High Performance Implicit Solvers for Geodynamics

These slides:
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Outline

Role of implicit solvers

Common methods and algorithmic barriers

Failure modes and troubleshooting

Coupling approaches

Stokes problems

Performance considerations

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Why do we need solvers?

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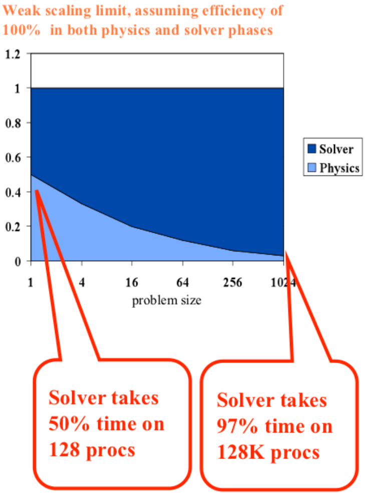
2. Convection insignificant compared to viscosity (unrelated to stiffness; Reynolds number)
3. Relaxation fast compared to dynamical time scale (depends on observational scale)

It’s *all* about algorithms (at the petascale)

- Given, for example:
  - a “physics” phase that scales as $O(N)$
  - a “solver” phase that scales as $O(N^{3/2})$
  - computation is almost all solver after several doublings
- Most applications groups have not yet “felt” this curve in their gut
  - as users actually get into queues with more than 4K processors, this will change



Weak scaling limit, assuming efficiency of 100% in both physics and solver phases

Solver takes 50% time on 128 procs

Solver takes 97% time on 128K procs

(c/o David Keyes)

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Evaluating methods

- Performance of methods will depend on grid resolution and model parameters (regime and heterogeneity).
- A method is:
  - scalable (also “optimal”) if its performance is independent of resolution and parallelism
  - robust if its performance is (nearly) independent of model parameters
  - efficient if it solves the problem in a small multiple of the cost to evaluate the residual[1]

[1] We’ll settle for “as fast as the best known method”.

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- Linear problems typically arise from linearizing a nonlinear problem. This step is not necessary, but it is convenient for reusing software and for debugging.

[1] We’ll settle for “as fast as the best known method”.

Taxonomy of implicit solvers

Global linearization: Picard and Newton

- Linear solve “$J(u)w = -F(u)$”
  - (sparse) direct vs. iterative (Krylov) with preconditioning
  - classical relaxation (Jacobi, Gauss-Seidel), incomplete factorization (ILU)
  - domain decomposition and multigrid
- Globalization: “$u_{\text{next}} = u + \alpha w$”
  - Line search, trust region, continuation

Inherently nonlinear methods

- Nonlinear GMRES, Nonlinear CG (can use preconditioning)
- Nonlinear domain decomposition
- Nonlinear multigrid: Full Approximation Scheme (FAS)

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- These methods can be **scalable**.

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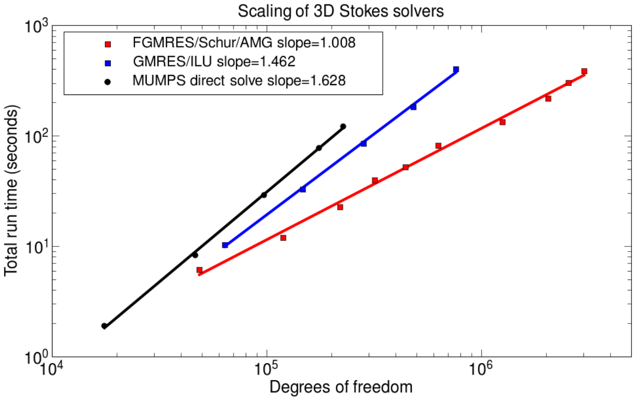
- How nonlinear are the scales? How expensive is setup?

What about direct linear solvers?



- By all means, start with a direct solver
- Direct solvers are robust, but not scalable
- **2D**: $\mathcal{O}(n^{1.5})$ flops, $\mathcal{O}(n \log n)$ memory.
- **3D**: $\mathcal{O}(n^2)$ flops, $\mathcal{O}(n^{4/3})$ memory
- We will focus on iterative linear solvers

Matrices

Definition (Matrix)

A matrix is a linear transformation between finite dimensional vector spaces.

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Definition (Forming a matrix)

Forming or assembling a matrix means defining it's action in terms of entries (usually stored in a sparse format).

Important matrices

1. Sparse (e.g. discretization of a PDE operator)
2. Inverse of *anything* interesting $B = A^{-1}$
3. Jacobian of a nonlinear function $Jy = \lim_{\varepsilon \to 0} \frac{F(x+\varepsilon y) - F(x)}{\varepsilon}$
4. Fourier transform $\mathscr{F}, \mathscr{F}^{-1}$
5. Other fast transforms, e.g. Fast Multipole Method
6. Low rank correction $B = A + uv^T$
7. Schur complement $S = D - CA^{-1}B$
8. Tensor product $A = \sum_e A_x^e \otimes A_y^e \otimes A_z^e$
9. Linearization of a few steps of an explicit integrator

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- These matrices are dense. Never form them.

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- These are not very sparse. Don't form them.

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- None of these matrices “have entries”

What can we do with a matrix that doesn't have entries?

Krylov solvers for $Ax = b$

- Krylov subspace: $\{b, Ab, A^2b, A^3b, \dots\}$
- Convergence rate depends on the spectral properties of the matrix
  - Existance of small polynomials $p_n(A) < \varepsilon$ where $p_n(0) = 1$.
  - condition number $\kappa(A) = \|A\| \left\|A^{-1}\right\| = \sigma_{\text{max}}/\sigma_{\text{min}}$
  - distribution of singular values, spectrum Λ, pseudospectrum Λ_ε
- For any popular Krylov method $\mathscr{K}$, there is a matrix of size m, such that $\mathscr{K}$ outperforms all other methods by a factor at least $\mathscr{O}(\sqrt{m})$ [Nachtigal et. al., 1992]

Typically...

- The action $y \leftarrow Ax$ can be computed in $\mathscr{O}(m)$
- Aside from matrix multiply, the n^{th} iteration requires at most $\mathscr{O}(mn)$

The $\mathfrak{p}$-Bratu equation

- 2-dimensional model problem

  $$-\nabla\cdot\big(|\nabla u|^{\mathfrak{p}-2}\nabla u\big) - \lambda e^u - f = 0, \qquad 1 \le \mathfrak{p} \le \infty, \quad \lambda < \lambda_{\text{crit}}(\mathfrak{p})$$

  Singular or degenerate when $\nabla u = 0$, turning point at λ_{crit}.
- Regularized variant

  $$-\nabla\cdot(\eta\nabla u) - \lambda e^u - f = 0$$

  $$\eta(\gamma) = (\epsilon^2 + \gamma)^{\frac{\mathfrak{p}-2}{2}} \qquad \gamma(u) = \frac{1}{2}|\nabla u|^2$$
- Jacobian

  $$J(u)w \sim -\nabla\cdot\big[(\eta 1 + \eta' \nabla u \otimes \nabla u)\nabla w\big] - \lambda e^u w$$

  $$\eta' = \frac{\mathfrak{p}-2}{2}\eta/(\epsilon^2 + \gamma)$$

  Interpretation: conductivity tensor flattened in direction ∇u
- Simple finite difference discretization in PETSc:

  ```
  $ cd petsc/src/snes/examples/tutorials/; make ex15
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- Step 1: Write the residual.

Step 1: Write the residual

- Start with $\mathfrak{p} = 2$ (standard Laplacian), define only residuals
- Matrix-free Jacobians, no preconditioning `-snes_mf`
- `$ ./ex15 -da_refine 1 -snes_mf -snes_monitor -ksp_converged_reason`
- `$ ./pbratu -da_refine 2 -snes_mf -snes_monitor -ksp_converged_reason`
- `$ ./pbratu -da_refine 3 -snes_mf -snes_monitor -ksp_converged_reason`
- `$ ./pbratu -da_refine 4 -snes_mf -snes_monitor -ksp_converged_reason`

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  ```
  $ ./ex15 -da_refine 1 -snes_mf -snes_monitor
  -ksp_converged_reason
  ```

  ```
  0 SNES Function norm 9.324361041196e-01
  Linear solve converged due to CONVERGED_RTOL iterations 7
  1 SNES Function norm 4.534365556764e-09

  CONVERGED_FNORM_RELATIVE Number of nonlinear iterations = 1
  ```

-
  ```
  $ ./pbratu -da_refine 2 -snes_mf -snes_monitor
  -ksp_converged_reason
  ```

-
  ```
  $ ./pbratu -da_refine 3 -snes_mf -snes_monitor
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  ```
  0 SNES Function norm 5.363535697720e-01
  Linear solve converged due to CONVERGED_RTOL iterations 18
  1 SNES Function norm 1.276738526722e-06
  Linear solve converged due to CONVERGED_RTOL iterations 18
  2 SNES Function norm 1.263046904535e-11

  CONVERGED_FNORM_RELATIVE Number of nonlinear iterations = 2
  ```
- `$ ./pbratu -da_refine 3 -snes_mf -snes_monitor -ksp_converged_reason`
- `$ ./pbratu -da_refine 4 -snes_mf -snes_monitor -ksp_converged_reason`

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- `$ ./pbratu -da_refine 3 -snes_mf -snes_monitor -ksp_converged_reason`

  ```
  0 SNES Function norm 2.820917170607e-01
  Linear solve converged due to CONVERGED_RTOL iterations 42
  1 SNES Function norm 2.782839451653e-06
  Linear solve converged due to CONVERGED_RTOL iterations 45
  2 SNES Function norm 2.682642095006e-11

  CONVERGED_FNORM_RELATIVE Number of nonlinear iterations = 2
  ```

- `$ ./pbratu -da_refine 4 -snes_mf -snes_monitor -ksp_converged_reason`

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```
0 SNES Function norm 1.441189193029e-01
Linear solve converged due to CONVERGED_RTOL iterations 101
1 SNES Function norm 1.409860069506e-06
Linear solve converged due to CONVERGED_RTOL iterations 154
2 SNES Function norm 1.390912345257e-11

CONVERGED_FNORM_RELATIVE Number of nonlinear iterations = 2
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  ```

- The number of iterations is growing with grid refinement.

Experimenting with algorithms

- `-pc_type asm -sub_pc_type lu`
- `-pc_type gamg -pc_gamg_agg_nsmooths 1`
- `-jtype PICARD -pc_type lu`
- `-snes_mf_operator -jtype PICARD -pc_type ml`

-
  ```
  -snes_type ngmres -snes_ngmres_m 10
      -npc_snes_max_it 1 -npc_snes_type fas
  ```

Barriers

- Krylov method: $(\text{iteration count}) \sim \sqrt{\text{condition number}}$
- Elliptic ill-conditioning
  - $\kappa(A) \sim h^{-2}$ for second order elliptic problems
  - *Asymptotics* not improved for standard methods:
    `-pc_type jacobi`, `-pc_type sor`, `-pc_type ilu`
  - 1-level Domain Decomposition: $\kappa \sim H^{-2}\phi(H/h)$
    `-pc_type bjacobi`, `-pc_type asm`
  - Multilevel/multigrid: $\kappa \sim 1$
    `-pc_type gamg`, `-pc_type ml`, `-pc_type hypre`, `-pc_type mg`
- Heterogeneity
  - Conditioning proportional to maximum material contrast
  - In friendly circumstances, a local preconditioner restores $\sim h^{-2}$ ill-conditioning
  - Coarse approximations and subdomain transmission conditions become difficult
  - Fine grids necessary *because of* heterogeneity
  - Coarse grid must accurately represent long-range coupling

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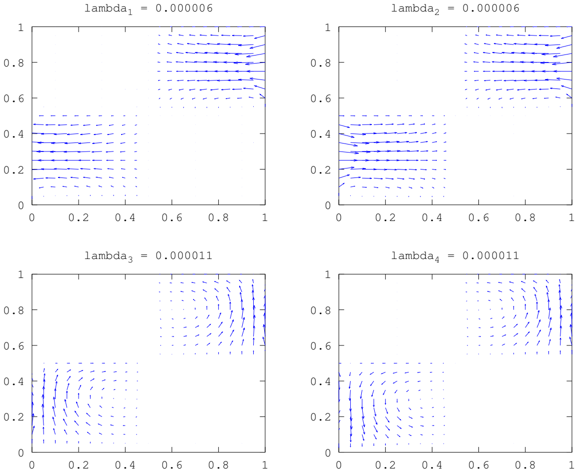
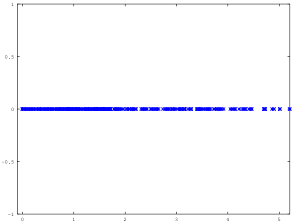
Low energy modes of preconditioned operator $P^{-1}A$

2×2 checkerboard elasticity problem, Neumann condition on right boundary

- Original operator, stiff blocks don't move

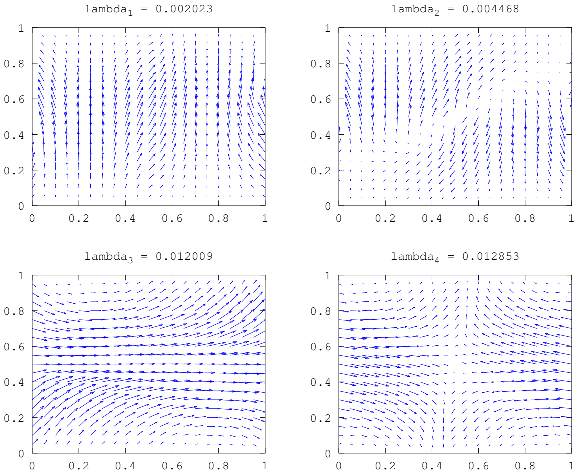


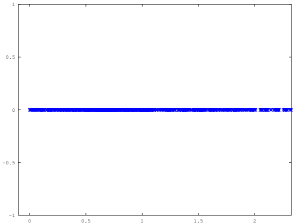


Low energy modes of preconditioned operator $P^{-1}A$

2×2 checkerboard elasticity problem, Neumann condition on right boundary

- With Jacobi preconditioning, balances stiffness, not $\mathcal{O}(\Delta x^2)$ elliptic ill-conditioning





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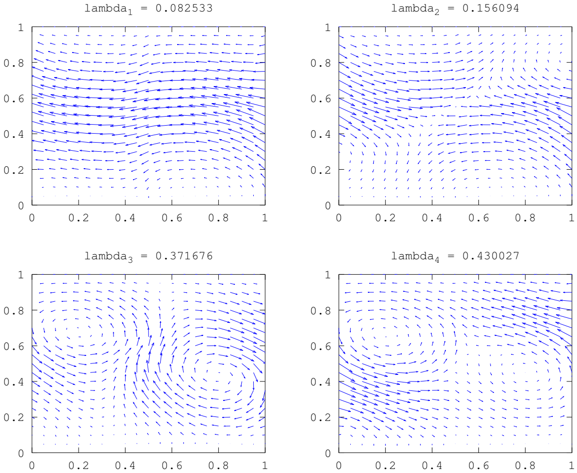
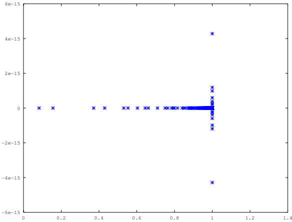
2×2 checkerboard elasticity problem, Neumann condition on right boundary

- With BoomerAMG preconditioning, does not find all rotations





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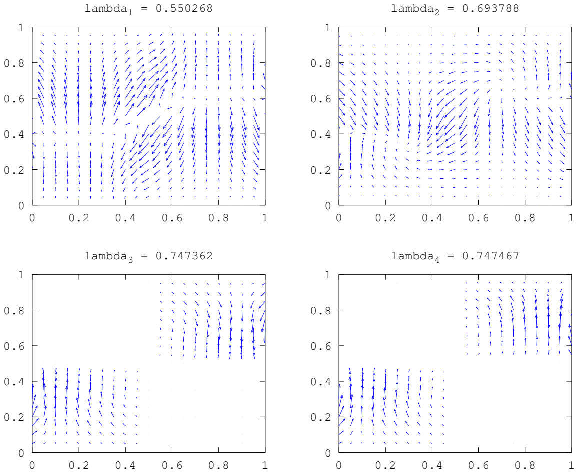
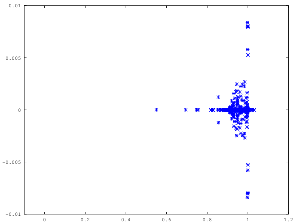
- With geometric MG, Galerkin coarse operators, Chebychev smoother





Low energy modes of preconditioned operator $P^{-1}A$

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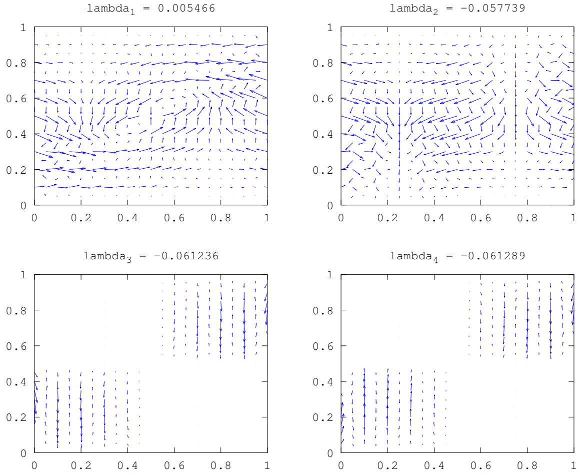
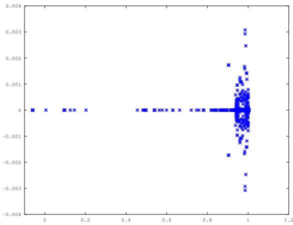
- With geometric MG, Galerkin coarse operators, unstable Chebychev smoother





Linear solver convergence problems[2]

- Watch the true residual `-ksp_monitor_true_residual`
- Make the problem small and create an environment to test rapidly
- Are boundary conditions correct?
  `-pc_type svd -pc_svd_monitor` and `-pc_type lu`
- Is the system singular? Known nullspace?
- Is the condition number reasonable?
  `-ksp_monitor_singular_value`
- Compare preconditioned residual to true residual (unstable preconditioner)
- Is GMRES restart a problem? `-ksp_gmres_restart 300`
- Is preconditioner nonlinear? `-ksp_type gcr`,
  `-ksp_type fgmres`
- Geometric multigrid with rediscretization: boundary condition scaling.

[2] `http://scicomp.stackexchange.com/questions/513`

Nonlinear solver convergence problems[3]

- Is the Jacobian assembled correctly?
  - `-snes_mf_operator -pc_type lu`
  - `-snes_type test` or `-snes_compare_explicit`
  - `-snes_mf_type ds`
- Is the linear system solved accurately enough?
- Does the linear system become singular?
- Is there a bug in residual evaluation?
- Is the residual function discontinuous?
- `-snes_linesearch_monitor`
- `./configure --with-precision=__float128`

[3] http://scicomp.stackexchange.com/questions/30

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The Great Solver Schism: Monolithic or Split?

Monolithic

- Direct solvers
- Coupled Schwarz
- Coupled Neumann-Neumann (need unassembled matrices)
- Coupled multigrid

X Need to understand local spectral and compatibility properties of the coupled system

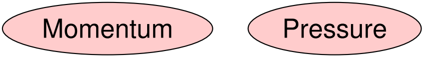
Split

- Physics-split Schwarz (based on relaxation)
- Physics-split Schur (based on factorization)
  - approximate commutators SIMPLE, PCD, LSC
  - segregated smoothers
  - Augmented Lagrangian
  - “parabolization” for stiff waves

X Need to understand global coupling strengths

- Preferred data structures depend on which method is used.
- Interplay with geometric multigrid.

Multi-physics coupling in PETSc

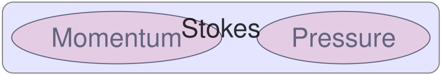


Momentum

Pressure

- package each “physics” independently
- solve single-physics and coupled problems
- semi-implicit and fully implicit
- reuse residual and Jacobian evaluation unmodified
- direct solvers, fieldsplit inside multigrid, multigrid inside fieldsplit without recompilation
- use the best possible matrix format for each physics (e.g. symmetric block size 3)
- matrix-free anywhere
- multiple levels of nesting

Multi-physics coupling in PETSc



- package each “physics” independently
- solve single-physics and coupled problems
- semi-implicit and fully implicit
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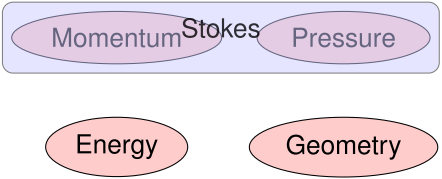

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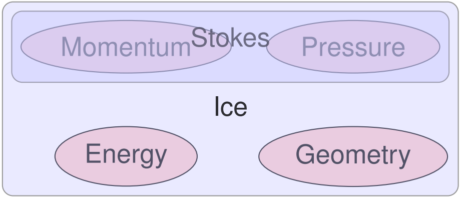

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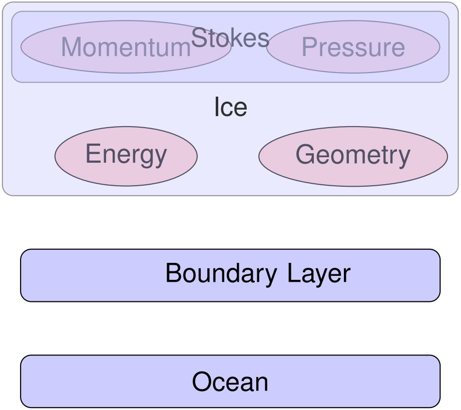

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- matrix-free anywhere
- multiple levels of nesting

Splitting for Multiphysics

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} f \\ g \end{bmatrix}$$

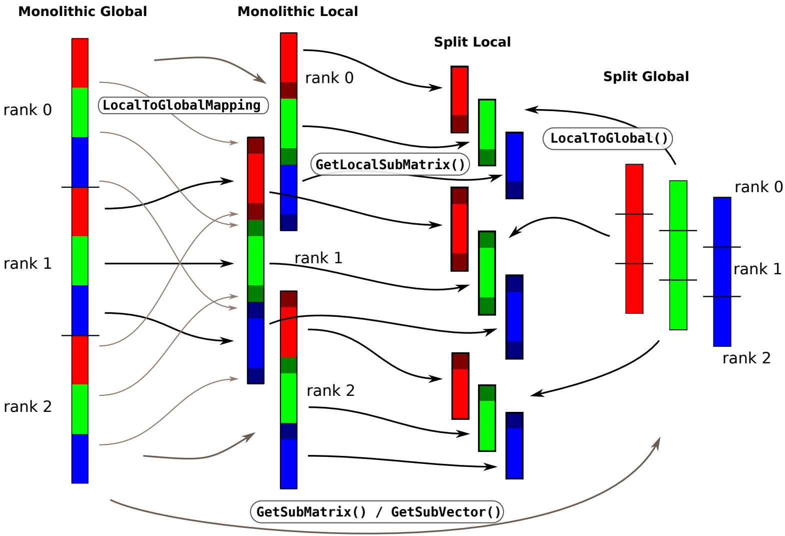
- Relaxation: `-pc_fieldsplit_type [additive,multiplicative,symmetric_multiplicative]`

$$\begin{bmatrix} A & \\ & D \end{bmatrix}^{-1} \qquad \begin{bmatrix} A & \\ C & D \end{bmatrix}^{-1} \qquad \begin{bmatrix} A & \\ & 1 \end{bmatrix}^{-1} \left(1 - \begin{bmatrix} A & B \\ & 1 \end{bmatrix} \begin{bmatrix} A & \\ C & D \end{bmatrix}^{-1} \right)$$

  - Gauss-Seidel inspired, works when fields are loosely coupled
- Factorization: `-pc_fieldsplit_type schur`

$$\begin{bmatrix} A & B \\ & S \end{bmatrix}^{-1} \begin{bmatrix} 1 & \\ CA^{-1} & 1 \end{bmatrix}^{-1}, \qquad S = D - CA^{-1}B$$

  - robust (exact factorization), can often drop lower block
  - how to precondition S which is usually dense?
    - interpret as differential operators, use approximate commutators



Work in Split Local space, matrix data structures reside in any space.

Multiphysics Assembly Code: Jacobians

```
FormJacobian_Coupled(SNES snes,Vec X,Mat J,Mat B,...) {
  // Access components as for residuals
  MatGetLocalSubMatrix(B,is[0],is[0],&Buu);
  MatGetLocalSubMatrix(B,is[0],is[1],&Buk);
  MatGetLocalSubMatrix(B,is[1],is[0],&Bku);
  MatGetLocalSubMatrix(B,is[1],is[1],&Bkk);
  FormJacobianLocal_U(user,&infou,u,k,Buu);         // single physics
  FormJacobianLocal_UK(user,&infou,&infok,u,k,Buk); // coupling
  FormJacobianLocal_KU(user,&infou,&infok,u,k,Bku); // coupling
  FormJacobianLocal_K(user,&infok,u,k,Bkk);         // single physics
  MatRestoreLocalSubMatrix(B,is[0],is[0],&Buu);
  // More restores
```

- Assembly code is independent of matrix format
- Single-physics code is used unmodified for coupled problem
- No-copy fieldsplit:

  ```
  -pack_dm_mat_type nest -pc_type fieldsplit
  ```

- Coupled direct solve:

  ```
  -pack_dm_mat_type aij -pc_type lu -pc_factor_mat_solver_package mumps
  ```

Outline

Role of implicit solvers

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Stokes problems

Performance considerations

Stokes example

The common block preconditioners for Stokes require only options:

The Stokes System

$$\begin{pmatrix} A & B \\ B^T & 0 \end{pmatrix}$$

Stokes example

The common block preconditioners for Stokes require only options:

```
-pc_type fieldsplit
-pc_fieldsplit_type additive

-fieldsplit_0_pc_type ml
-fieldsplit_0_ksp_type preonly

-fieldsplit_1_pc_type jacobi
-fieldsplit_1_ksp_type preonly
```

PC

$$\begin{pmatrix} \hat{A} & 0 \\ 0 & I \end{pmatrix}$$

Cohouet and Chabard, *Some fast 3D finite element solvers for the generalized Stokes problem*, 1988.

Stokes example

The common block preconditioners for Stokes require only options:

```
-pc_type fieldsplit
-pc_fieldsplit_type
multiplicative
-fieldsplit_0_pc_type hypre
-fieldsplit_0_ksp_type preonly
-fieldsplit_1_pc_type jacobi
-fieldsplit_1_ksp_type preonly
```

PC

$$\begin{pmatrix} \hat{A} & B \\ 0 & I \end{pmatrix}$$

Elman, *Multigrid and Krylov subspace methods for the discrete Stokes equations*, 1994.

Stokes example

The common block preconditioners for Stokes require only options:

```
-pc_type fieldsplit
-pc_fieldsplit_type schur

-fieldsplit_0_pc_type gamg
-fieldsplit_0_ksp_type preonly

-fieldsplit_1_pc_type none
-fieldsplit_1_ksp_type minres
 -pc_fieldsplit_schur_factorization_type diag
```

PC

$$\begin{pmatrix} \hat{A} & 0 \\ 0 & -\hat{S} \end{pmatrix}$$

May and Moresi, *Preconditioned iterative methods for Stokes flow problems arising in computational geodynamics*, 2008.

Olshanskii, Peters, and Reusken, *Uniform preconditioners for a parameter dependent saddle point problem with application to generalized Stokes interface equations*, 2006.

Stokes example

The common block preconditioners for Stokes require only options:

```
-pc_type fieldsplit
-pc_fieldsplit_type schur

-fieldsplit_0_pc_type gamg
-fieldsplit_0_ksp_type preonly

-fieldsplit_1_pc_type none
-fieldsplit_1_ksp_type minres
 -pc_fieldsplit_schur_factorization_type lower
```

PC

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

May and Moresi, *Preconditioned iterative methods for Stokes flow problems arising in computational geodynamics*, 2008.

Stokes example

The common block preconditioners for Stokes require only options:

```
-pc_type fieldsplit
-pc_fieldsplit_type schur

-fieldsplit_0_pc_type gamg
-fieldsplit_0_ksp_type preonly

-fieldsplit_1_pc_type none
-fieldsplit_1_ksp_type minres
 -pc_fieldsplit_schur_factorization_type upper
```

PC

$$\begin{pmatrix} \hat{A} & B \\ 0 & \hat{S} \end{pmatrix}$$

May and Moresi, *Preconditioned iterative methods for Stokes flow problems arising in computational geodynamics*, 2008.

Stokes example

The common block preconditioners for Stokes require only options:

```
-pc_type fieldsplit
-pc_fieldsplit_type schur

-fieldsplit_0_pc_type gamg
-fieldsplit_0_ksp_type preonly

-fieldsplit_1_pc_type lsc
-fieldsplit_1_ksp_type minres
 -pc_fieldsplit_schur_factorization_type upper
```

PC

$$\begin{pmatrix} \hat{A} & B \\ 0 & \hat{S}_{\mathrm{LSC}} \end{pmatrix}$$

May and Moresi, *Preconditioned iterative methods for Stokes flow problems arising in computational geodynamics*, 2008.

Kay, Loghin and Wathen, *A Preconditioner for the Steady-State N-S Equations*, 2002.
Elman, Howle, Shadid, Shuttleworth, and Tuminaro, *Block preconditioners based on approximate commutators*, 2006.

Stokes example

The common block preconditioners for Stokes require only options:

```
-pc_type fieldsplit
-pc_fieldsplit_type schur
 -pc_fieldsplit_schur_factorization_type full
```

PC

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

Stokes example

All block preconditioners can be *embedded* in MG using only options:

```
-pc_type mg -pc_mg_levels 5 -pc_mg_galerkin
```

System on each Coarse Level

$$R \begin{pmatrix} A & B \\ B^T & 0 \end{pmatrix} P$$

Stokes example

All block preconditioners can be *embedded* in MG using only options:

```
-pc_type mg -pc_mg_levels 5 -pc_mg_galerkin
-mg_levels_pc_type fieldsplit
-mg_levels_pc_fieldsplit_type additive

-mg_levels_fieldsplit_0_pc_type sor
-mg_levels_fieldsplit_0_ksp_type preonly

-mg_levels_fieldsplit_1_pc_type jacobi
-mg_levels_fieldsplit_1_ksp_type preonly
```

Smoother

PC

$$\begin{pmatrix} \hat{A} & 0 \\ 0 & I \end{pmatrix}$$

Stokes example

All block preconditioners can be *embedded* in MG using only options:

```
-pc_type mg -pc_mg_levels 5 -pc_mg_galerkin
-mg_levels_pc_type fieldsplit
-mg_levels_pc_fieldsplit_type
multiplicative

-mg_levels_fieldsplit_0_pc_type sor
-mg_levels_fieldsplit_0_ksp_type preonly

-mg_levels_fieldsplit_1_pc_type jacobi
-mg_levels_fieldsplit_1_ksp_type preonly
```

Smoother

PC

$$\begin{pmatrix} \hat{A} & B \\ 0 & I \end{pmatrix}$$

Stokes example

All block preconditioners can be *embedded* in MG using only options:

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-pc_type mg -pc_mg_levels 5 -pc_mg_galerkin
-mg_levels_pc_type fieldsplit
-mg_levels_pc_fieldsplit_type schur

-mg_levels_fieldsplit_0_pc_type sor
-mg_levels_fieldsplit_0_ksp_type preonly

-mg_levels_fieldsplit_1_pc_type none
-mg_levels_fieldsplit_1_ksp_type minres
```

Smoother

PC

$$\begin{pmatrix} \hat{A} & 0 \\ 0 & -\hat{S} \end{pmatrix}$$

```
-mg_levels_pc_fieldsplit_schur_factorization_type diag
```

Stokes example

All block preconditioners can be *embedded* in MG using only options:

```
-pc_type mg -pc_mg_levels 5 -pc_mg_galerkin
-mg_levels_pc_type fieldsplit
-mg_levels_pc_fieldsplit_type schur

-mg_levels_fieldsplit_0_pc_type sor
-mg_levels_fieldsplit_0_ksp_type preonly

-mg_levels_fieldsplit_1_pc_type none
-mg_levels_fieldsplit_1_ksp_type minres
```

Smoother

PC

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

```
-mg_levels_pc_fieldsplit_schur_factorization_type lower
```

Stokes example

All block preconditioners can be *embedded* in MG using only options:

```
-pc_type mg -pc_mg_levels 5 -pc_mg_galerkin
-mg_levels_pc_type fieldsplit
-mg_levels_pc_fieldsplit_type schur

-mg_levels_fieldsplit_0_pc_type sor
-mg_levels_fieldsplit_0_ksp_type preonly

-mg_levels_fieldsplit_1_pc_type none
-mg_levels_fieldsplit_1_ksp_type minres
```

Smoother

PC

$$\begin{pmatrix} \hat{A} & B \\ 0 & \hat{S} \end{pmatrix}$$

```
-mg_levels_pc_fieldsplit_schur_factorization_type upper
```

Stokes example

All block preconditioners can be *embedded* in MG using only options:

```
-pc_type mg -pc_mg_levels 5 -pc_mg_galerkin
-mg_levels_pc_type fieldsplit
-mg_levels_pc_fieldsplit_type schur

-mg_levels_fieldsplit_0_pc_type sor
-mg_levels_fieldsplit_0_ksp_type preonly

-mg_levels_fieldsplit_1_pc_type lsc
-mg_levels_fieldsplit_1_ksp_type minres
```

Smoother

PC

$$\begin{pmatrix} \hat{A} & B \\ 0 & \hat{S}_{\mathrm{LSC}} \end{pmatrix}$$

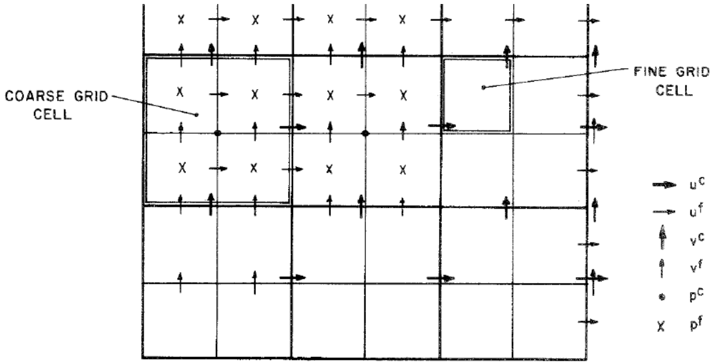
```
-mg_levels_pc_fieldsplit_schur_factorization_type upper
```

Smoothing for saddle point systems

$$\begin{pmatrix} A & B^T \\ B & 0 \end{pmatrix} \begin{pmatrix} u \\ p \end{pmatrix} = \begin{pmatrix} b \\ 0 \end{pmatrix}$$

- pressure has no self-coupling
- pressure error modes not spectrally separated
- approaches
  - block smoothers (Vanka)
  - amplify fine-grid modes (distributive relaxation)
  - splitting with approximate Schur complement

Vanka block smoothers



- solve pressure-centered cell problems
  (better for discontinuous pressure)
- robust convergence factor ~ 0.3 *if* coarse grids are accurate
- 1D energy minimizing interpolants easy and effective
- can use assembled sparse matrices, but more efficient without

Changing Associativity: Distributive Smoothing

$$PAx = Pb \qquad\qquad APy = b, \quad x = Py$$

- Normal Preconditioning: make PA or AP well-conditioned
- Alternative: amplify high-frequency modes
  - Multigrid smoothers only need to relax high-frequency modes
  - Easier to do when spectrally separated: h-ellipticity
    - pointwise smoothers (Gauss-Seidel) and polynomial/multistage methods
  - Mechanics: form the product PA or AP and apply “normal” method
  - Example (Stokes)

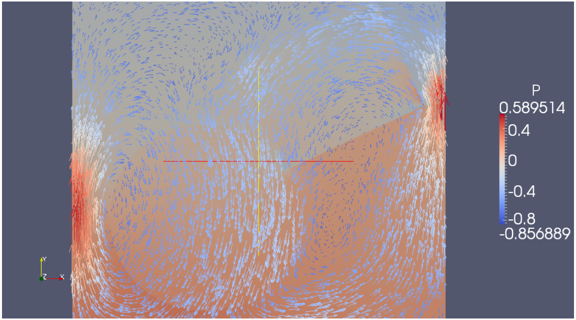
$$A \sim \begin{pmatrix} -\nabla^2 & \nabla \\ \nabla\cdot & 0 \end{pmatrix} \quad P \sim \begin{pmatrix} 1 & -\nabla \\ 0 & -\nabla^2 \end{pmatrix} \quad AP \sim \begin{pmatrix} -\nabla^2 & \text{“0”} \\ \nabla\cdot & -\nabla^2 \end{pmatrix}$$

- Convergence factor 0.32 (as good as Laplace) for smooth problems

Coupled MG for Stokes, split smoothers

$$J = \begin{pmatrix} A & B^T \\ B & C \end{pmatrix}$$

$$P_{\text{smooth}} = \begin{pmatrix} A_{\text{SOR}} & 0 \\ B & M \end{pmatrix}$$



```
-pc_type mg -pc_mg_levels 5 -pc_mg_galerkin
-mg_levels_pc_type fieldsplit
-mg_levels_pc_fieldsplit_block_size 3
-mg_levels_pc_fieldsplit_0_fields 0,1
-mg_levels_pc_fieldsplit_1_fields 2
-mg_levels_fieldsplit_0_pc_type sor
```

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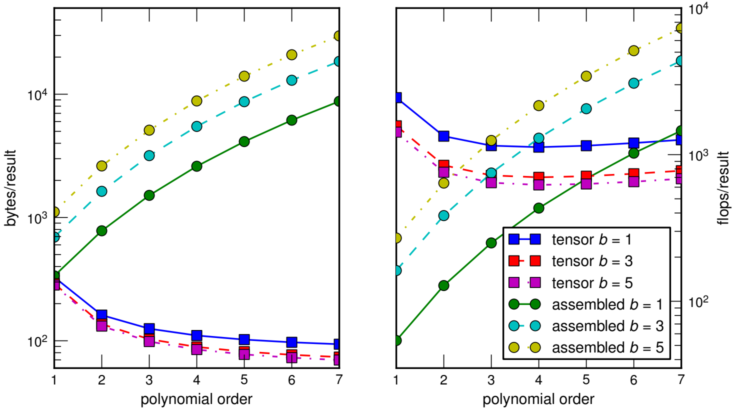
Profiling basics

- Get the math right
  - Choose an algorithm that gives robust iteration counts and really converges
- Look at where the time is spent
  - Run with `-log_summary` and look at events
  - `VecNorm`, `VecDot` measures latency
  - `MatMult` measures neighbor exchange and memory bandwidth
  - `PCSetUp` factorization, aggregation, matrix-matrix products, ...
  - `PCApply` V-cycles, triangular solves, ...
  - `KSPSolve` linear solve
  - `SNESFunctionEval` residual evaluation (user code)
  - `SNESJacobianEval` matrix assembly (user code)

Performance of assembled versus unassembled



- High order Jacobian stored unassembled using coefficients at quadrature points, can use local AD
- Choose approximation order at run-time, independent for each field
- Precondition high order using assembled lowest order method
- Implementation $> 70\%$ of FPU peak, SpMV bandwidth wall $< 4\%$

Hardware Arithmetic Intensity

Operation	Arithmetic Intensity (flops/B)
Sparse matrix-vector product	1/6
Dense matrix-vector product	1/4
Unassembled matrix-vector product	≈ 8
High-order residual evaluation	> 5

Processor	BW (GB/s)	Peak (GF/s)	Balanced AI (F/B)
E5-2670 8-core	35	166	4.7
Magny Cours 16-core	49	281	5.7
Blue Gene/Q node	43	205	4.8
Tesla M2090	120	665	5.5
Kepler K20Xm	160	1310	8.2
Xeon Phi	150	1248	8.3

Quasi-Newton revisited: ameliorating setup costs

- Newton-Krylov with analytic Jacobian

Lag	FunctionEval	JacobianEval	PCSetUp	PCApply
1 bt	12	8	8	31
1 cp	31	6	6	24
2 bt		— diverged —		
2 cp	41	4	4	35
3 cp	50	4	4	44

pseudo-plastic rheology

```
-snes_type qn
-snes_qn_scale_type
jacobian
```

- Jacobian-free Newton-Krylov with lagged preconditioner

Lag	FunctionEval	JacobianEval	PCSetUp	PCApply
1 bt	23	11	11	31
2 bt	48	4	4	36
3 bt	64	3	3	52
4 bt	87	3	3	75

- Limited-memory Quasi-Newton/BFGS with lagged solve for H_0

Restart	H_0	FunctionEval	JacobianEval	PCSetUp	PCApply
1 cp	10^{-5}	17	4	4	35
1 cp	preonly	21	5	5	10
3 cp	10^{-5}	21	3	3	43
3 cp	preonly	23	3	3	11
6 cp	10^{-5}	29	2	2	60
6 cp	preonly	29	2	2	14

Network latency

`MPI_Allreduce` is slow at large scale

- True on many machines, not on Blue Gene ($\sim 100\,\mu s$)
- Bottleneck for Krylov methods
- Pipelining allows overlap, uses `MPI_Iallreduce` from MPI-3
  `-ksp_type pgmres`, `-ksp_type pipecg`, `-ksp_type pipecr`

Coarse grid solves for multigrid

- Need to restrict active processor set
- Coarse levels have similar cost to finer levels
- Aggressive coarsening more important than tight iteration count
- Additive multigrid possible, but less robust

Outlook

- PETSc `http://mcs.anl.gov/petsc`
- Trilinos `http://trilinos.sandia.gov`
- Think about solution algorithms when designing discretization
- Learn how to evaluate solver quality and experiment
- Expect the best method to change with problem instance and machine

Contact

- `petsc-maint@mcs.anl.gov`
- `http://lists.mcs.anl.gov/pipermail/petsc-users/`