Geodynamic Simulator Building

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University at Buffalo

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

Main Idea

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,

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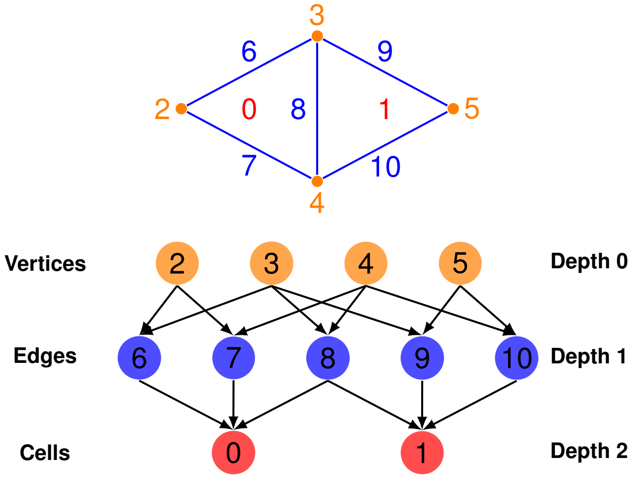
just **once**.

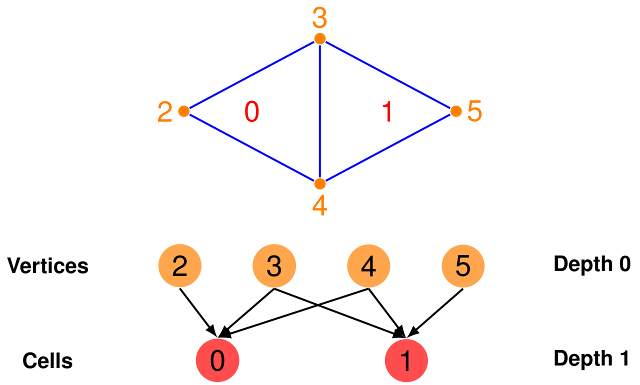
Sample Meshes

Interpolated triangular mesh



Sample Meshes

Optimized triangular mesh



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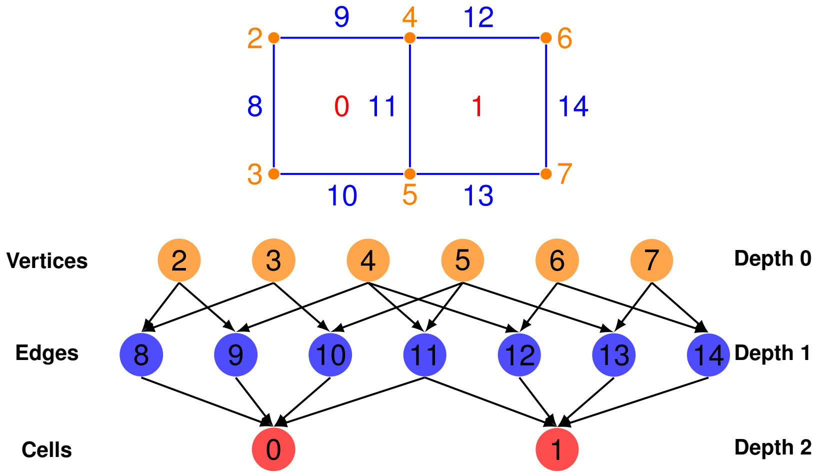
Interpolated quadrilateral mesh



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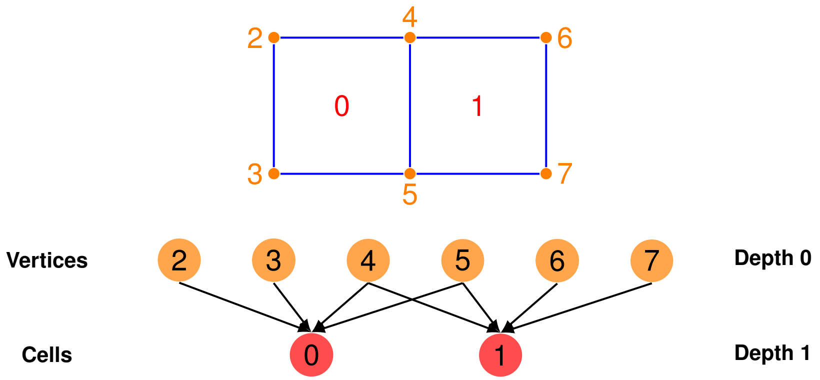
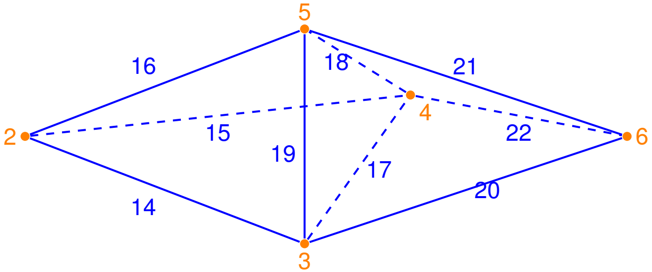
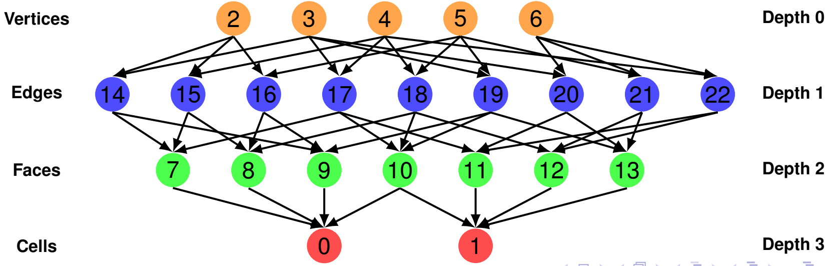


Sample Meshes

Interpolated tetrahedral mesh





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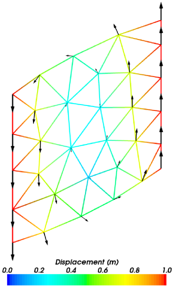
   - DMNetwork

Example: PyLith



Many cell types

Surface extraction

Hybrid meshes

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

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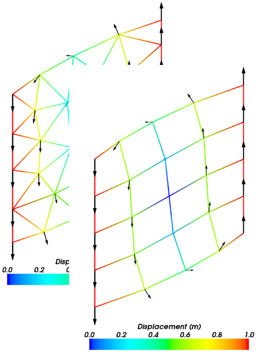

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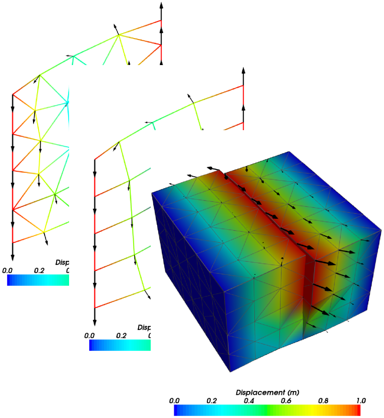

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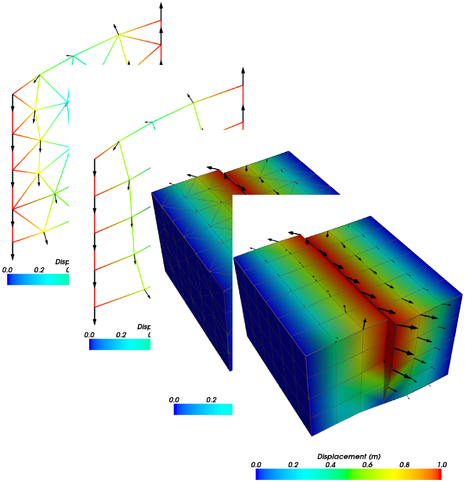

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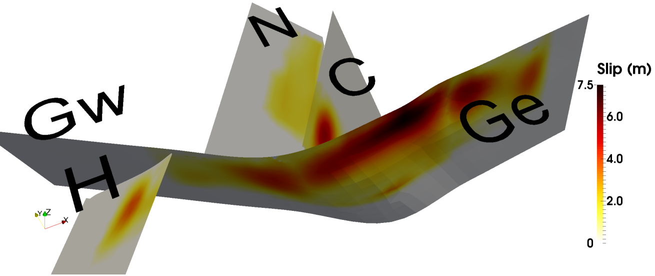

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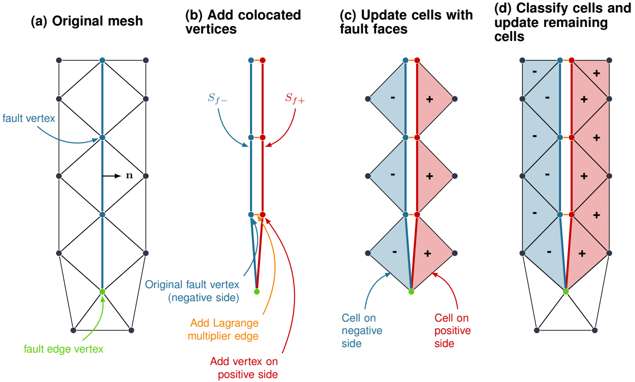

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Example: DMNetwork

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

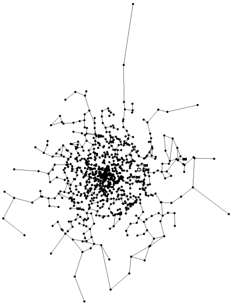

Table IV. Execution Time of Transient State on Edison

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

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

Outline

1. Flexible Meshing

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

Main Question

How do I handle

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Most packages handle one discretization,

FEniCS/Firedrake is a notable exception,

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The `Section` abstraction allows us to write code for

- parallel data layout,
- block/field decompositions,
- (variable) point-block decompositions,
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- (nonlinear) hierarchical rediscretization,
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A `Section` is a map

$$\text{mesh point} \Longrightarrow (\text{size}, \text{offset})$$

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Data Layout	mesh point $\Longrightarrow$ # dofs
Boundary conditions	mesh point $\Longrightarrow$ # constrained dofs
Fields	mesh point $\Longrightarrow$ # field dofs

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Decouples Mesh, Discretization, and Solver

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

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Decouples Mesh, Discretization, and Solver

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

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A `Section` is a map

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Decouples Mesh, Discretization, and Solver

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

Section

A `Section` is a map

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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

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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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`PCTelescope` abstracts the parallel distribution
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The paper shows scaling up to
32^3 processors on Piz Daint,
and also hybrid CPU-GPU solvers.

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Outline

2. Interaction of Discretizations and Solvers
    - PCTelescope
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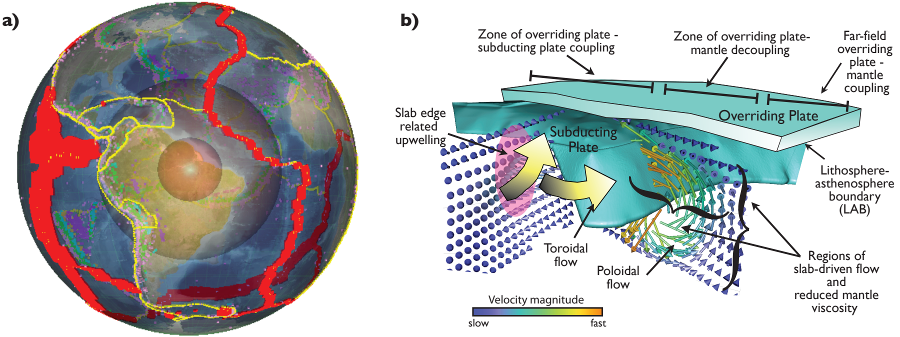
    - Comparison of Discretizations

Geometric Multigrid with a Coefficient

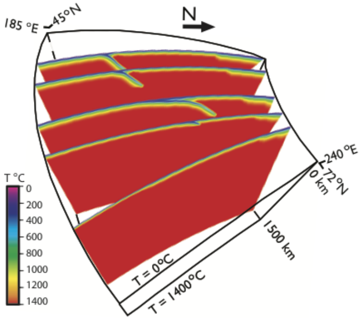
Regional mantle convection
has highly variable viscosity,
due to temperature and strain rate.



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.



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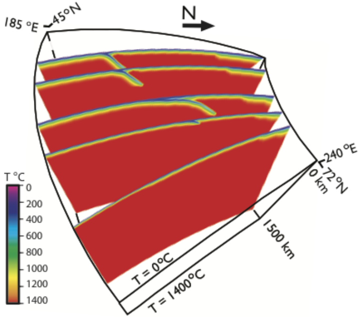
Geometric Multigrid with a Coefficient

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



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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, &I, &Rscale);
MatMult(I, coarseTemp, fineTemp);
```

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Now we restrict the input temperature to coarser meshes.

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DMCreateInterpolation(coarseMesh, fineMesh, &I, &Rscale);
MatMultTranspose(I, fineTemp, coarseTemp);
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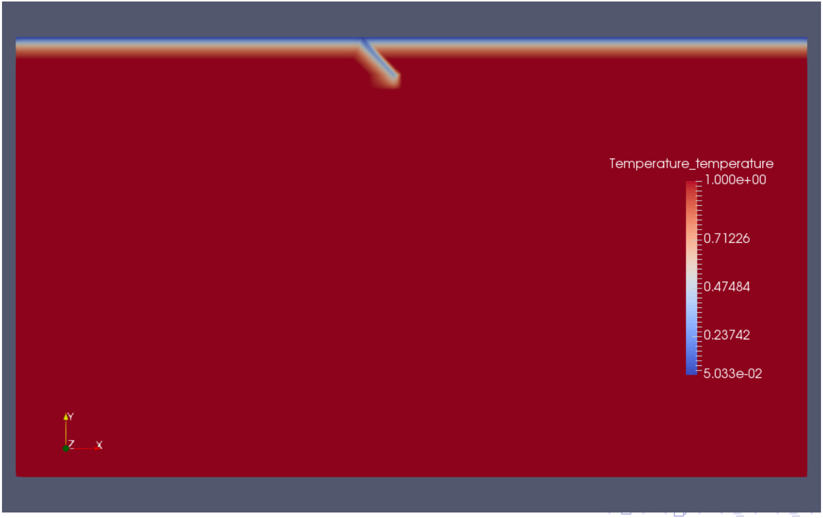
Mantle Temperature (Fine Grid, Level 3)



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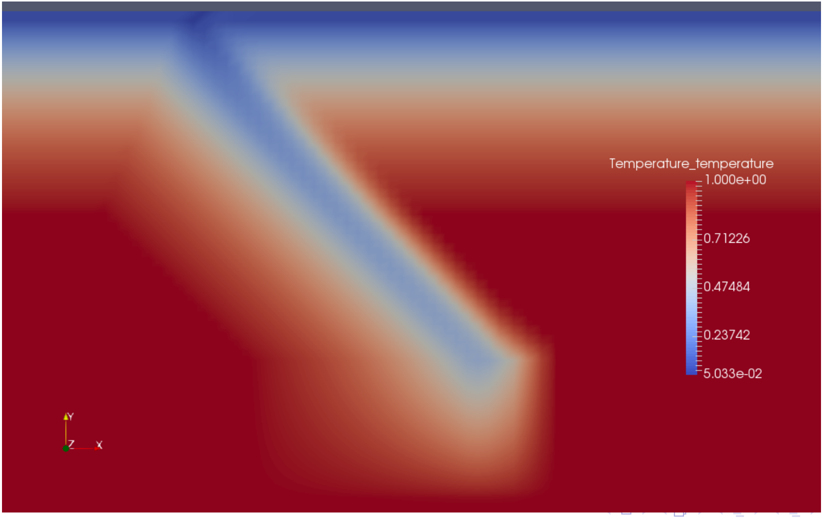
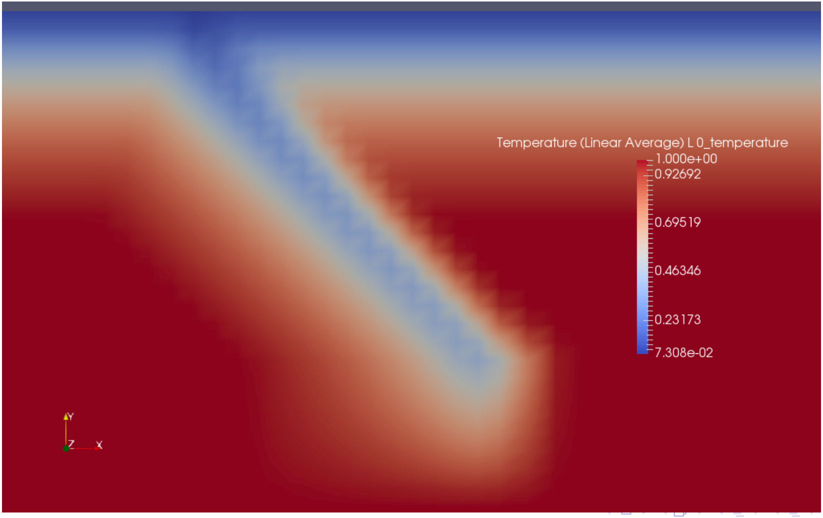


Geometric Multigrid with a Coefficient: Part II

Interpolation

Mantle Temperature (Level 2, Q1 Restriction)



Geometric Multigrid with a Coefficient: Part II

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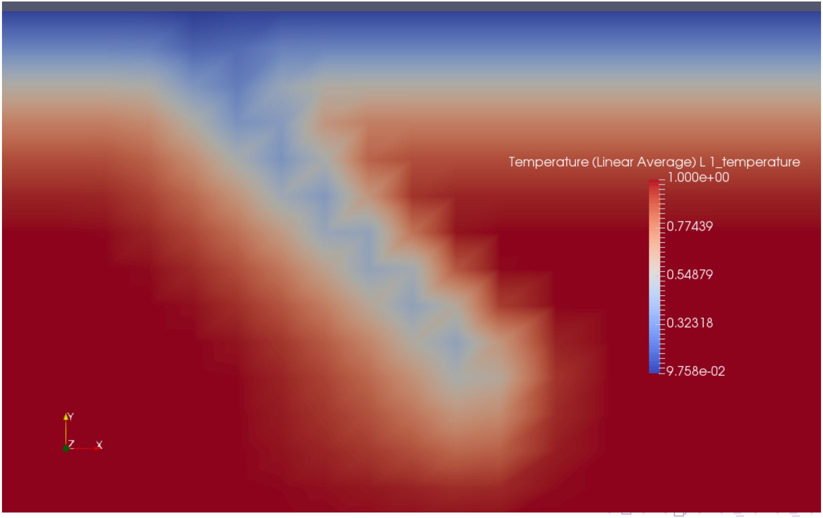
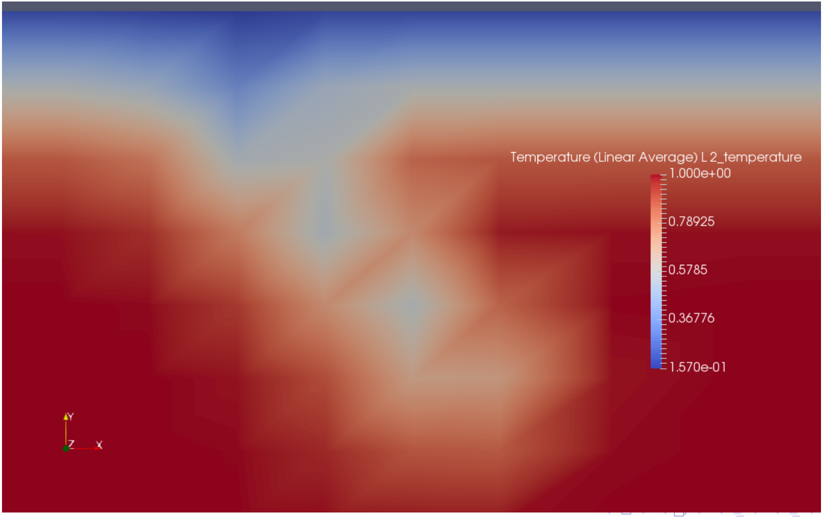
Mantle Temperature (Level 1, Q1 Restriction)



Geometric Multigrid with a Coefficient: Part II

Interpolation

Mantle Temperature (Level 0, Q1 Restriction)



Geometric Multigrid with a Coefficient: Part II

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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

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The power mean could better preserve low temperatures

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

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

Geometric Multigrid with a Coefficient: Part II

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The power mean could better preserve low temperatures

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

```
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);
  }
}
```

It reuses the parallel `MatMultTranspose()` implementation.

Geometric Multigrid with a Coefficient: Part II

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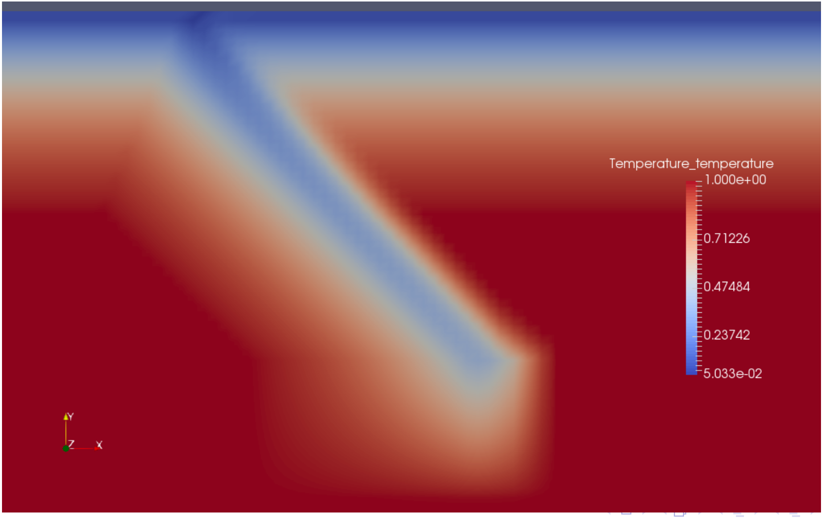

Geometric Multigrid with a Coefficient: Part II

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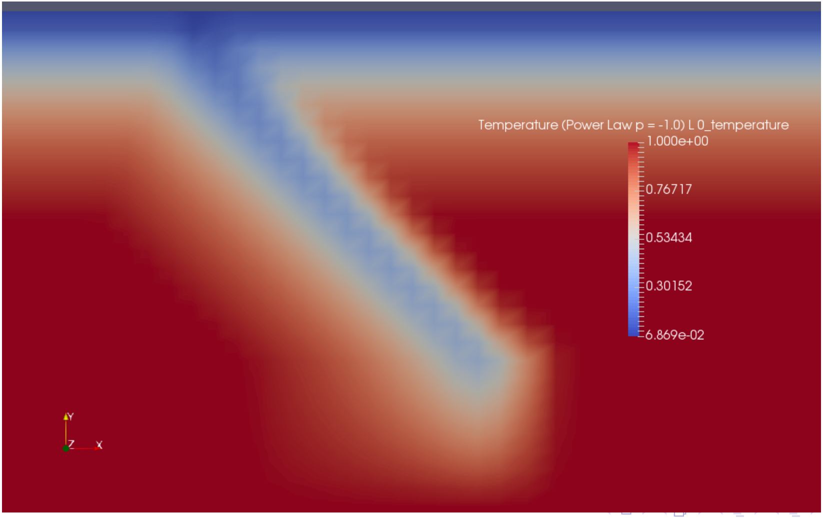
Mantle Temperature (Level 2, Harmonic Restriction)



Geometric Multigrid with a Coefficient: Part II

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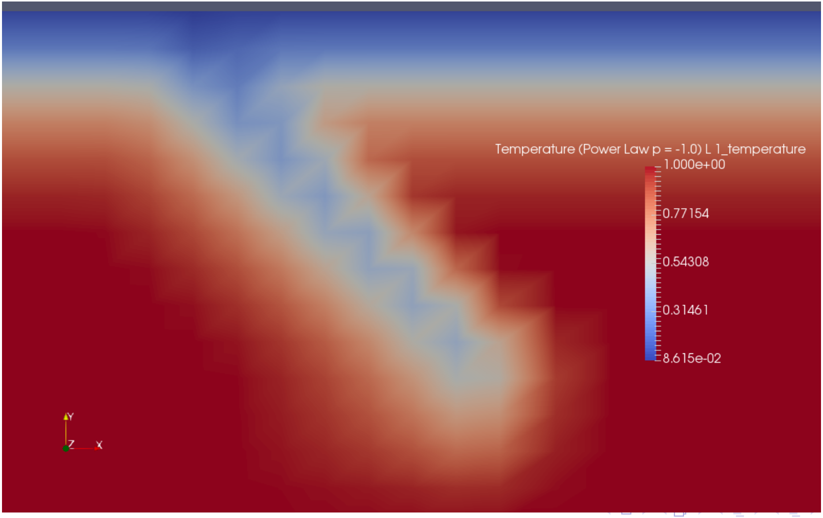
Mantle Temperature (Level 1, Harmonic Restriction)



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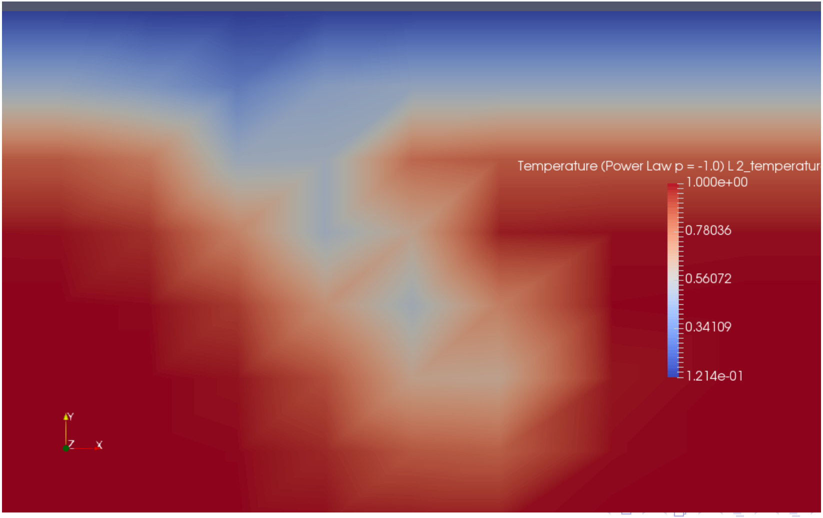
Interpolation

Mantle Temperature (Level 0, Harmonic Restriction)



Geometric Multigrid with a Coefficient: Part II

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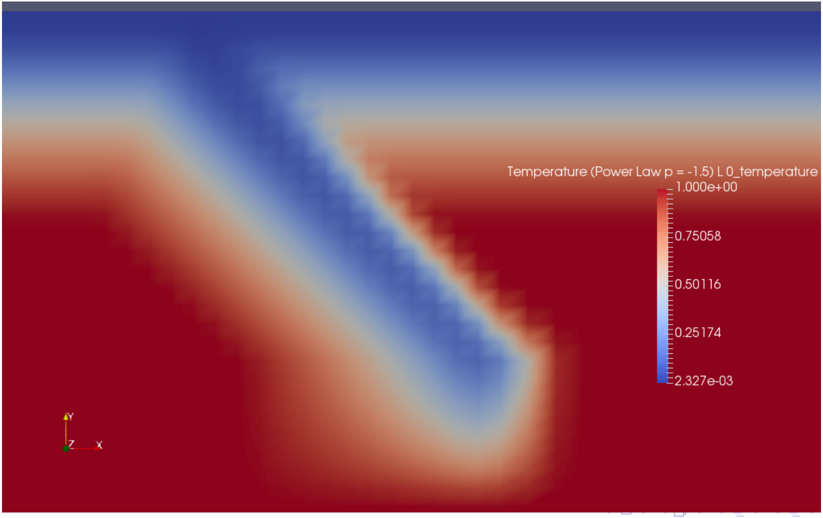
Mantle Temperature (Level 2, $p = -1.5$ Restriction)



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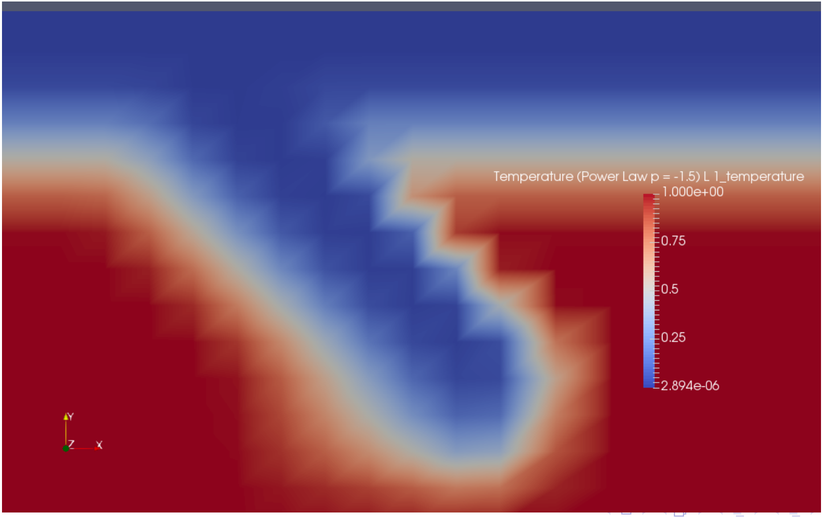

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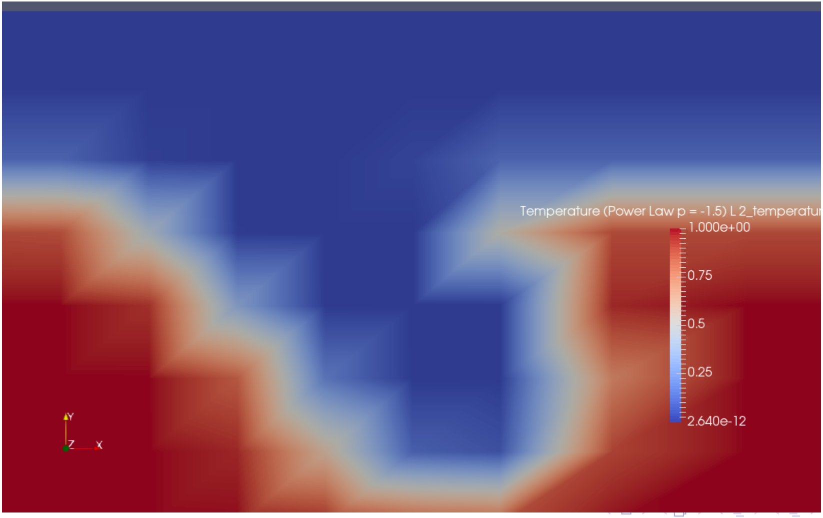

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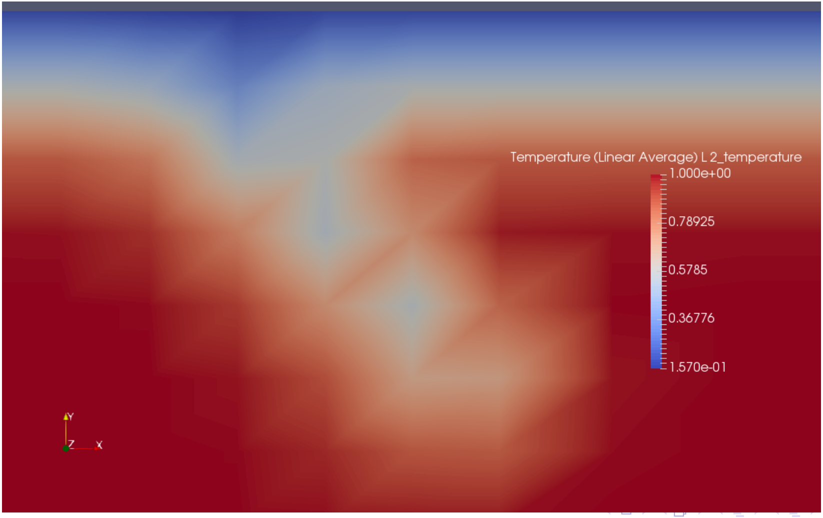

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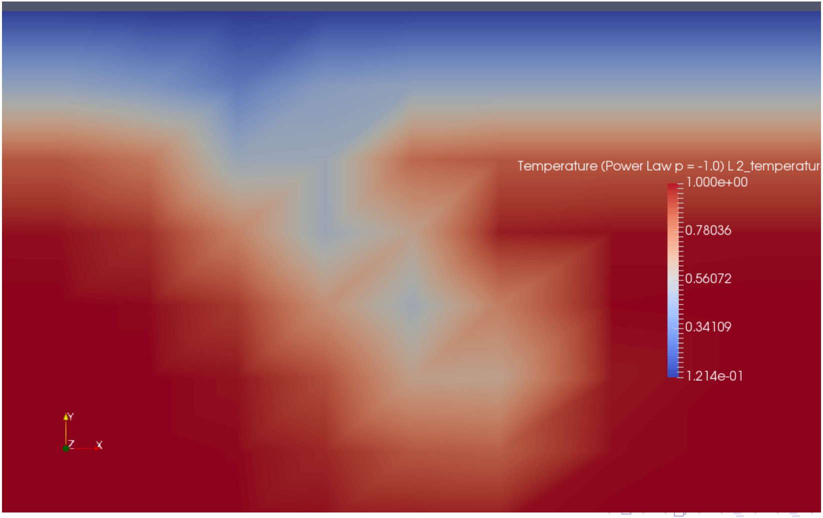
Interpolation

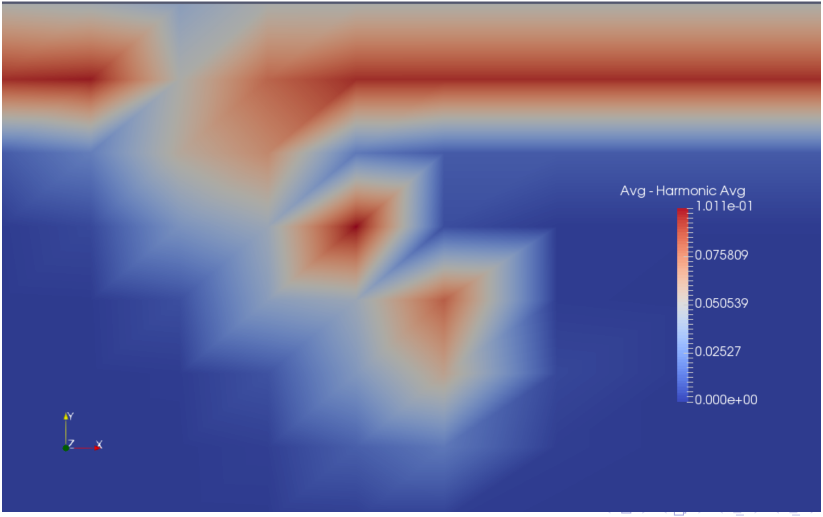
Mantle Temperature (Level 0, Harmonic Restriction)



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 a11
      -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 a11
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            -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
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Geometric Multigrid with a Coefficient: Part III

Solving

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            -fieldsplit_velocity_mg_levels_pc_pbjacobi_variable
            -fieldsplit_velocity_mg_levels_pc_use_amat
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Geometric Multigrid with a Coefficient: Part III

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            -fieldsplit_velocity_mg_levels_pc_pbjacobi_variable
            -fieldsplit_velocity_mg_levels_pc_use_amat
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Geometric Multigrid with a Coefficient: Part III

Solving

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Geometric Multigrid with a Coefficient: Part III

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        -fieldsplit_pressure_sub_pc_type ilu
        -fieldsplit_pressure_ksp_rtol 1e-4
        -fieldsplit_pressure_ksp_max_it 20
```
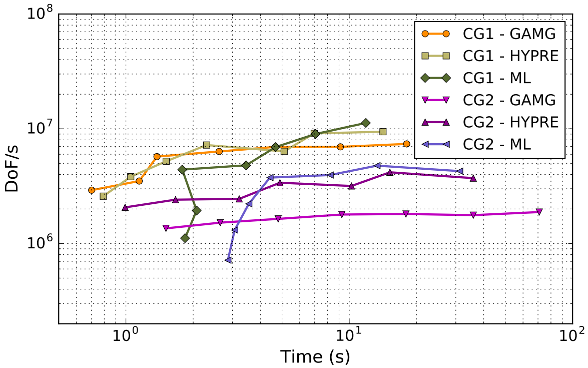

Outline

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

Example: TAS Performance Analysis

Static Scaling (1K procs)



Measure dof/s,

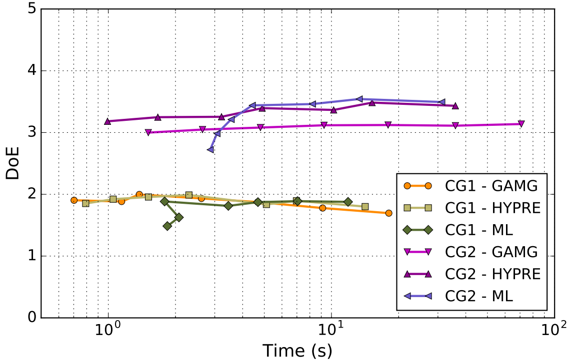
fixed parallelism,

different sizes.

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

Example: TAS Performance Analysis

Accuracy Scaling (1K procs)



Measure
error × 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.