Commuting Block Preconditioned Splitting with Multigrid within the Same Code Base

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Multiphysics problems

Examples

- Saddle-point problems (e.g. incompressibility, contact)
- Stiff waves (e.g. low-Mach combustion)
- Mixed type (e.g. radiation hydrodynamics, ALE free-surface flows)
- Multi-domain problems (e.g. fluid-structure interaction)
- Full space PDE-constrained optimization

Software/algorithmic considerations

- Separate groups develop different “physics” components
- Do not know a priori which methods will have good algorithmic properties
- Achieving high throughput is more complicated
- Multiple time and/or spatial scales
  - Splitting methods are delicate, often not in asymptotic regime
  - Strongest nonlinearities usually non-stiff: prefer explicit for TVD limiters/shocks

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

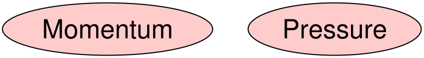
Split

- 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



- 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

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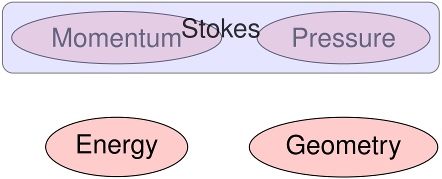

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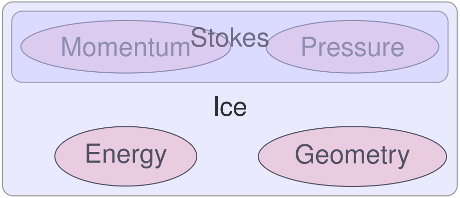

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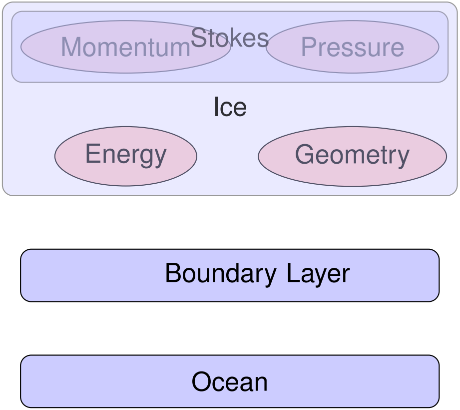

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Splitting for Multiphysics

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

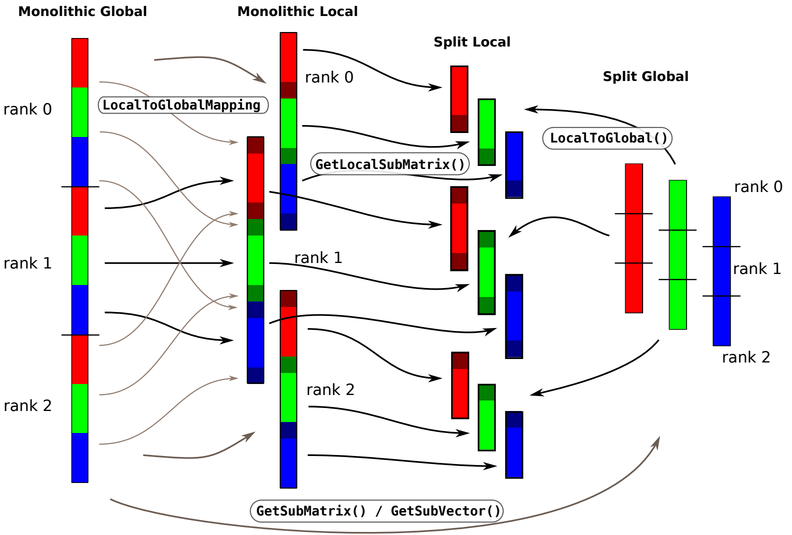
- Relaxation: `-pc_fieldsplit_type [additive,multiplicative,symmetric_multiplicative]`

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

  - 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: Residuals

```
FormFunction_Coupled(SNES snes,Vec X,Vec F,void *ctx) {
  struct UserCtx *user = ctx;
  // ...
  SNESGetDM(snes,&pack);
  DMCompositeGetEntries(pack,&dau,&dak);
  DMCompositeScatter(pack,X,Uloc,Kloc);
  DMDAVecGetArray(dau,Uloc,&u);
  DMDAVecGetArray(dak,Kloc,&k);
  DMCompositeGetAccess(pack,F,&Fu,&Fk);
  DMDAVecGetArray(dau,Fu,&fu);
  DMDAVecGetArray(dak,Fk,&fk);
  FormFunctionLocal_U(user,&infou,u,k,fu); // u residual with k given
  FormFunctionLocal_K(user,&infok,u,k,fk); // k residual with u given
  DMDAVecRestoreArray(dau,Fu,&fu);
  // More restores
```

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`

`MatGetLocalSubMatrix(Mat A,IS rows,IS cols,Mat *B);`

- Primarily for assembly
  - `B` is not guaranteed to implement `MatMult`
  - The communicator for `B` is not specified, only safe to use non-collective ops (unless you check)
- `IS` represents an index set, includes a block size and communicator
- `MatSetValuesBlockedLocal()` is implemented
- MatNest returns nested submatrix, no-copy
- No-copy for Neumann-Neumann formats (unassembled across procs, e.g. BDDC, FETI-DP)
- Most other matrices return a lightweight proxy `Mat`
  - `COMM_SELF`
  - Values not copied, does not implement `MatMult`
  - Translates indices to the language of the parent matrix
  - Multiple levels of nesting are flattened

Monolithic nonlinear solvers

Coupled nonlinear multigrid accelerated by NGMRES with multi-stage smoothers

```
-lidvelocity 200 -grashof 1e4
-snes_grid_sequence 5 -snes_monitor -snes_view
-snes_type ngmres
-npc_snes_type fas
-npc_snes_max_it 1
-npc_fas_coarse_snes_type ls
-npc_fas_coarse_ksp_type preonly
-npc_fas_snes_type ms
-npc_fas_snes_max_it 1
-npc_fas_ksp_type preonly
-npc_fas_pc_type pbjacobi
-npc_fas_snes_ms_type vltp61
-npc_fas_snes_max_it 1
```

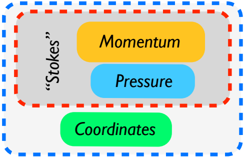
- Uses only residuals and point-block diagonal
- High arithmetic intensity and parallelism

Stokes + Implicit Free Surface

$$\left[\eta D_{ij}(\boldsymbol{u})\right]_{,j} - p_{,i} = f_i$$

$$u_{k,k} = 0$$

$$\hat{x}_i = \hat{x}_i^{t-\Delta t} + \Delta t \, u_i(\hat{x}_i)$$



COORDINATE RESIDUALS

$$F_x := -u_i + \frac{\hat{x}_i}{\Delta t} - \frac{\hat{x}_i^{t-\Delta t}}{\Delta t}$$

[We use a full Lagrangian update of our mesh, with no remeshing]

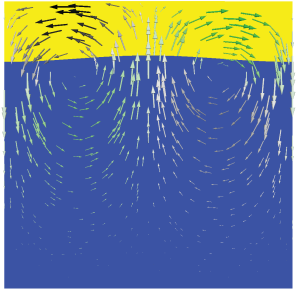
JACOBIAN

$$\mathcal{J}_{si} = \begin{bmatrix} A + \delta_{\hat{x}} A & B + \delta_{\hat{x}} B & J_{ac} \\ B^T + \delta_{\hat{x}} B^T & 0 & J_{bc} \\ -I & 0 & \frac{I}{\Delta t} \end{bmatrix}$$

Reuse stokes operators and saddle point preconditioners

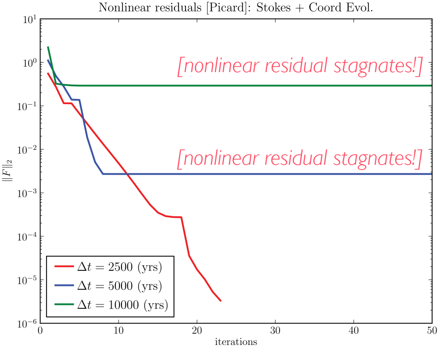
NESTED PRECONDITIONER

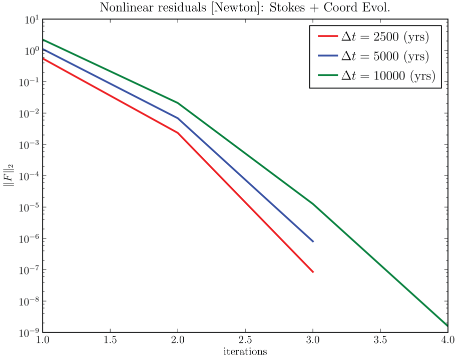
$$\mathcal{P}_{si} = \begin{bmatrix} \left[\ \mathcal{P}_s^l\ \right] & \\ \left[\ I\ \right] & \left[\ -\frac{I}{\Delta t}\ \right] \end{bmatrix} \qquad \mathcal{P}_s^l = \begin{bmatrix} A & 0 \\ B^T & -S \end{bmatrix}$$



"Drunken seaman", Rayleigh Taylor instability test case from Kaus et al., 2010. Dense, viscous material (yellow) overlying less dense, less viscous material (blue).

Stokes + Implicit Free Surface

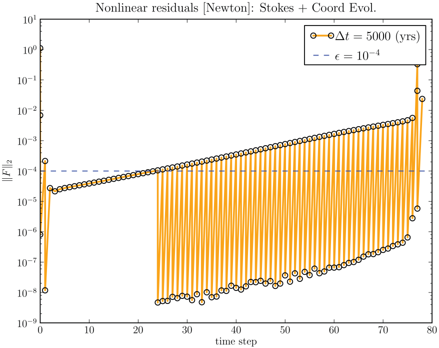


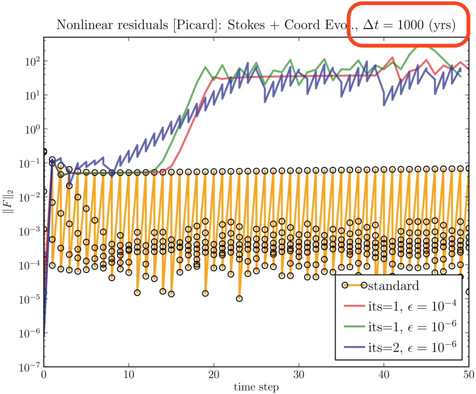


* Picard fails to converge for large time steps sizes.

* Newton is robust for a wide range of time step sizes.

Stokes + Implicit Free Surface





* The nonlinear residual *ALWAYS* increases from one step to the next.

* A nonlinear solve is required to control the error.

* An accurate nonlinear solve on the first time step, combined with 1 or 2 nonlinear iterations on subsequent steps still results in severe errors. *This is true even when dt is small.*

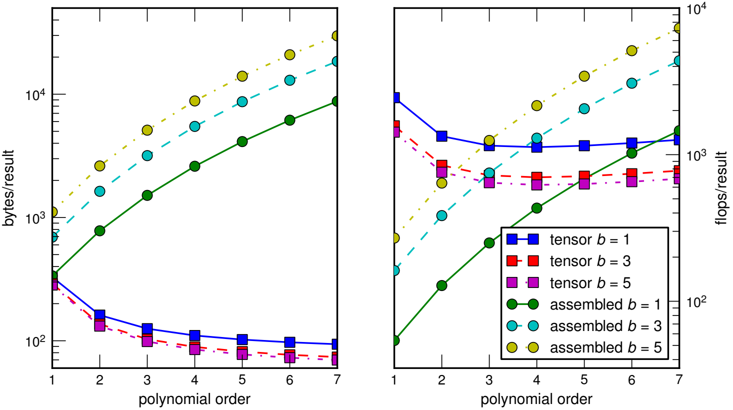
Conservative (non-Boussinesq) two-phase ice flow

Find momentum density ρu, pressure p, and total energy density E:

$$(\rho u)_t + \nabla\cdot(\rho u \otimes u - \eta D u_i + p1) - \rho g = 0$$
$$\rho_t + \nabla\cdot\rho u = 0$$
$$E_t + \nabla\cdot\big((E+p)u - k_T \nabla T - k_\omega \nabla \omega\big) - \eta D u_i : D u_i - \rho u \cdot g = 0$$

- Solve for density ρ, ice velocity u_i, temperature T, and melt fraction ω using constitutive relations.
  - Simplified constitutive relations can be solved explicitly.
  - Temperature, moisture, and strain-rate dependent rheology η.
  - High order FEM, typically Q_3 momentum & energy
- DAEs solved implicitly after semidiscretizing in space.
- Preconditioning using nested fieldsplit

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 $< 4\%$

Relative effect of the blocks

$$J = \begin{pmatrix} J_{uu} & J_{up} & J_{uE} \\ J_{pu} & 0 & 0 \\ J_{Eu} & J_{Ep} & J_{EE} \end{pmatrix}.$$

- J_{uu} Viscous/momentum terms, nearly symmetric, variable coefficionts, anisotropy from Newton.
- J_{up} Weak pressure gradient, viscosity dependence on pressure (small), gravitational contribution (pressure-induced density variation). Large, nearly balanced by gravitational forcing.
- J_{uE} Viscous dependence on energy, very nonlinear, not very large.
- J_{pu} Divergence (mass conservation), nearly equal to J_{up}^T.
- J_{Eu} Sensitivity of energy on momentum, mostly advective transport. Large in boundary layers with large thermal/moisture gradients.
- J_{Ep} Thermal/moisture diffusion due to pressure-melting, $u \cdot \nabla$.
- J_{EE} Advection-diffusion for energy, very nonlinear at small regularization. Advection-dominated except in boundary layers and stagnant ice, often balanced in vertical.

How much nesting?

$$P_1 = \begin{pmatrix} J_{uu} & J_{up} & J_{uE} \\ 0 & B_{pp} & 0 \\ 0 & 0 & J_{EE} \end{pmatrix}$$

- B_{pp} is a mass matrix in the pressure space weighted by inverse of kinematic viscosity.
- Elman, Mihajlović, Wathen, JCP 2011 for non-dimensional isoviscous Boussinesq.
- Works well for non-dimensional problems on the cube, not for realistic parameters.

$$P = \begin{bmatrix} \begin{pmatrix} J_{uu} & J_{up} \\ J_{pu} & 0 \end{pmatrix} & \\ \begin{pmatrix} J_{Eu} & J_{Ep} \end{pmatrix} & J_{EE} \end{bmatrix}$$

- Inexact inner solve using upper-triangular with B_{pp} for Schur.
- Another level of nesting.
- GCR tolerant of inexact inner solves.
- Outer converges in 1 or 2 iterations.

- Low-order preconditioning full-accuracy unassembled high order operator.
- Build these on command line with PETSc `PCFieldSplit`.

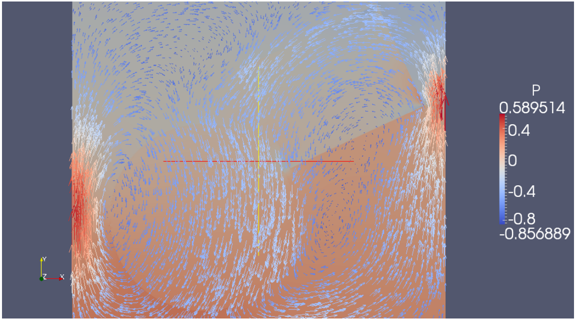
Example 3×3 problem with nested 2×2 split

```
-fieldsplit_s_ksp_type gcr
-fieldsplit_s_ksp_rtol 1e-1
-fieldsplit_s_ksp_monitor_vht
-fieldsplit_s_ksp_monitor_singular_value
-fieldsplit_s_pc_type fieldsplit
-fieldsplit_s_pc_fieldsplit_type schur
-fieldsplit_s_pc_fieldsplit_real_diagonal
-fieldsplit_s_pc_fieldsplit_schur_factorization_type lower
-fieldsplit_s_fieldsplit_u_ksp_type gmres
-fieldsplit_s_fieldsplit_u_ksp_max_it 10
-fieldsplit_s_fieldsplit_u_pc_type asm
-fieldsplit_s_fieldsplit_u_sub_pc_type ilu
-fieldsplit_s_fieldsplit_u_sub_pc_factor_levels 1
-fieldsplit_s_fieldsplit_u_ksp_converged_reason
-fieldsplit_s_fieldsplit_p_ksp_type preonly
-fieldsplit_s_fieldsplit_p_ksp_max_it 1
-fieldsplit_s_fieldsplit_p_pc_type jacobi
-fieldsplit_e_ksp_type gmres
-fieldsplit_e_ksp_converged_reason
-fieldsplit_e_pc_type asm
-fieldsplit_e_sub_pc_type ilu
-fieldsplit_e_sub_pc_factor_levels 2
```

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
```

Phase field models

State variables $u = (u_1, \ldots, u_N)^T$ are concentrations of different phases satisfying the inequality and sum constraints

$$u(x,t) \in G = \{v \in \mathbb{R}^d | v_i \geq 0, \sum_{i=1}^{N} v_i = 1\}, \quad \forall (x,t) \in Q.$$

Minimize free energy, reduced space active set method

$$J = \begin{pmatrix} A & 0 & 0 & -I \\ 0 & A & 0 & -I \\ 0 & 0 & A & -I \\ -I & -I & -I & 0 \end{pmatrix}, \qquad P = \begin{pmatrix} A & 0 & 0 & 0 \\ 0 & A & 0 & 0 \\ 0 & 0 & A & 0 \\ -I & -I & -I & S_{\text{LSC}} \end{pmatrix}$$

```
-ksp_type fgmres -pc_type fieldsplit
-pc_fieldsplit_detect_saddle_point
-pc_fieldsplit_type schur
-pc_fieldsplit_schur_precondition self
-fieldsplit_0_ksp_type preonly
-fieldsplit_0_pc_type hypre
-fieldsplit_1_ksp_type fgmres
-fieldsplit_1_pc_type lsc
```

Outlook

- Unintrusive composition of multigrid and block preconditioning
- We can build many preconditioners from the literature *on the command line*
- User code does not depend on matrix format, preconditioning method, nonlinear solution method, time integration method (implicit or IMEX), or size of coupled system (except for driver).

In development

- Distributive relaxation, Vanka smoothers
- Algebraic coarsening of “dual” variables
- Improving operator-dependent semi-geometric multigrid
- More automatic spectral analysis and smoother optimization
- Better interaction with IMEX time integration
  - Additive Runge-Kutta, Rosenbrock-W, linear multistep
  - Composability with FAS
  - Possible parallel-in-time approaches