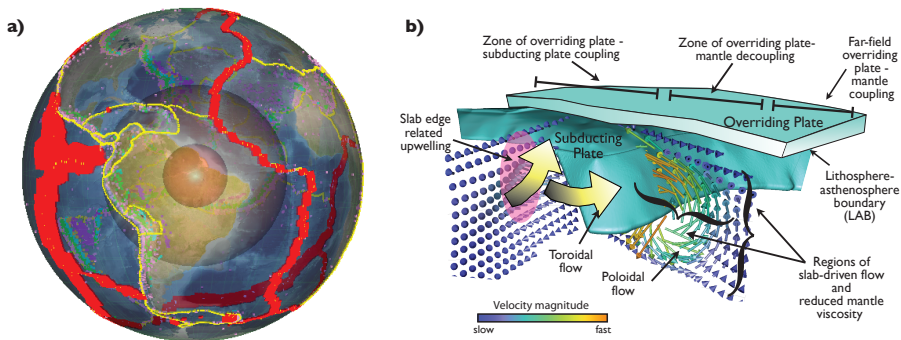
Outline

2 Interaction of Discretizations and Solvers

- PCTelescope
- **GMG with coefficients**
- Comparison of Discretizations

Geometric Multigrid with a Coefficient

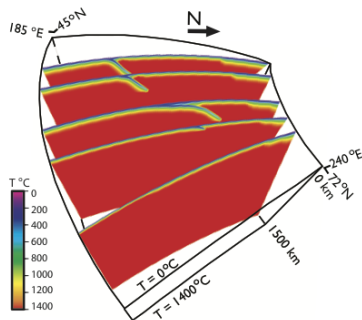
Regional mantle convection
has highly variable viscosity,
due to temperature and strain rate.



Jadamec, Billen, Nature, 2009.

Geometric Multigrid with a Coefficient

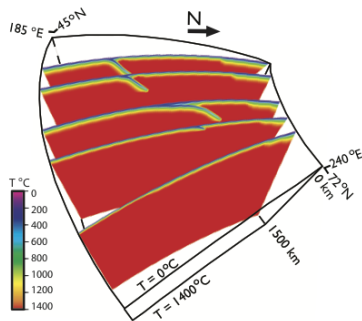
We will specify an initial temperature, on some initial mesh, and let strain develop self-consistently.



Jadamec, Billen, Nature, 2009.

Geometric Multigrid with a Coefficient

This temperature must be distributed,
matching the mesh partition,
and interpolate/restrict to meshes.



Jadamec, Billen, Nature, 2009.

Geometric Multigrid with a Coefficient: Part I

Distribution

Create Section mapping temperature to coarse cells,
using `PetscFECreateDefault()` for a DG function space

Distribute the coarse mesh,
using `DMPlexDistribute()`

Distribute the cell temperatures,
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Transfer cell temperatures to finer cells (purely local)

Transfer cell temperatures to vertices on fine grid (purely local)

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Geometric Multigrid with a Coefficient: Part II

Interpolation

Interpolation is straightforward

```
DMRefine(coarseMesh, comm, &fineMesh);  
DMCreateInterpolation(coarseMesh, fineMesh, &l, &Rscale);  
MatMult(l, coarseTemp, fineTemp);
```

Geometric Multigrid with a Coefficient: Part II

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Geometric Multigrid with a Coefficient: Part II

Interpolation

Now we restrict the input temperature to coarser meshes.

```
DMCreateInterpolation(coarseMesh, fineMesh, &I, &Rscale);  
MatMultTranspose(I, fineTemp, coarseTemp);  
VecPointwiseMult(coarseTemp, coarseTemp, Rscale);
```

Geometric Multigrid with a Coefficient: Part II

Interpolation

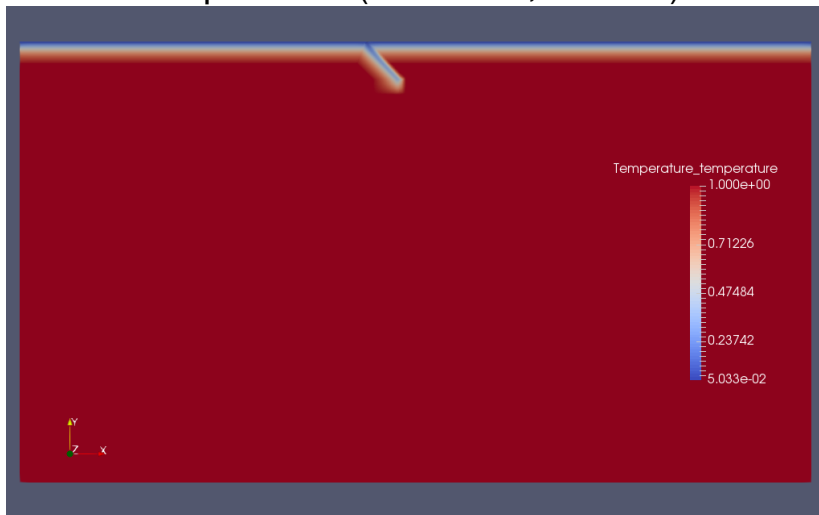
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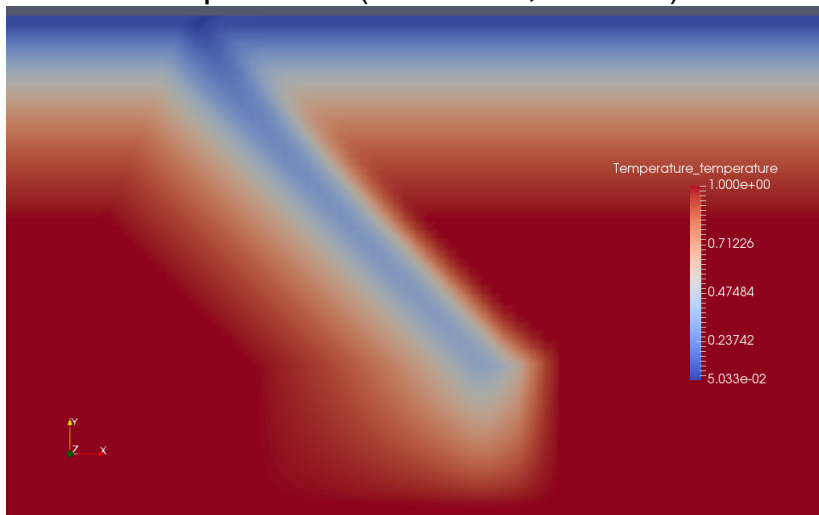
Mantle Temperature (Fine Grid, Level 3)



Geometric Multigrid with a Coefficient: Part II

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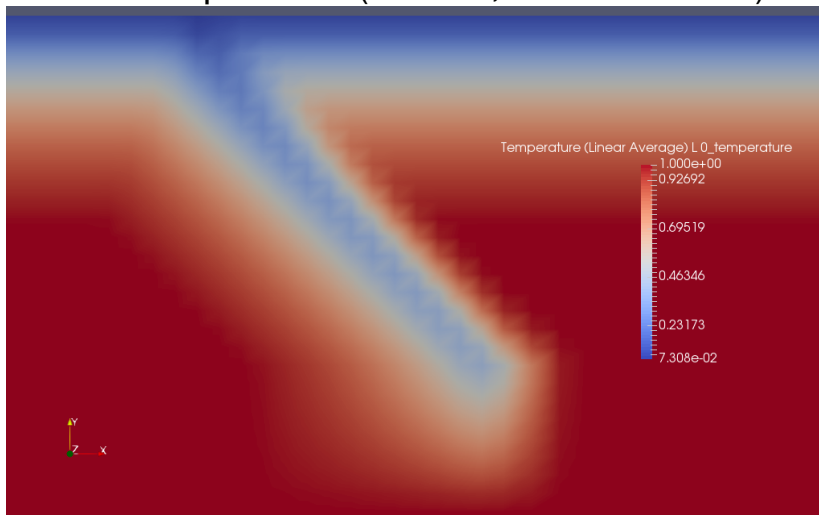
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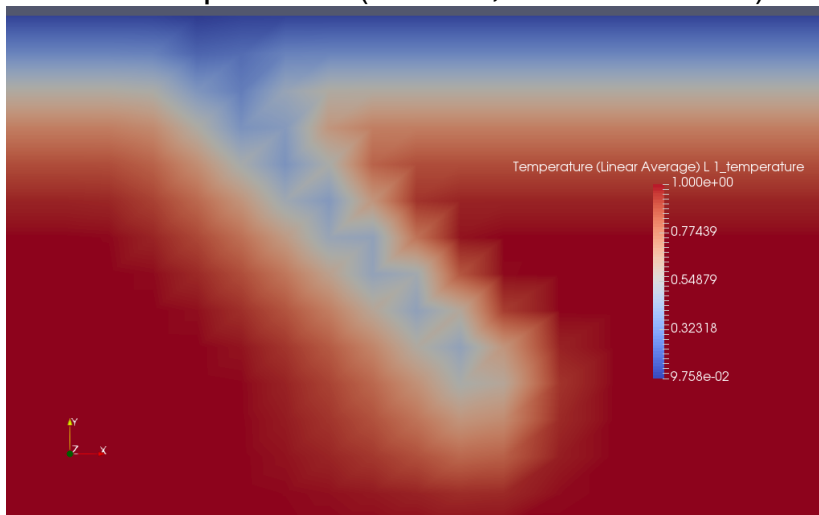
Mantle Temperature (Level 2, Q1 Restriction)



Geometric Multigrid with a Coefficient: Part II

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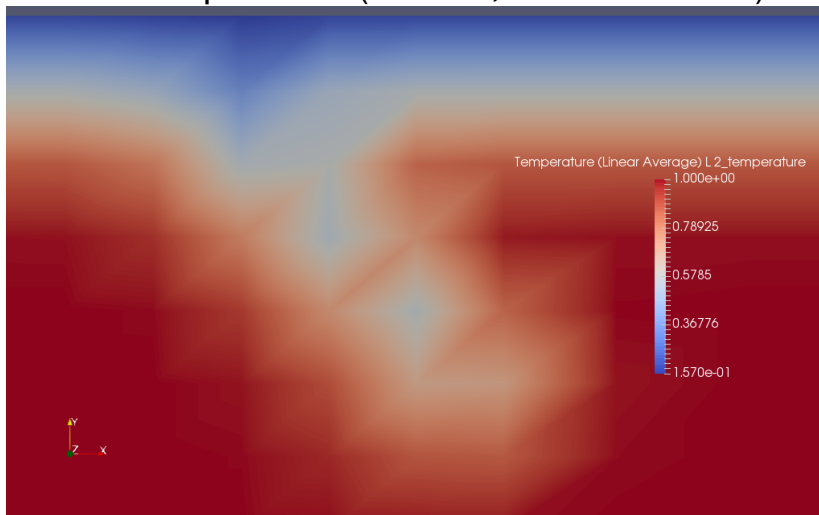
Mantle Temperature (Level 1, Q1 Restriction)



Geometric Multigrid with a Coefficient: Part II

Interpolation

Mantle Temperature (Level 0, Q1 Restriction)



Geometric Multigrid with a Coefficient: Part II

Interpolation

The power mean could better preserve low temperatures

$$\bar{x} = \left(\sum_i x_i^p \right)^{\frac{1}{p}}$$

Geometric Multigrid with a Coefficient: Part II

Interpolation

The power mean could better preserve low temperatures

$$\bar{x} = \left(\sum_i x_i^p \right)^{\frac{1}{p}}$$

```
DMCreateInterpolation(coarseMesh, fineMesh, &l, &Rscale);  
MatShellSetOperation(l, MATOP_MULT_TRANSPOSE,  
    MatMultTransposePowerMean_SeqAIJ);  
MatMultTranspose(l, fineTemp, coarseTemp);  
VecPointwiseMult(coarseTemp, coarseTemp, Rscale);  
VecPow(coarseTemp, p);
```

Geometric Multigrid with a Coefficient: Part II

Interpolation

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$$\bar{x} = \left(\sum_i x_i^p \right)^{\frac{1}{p}}$$

```

for (i = 0; i < m; ++i) {
    idx = a->j + a->i[i];
    v    = a->a + a->i[i];
    n    = a->i[i+1] - a->i[i];
    xi   = x[i];
    for (j = 0; j < n; ++j) {
        y[idx[j]] += v[j]*PetscPowScalarReal(xi, p);
    }
}

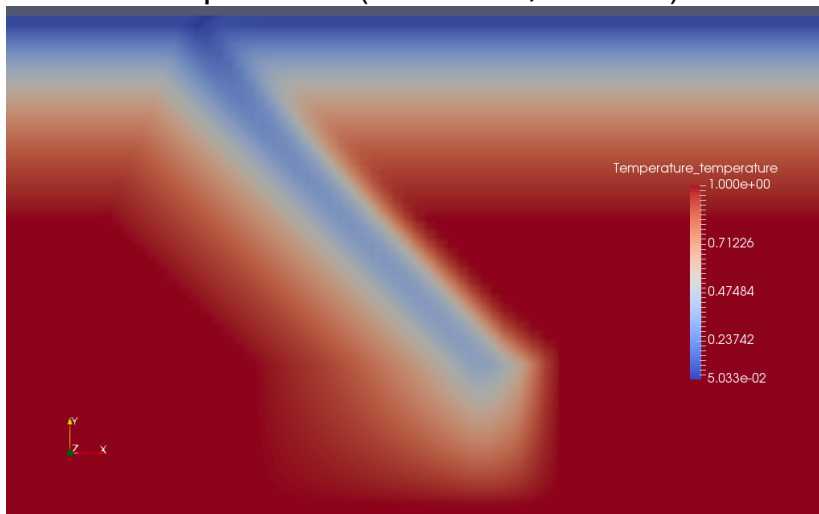
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It reuses the parallel `MatMultTranspose()` implementation.

Geometric Multigrid with a Coefficient: Part II

Interpolation

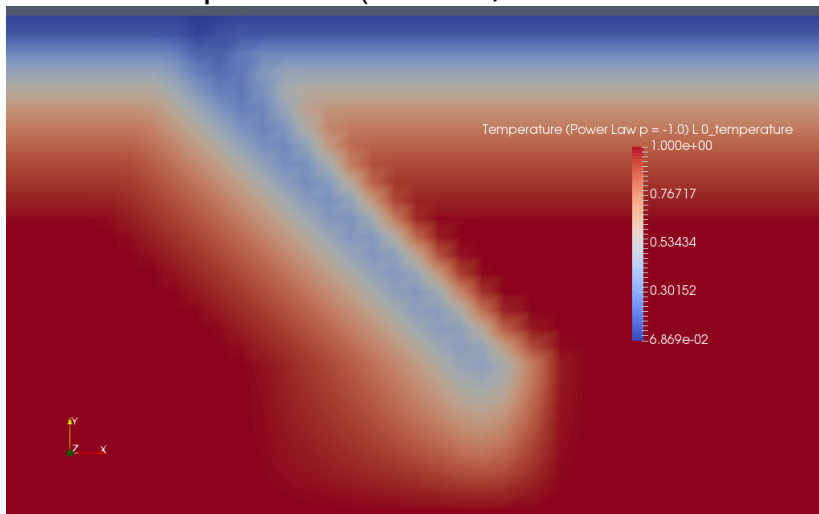
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Geometric Multigrid with a Coefficient: Part II

Interpolation

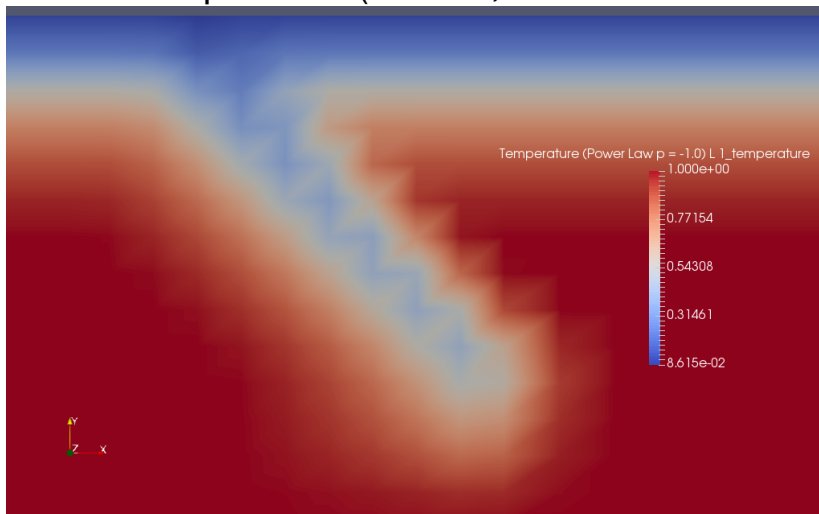
Mantle Temperature (Level 2, Harmonic Restriction)



Geometric Multigrid with a Coefficient: Part II

Interpolation

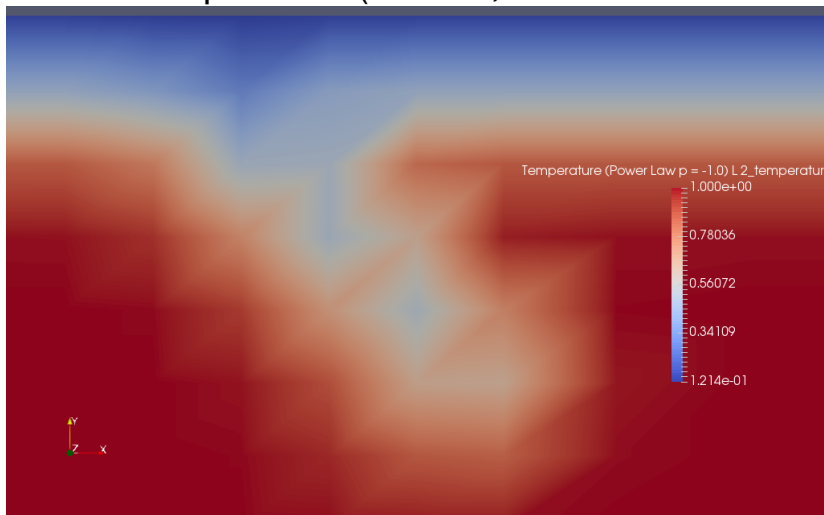
Mantle Temperature (Level 1, Harmonic Restriction)



Geometric Multigrid with a Coefficient: Part II

Interpolation

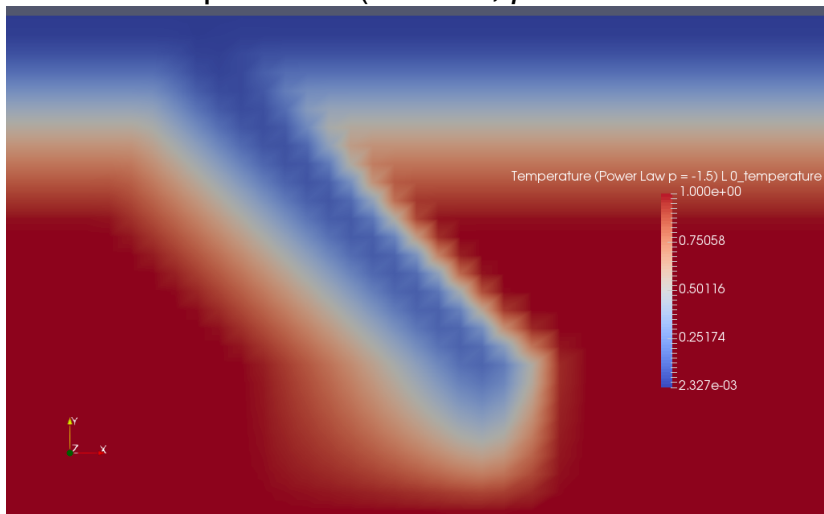
Mantle Temperature (Level 0, Harmonic Restriction)



Geometric Multigrid with a Coefficient: Part II

Interpolation

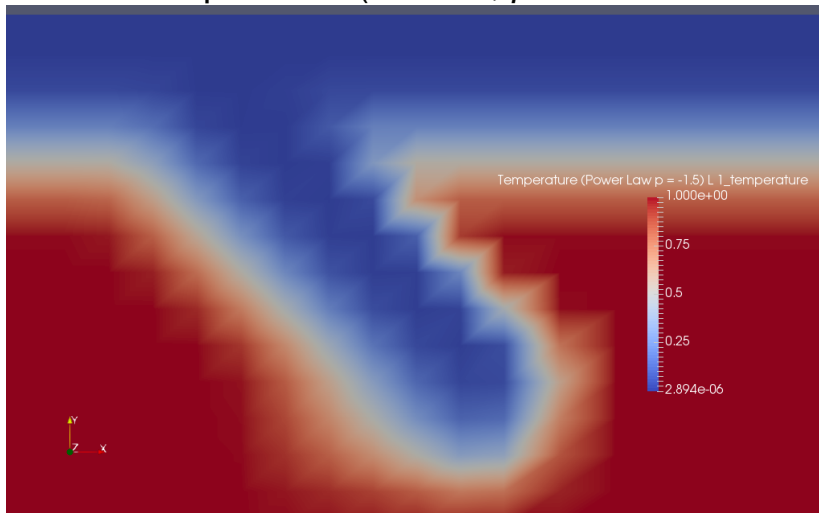
Mantle Temperature (Level 2, $p = -1.5$ Restriction)



Geometric Multigrid with a Coefficient: Part II

Interpolation

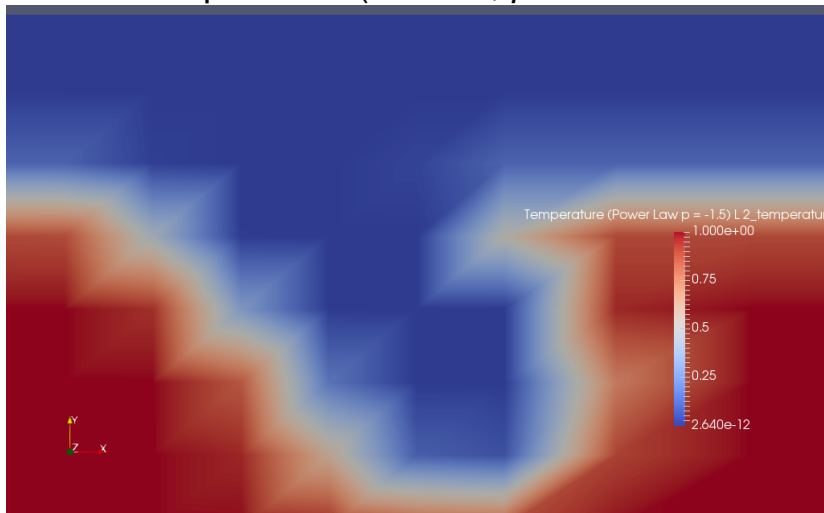
Mantle Temperature (Level 1, $p = -1.5$ Restriction)



Geometric Multigrid with a Coefficient: Part II

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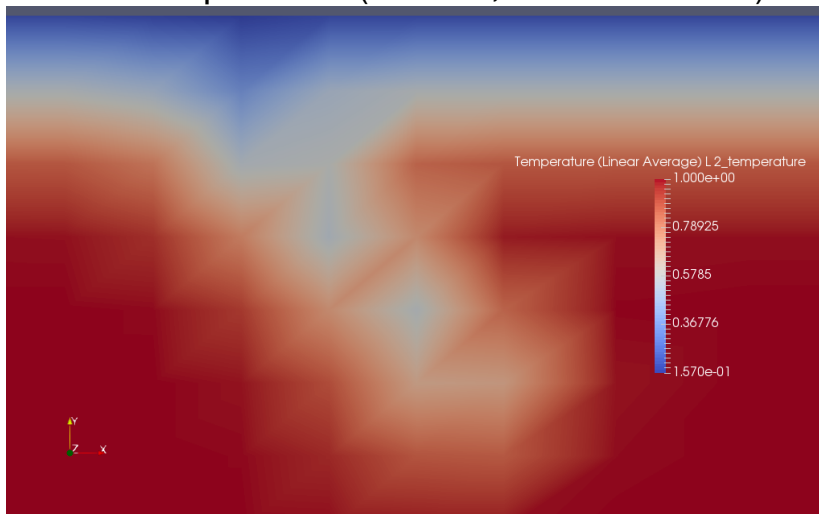
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Geometric Multigrid with a Coefficient: Part II

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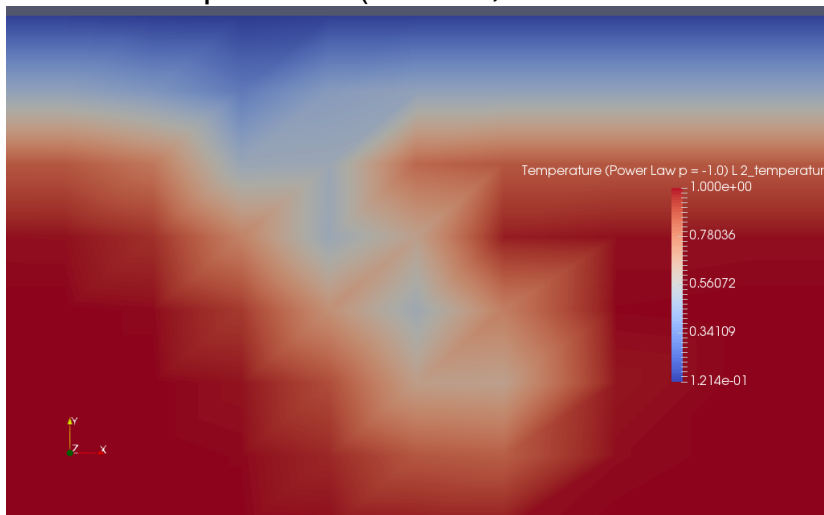
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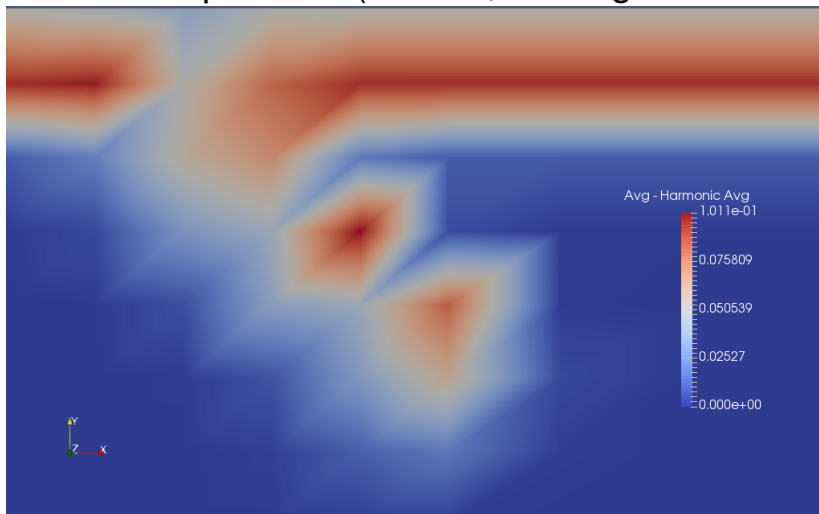
Mantle Temperature (Level 0, Harmonic Restriction)



Geometric Multigrid with a Coefficient: Part II

Interpolation

Mantle Temperature (Level 0, Q1 Avg - Harmonic Avg)



Geometric Multigrid with a Coefficient: Part III

Solving

```
-snes_rtol 1e-7 -snes_atol 1e-12 -snes_linesearch_maxstep 1e20
-ksp_rtol 1e-5
-pc_type fieldsplit
  -pc_fieldsplit_diag_use_amat
  -pc_fieldsplit_type schur
  -pc_fieldsplit_schur_factorization_type full
  -pc_fieldsplit_schur_precondition all
    -fieldsplit_velocity_ksp_type gmres
    -fieldsplit_velocity_ksp_rtol 1e-8
  -fieldsplit_velocity_pc_type mg
    -fieldsplit_velocity_pc_mg_levels n
    -fieldsplit_velocity_mg_levels_ksp_type gmres
    -fieldsplit_velocity_mg_levels_ksp_max_it 4
    -fieldsplit_velocity_mg_levels_pc_type pbjacobi
    -fieldsplit_velocity_mg_levels_pc_pbjacobi_variable
    -fieldsplit_velocity_mg_levels_pc_use_amat
  -fieldsplit_pressure_pc_type asm
    -fieldsplit_pressure_sub_pc_type ilu
    -fieldsplit_pressure_ksp_rtol 1e-4
    -fieldsplit_pressure_ksp_max_it 20
```

Geometric Multigrid with a Coefficient: Part III

Solving

```
-snes_rtol 1e-7 -snes_atol 1e-12 -snes_linesearch_maxstep 1e20
-ksp_rtol 1e-5
-pc_type fieldsplit
-pc_fieldsplit_diag_use_amat
-pc_fieldsplit_type schur
-pc_fieldsplit_schur_factorization_type full
-pc_fieldsplit_schur_precondition all
-fieldsplit_velocity_ksp_type gmres
-fieldsplit_velocity_ksp_rtol 1e-8
-fieldsplit_velocity_pc_type mg
-fieldsplit_velocity_pc_mg_levels n
-fieldsplit_velocity_mg_levels_ksp_type gmres
-fieldsplit_velocity_mg_levels_ksp_max_it 4
-fieldsplit_velocity_mg_levels_pc_type pbjacobi
-fieldsplit_velocity_mg_levels_pc_pbjacobi_variable
-fieldsplit_velocity_mg_levels_pc_use_amat
-fieldsplit_pressure_pc_type asm
-fieldsplit_pressure_sub_pc_type ilu
-fieldsplit_pressure_ksp_rtol 1e-4
-fieldsplit_pressure_ksp_max_it 20
```

Geometric Multigrid with a Coefficient: Part III

Solving

```
-snes_rtol 1e-7 -snes_atol 1e-12 -snes_linesearch_maxstep 1e20
-ksp_rtol 1e-5
-pc_type fieldsplit
-pc_fieldsplit_diag_use_amat
-pc_fieldsplit_type schur
-pc_fieldsplit_schur_factorization_type full
-pc_fieldsplit_schur_precondition all
-fieldsplit_velocity_ksp_type gmres
-fieldsplit_velocity_ksp_rtol 1e-8
-fieldsplit_velocity_pc_type mg
-fieldsplit_velocity_pc_mg_levels n
-fieldsplit_velocity_mg_levels_ksp_type gmres
-fieldsplit_velocity_mg_levels_ksp_max_it 4
-fieldsplit_velocity_mg_levels_pc_type pbjacobi
-fieldsplit_velocity_mg_levels_pc_pbjacobi_variable
-fieldsplit_velocity_mg_levels_pc_use_amat
-fieldsplit_pressure_pc_type asm
-fieldsplit_pressure_sub_pc_type ilu
-fieldsplit_pressure_ksp_rtol 1e-4
-fieldsplit_pressure_ksp_max_it 20
```

Geometric Multigrid with a Coefficient: Part III

Solving

```
-snes_rtol 1e-7 -snes_atol 1e-12 -snes_linesearch_maxstep 1e20
-ksp_rtol 1e-5
-pc_type fieldsplit
  -pc_fieldsplit_diag_use_amat
  -pc_fieldsplit_type schur
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    -fieldsplit_velocity_mg_levels_ksp_type gmres
    -fieldsplit_velocity_mg_levels_ksp_max_it 4
    -fieldsplit_velocity_mg_levels_pc_type pbjacobi
    -fieldsplit_velocity_mg_levels_pc_pbjacobi_variable
    -fieldsplit_velocity_mg_levels_pc_use_amat
-fieldsplit_pressure_pc_type asm
  -fieldsplit_pressure_sub_pc_type ilu
  -fieldsplit_pressure_ksp_rtol 1e-4
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```

Geometric Multigrid with a Coefficient: Part III

Solving

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-fieldsplit_velocity_pc_mg_levels n
-fieldsplit_velocity_mg_levels_ksp_type gmres
-fieldsplit_velocity_mg_levels_ksp_max_it 4
-fieldsplit_velocity_mg_levels_pc_type pbjacobi
-fieldsplit_velocity_mg_levels_pc_pbjacobi_variable
-fieldsplit_velocity_mg_levels_pc_use_amat
-fieldsplit_pressure_pc_type asm
-fieldsplit_pressure_sub_pc_type ilu
-fieldsplit_pressure_ksp_rtol 1e-4
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Geometric Multigrid with a Coefficient: Part III

Solving

```
-snes_rtol 1e-7 -snes_atol 1e-12 -snes_linesearch_maxstep 1e20
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-fieldsplit_velocity_mg_levels_ksp_type gmres
-fieldsplit_velocity_mg_levels_ksp_max_it 4
-fieldsplit_velocity_mg_levels_pc_type pbjacobi
-fieldsplit_velocity_mg_levels_pc_pbjacobi_variable
-fieldsplit_velocity_mg_levels_pc_use_amat
-fieldsplit_pressure_pc_type asm
-fieldsplit_pressure_sub_pc_type ilu
-fieldsplit_pressure_ksp_rtol 1e-4
-fieldsplit_pressure_ksp_max_it 20
```

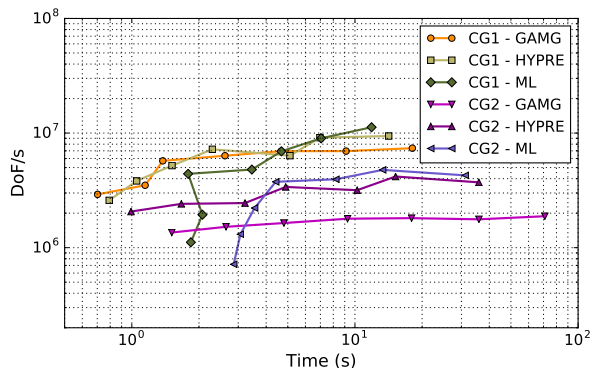

Outline

2 Interaction of Discretizations and Solvers

- PCTelescope
- GMG with coefficients
- Comparison of Discretizations

Example: TAS Performance Analysis

Static Scaling (1K procs)



Measure
dof/s,

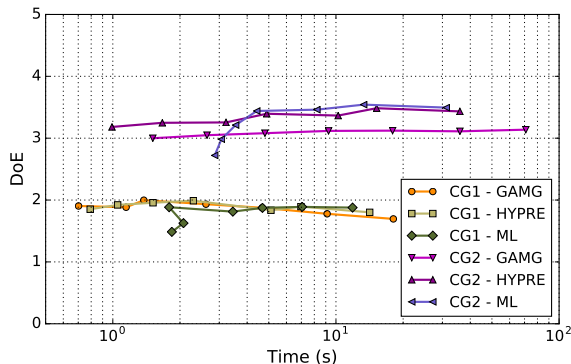
fixed parallelism,

different sizes.

Chang, Fabien, Knepley, Mills, submitted, 2018.

Example: TAS Performance Analysis

Accuracy Scaling (1K procs)



Measure
error \times time

fixed parallelism

different sizes.

Chang, Fabien, Knepley, Mills, submitted, 2018.

Conclusions

Abstractions for
Topology and Geometry,
Data Layout, and
Operator Composition
let the
User construct the Simulator.

Conclusions

<http://bitbucket.org/petsc/petsc>

<http://github.com/petsc/petsc>

Example: Magma Dynamics

Show magma performance using FAS

Knepley, Melt in the Mantle Program, Newton Institute, 2016.