Numerical Libraries and Frameworks (PETSc)

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ENES Workshop on Exascale Technologies, 2014-03-18

What can libraries offer?

- Code reuse
  - Porting/optimization to new architectures
  - . . . but only the part of the problem solved by the library
- Easy experimentation with different methods
  - via run-time options (PETSc)
  - “black box” solvers are not sustainable
  - preconditioners, linear and nonlinear accelerators, time integrators
- Diagnostic and debugging support
  - Convergence monitors, error estimators, adaptive controllers
  - Compatibility checks
  - Eigen-analysis
- Communication with algorithm developers
  - Precise language to describe methods
  - Performance diagnostics
- Flexible coupling algorithms: beyond “first-order” splitting

Library or Framework?

Library

- Libraries provide a toolbox
- No assumptions about usage
- Any selection of libraries should be usable in combination
- *Extensible* libraries enable user to implement/extend

Framework

- Rapid development within a problem class
- End-to-end solution provides guidance and auxiliary tools
- Opinionated
- Hard to use in combination with other Frameworks1

PETSc is a Library

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PETSc is a Library

Portable **Extensible** Toolkit for Scientific computing

Portable

- Runs *performantly* from laptop and iPhone to BG/Q and Titan
- Any compiler, any OS
- C, C++, Fortran 77 & 90+, Python, MATLAB
- Free to everyone: BSD-style license, open development

Philosophy: Everything has a plugin architecture

- Vectors, Matrices, Coloring/ordering/partitioning algorithms
- Preconditioners, Krylov accelerators, Nonlinear solvers, Time integrators
- Spatial discretizations/topology*
- Example: Third party supplies matrix format and associated preconditioner, distributes compiled shared library. Application user loads plugin at runtime, no source code in sight.

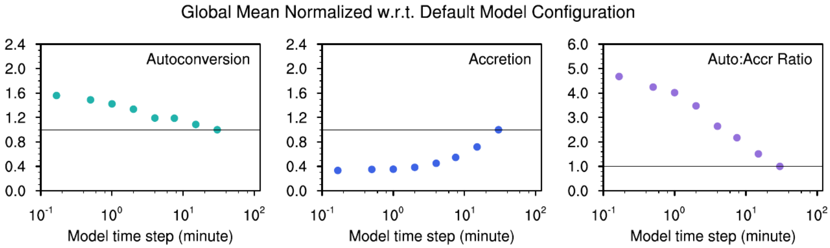
Portable Extensible Toolkit for **Scientific computing**

- Computational Scientists and Engineers
  - Structural mechanics, CFD, Geodynamics, Subsurface flow, Reactor engineering, Fusion
  - Research (many countries, many agencies) and industry (oil and gas, aerospace, ABAQUS)
- Algorithm Developers (iterative methods and preconditioning)
  - Example: Ghysels' pipelined Krylov methods
- Package Developers
  - SLEPc, TAO, Libmesh, MOOSE, FEniCS, Deal.II, etc
- Funding
  - Department of Energy (SciDAC, ASCR, collaborations)
  - National Science Foundation (CIG and others)
- Active development team with long-term commitment
- Hundreds of tutorial-style examples
- Hyperlinked manual, examples, and manual pages for all routines
- Lists: `petsc-users@mcs.anl.gov`, `petsc-dev@mcs.anl.gov`
- Support from `petsc-maint@mcs.anl.gov`

Solvers in climate

- "Pressure" solves for semi-implicit methods
  - Depends on separation between fastest wave and dynamics
- Time integration for atmospheric column physics
  - Currently swamped with splitting error
  - Stiff, positivity constraints, non-smoothness (freezing)
- Sea ice
  - Fast elastic wave speed ($v_p \approx 3\,\mathrm{km\,s^{-1}}$)
  - Damped EVP model not converged at 120 subcycles, nor at 1200 (Lemieux at al 2012)
- Land ice (Stokes and hydrostatic models with slippery bed)
  - PETSc: PISM (UAF, PIK), BISICLES (LBL, Chombo), ISSM (NASA)
- Improved stability for symplectic integration
- Accelerated spin-up (e.g., deep ocean)
  - Need to model unresolved-in-time processes

Impact of time step on autoconversion vs accretion partitioning (from Hui)



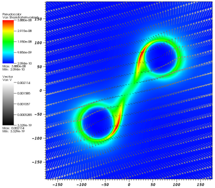
c/o Peter Caldwell (LLNL)

- Models calibrated for “efficient” time step
- No longer solving the PDEs we write down
- Expensive to recalibrate when discretization changes
- Calibration eats up a big chunk of the IPCC policy timeline

Sea Ice

$$(\rho h u)_t + \underbrace{\rho h f k \times u}_{\text{Coriolis}} - \underbrace{\tau}_{\text{water/air}} + \underbrace{\rho g h \nabla H_d}_{\text{surface gradient}} - \nabla \cdot (\underbrace{\rho h u \otimes u}_{\text{convection}} - \underbrace{\sigma}_{\text{viscoplastic}}) = 0$$

$$\sigma = 2\eta \dot{\varepsilon} + \left[(\zeta - \eta) \operatorname{tr} \dot{\varepsilon} - P/2 \right] 1$$



- mildly nonsymmetric due to Coriolis (quasi-diagonal) and convection (small compared to viscous stresses)
- Nonlinear multigrid is less synchronous

Method	Nonlinear its/stage	Linear its/stage	V-cycles
Newton-Krylov MG	6	30.44	30.44
FAS Newton/BJacobi/SOR	18.33	—	18.33

- Additive Runge-Kutta IMEX, error-based adaptivity, solver rtol 10^{-8}
- Preliminary tests to 4096 cores of BG/Q and 64 fine-grid elements/process, less than 0.1 seconds/time step.

IMEX time integration in PETSc

- Additive Runge-Kutta IMEX methods

$$G(t, x, \dot{x}) = F(t, x)$$
$$J_\alpha = \alpha G_{\dot{x}} + G_x$$

  - User provides:
    - `FormRHSFunction(ts,`t`,`x`,`F`,void *ctx);`
    - `FormIFunction(ts,`t`,`x`,`$\dot{x}$`,`G`,void *ctx);`
    - `FormIJacobian(ts,`t`,`x`,`$\dot{x}$`,`α`,`J`,`J_p`,mstr,void *ctx);`
  - Can have L-stable DIRK for stiff part G, SSP explicit part, etc.
  - Orders 2 through 5, embedded error estimates
  - Dense output, hot starts for Newton
  - More accurate methods if G is linear, also Rosenbrock-W
  - Can use preconditioner from classical “semi-implicit” methods
  - FAS nonlinear solves supported
  - Extensible adaptive controllers, can change order within a family
  - Easy to register new methods: `TSARKIMEXRegister()`
- Single step interface so user can have own time loop
- Same interface for Extrapolation IMEX, LMS IMEX (in development)

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

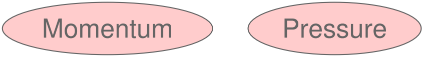
Split

- 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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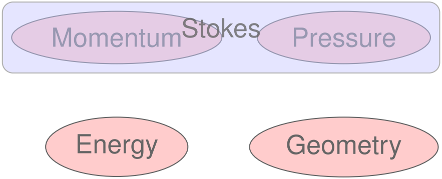

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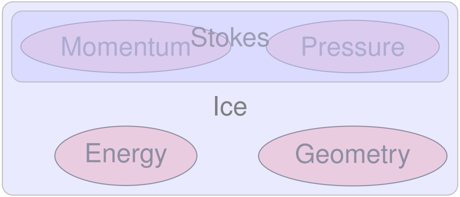

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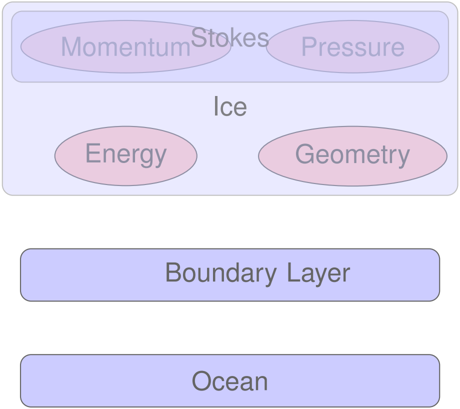

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Splitting for Multiphysics

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

- 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`

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

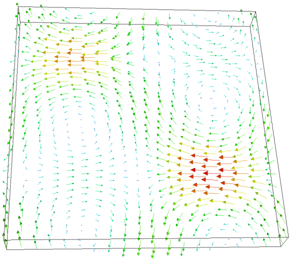
  - robust (exact factorization), can often drop lower block
  - how to precondition S which is usually dense?
    - interpret as differential operators, use approximate commutators
- "Composable Linear Solvers for Multiphysics" ISPDC 2012

Eigen-analysis plugin for solver design

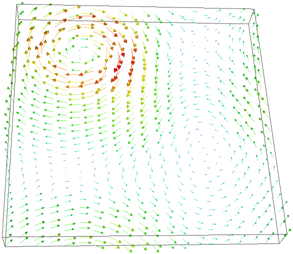
Hydrostatic ice flow (nonlinear rheology and slip conditions)

$$-\nabla\left[\eta\begin{pmatrix}4u_x+2v_y & u_y+v_x & u_z\\ u_y+v_x & 2u_x+4v_y & v_z\end{pmatrix}\right]+\rho g\nabla s=0, \tag{1}$$

- Many solvers converge easily with no-slip/frozen bed, more difficult for slippery bed (ISMIP HOM test C)
- Geometric MG is good: $\lambda \in [0.805, 1]$ (SISC 2013)



(a) $\lambda_0 = 0.0268$



(b) $\lambda_1 = 0.0409$

Implicit Runge-Kutta for advection

Table: Total number of iterations (communications or accesses of J) to solve linear advection to $t = 1$ on a 1024-point grid using point-block Jacobi preconditioning of implicit Runge-Kutta matrix. The relative algebraic solver tolerance is 10^{-8}.

Family	Stages	Order	Iterations
Crank-Nicolson/Gauss	1	2	3627
Gauss	2	4	2560
Gauss	4	8	1735
Gauss	8	16	1442

- Naive centered-difference discretization

A case for run-time configuration

- Simple build process
- Complete test suite without recompilation
- Cleaner provenance
  - Only need run-time configuration
  - No recompiles, only one binary to keep track of
  - Consistency checks in one place
- Simplified analysis/uncertainty quantification
  - More algorithms accessible
- More automated calibration
- Interface granularity is key to performance

Outlook

- PETSc: flexible, extensible, unintrusive
  - `http://mcs.anl.gov/petsc`
- Verification (converging the equations) encourages mathematicians
- Climate model components *should* become more library-like
  - Remove assumptions about environment
  - Improved modularity
  - Interfaces for configuration/calibration
  - Remove global variables (Fortran module variables)
- Tools need to make hard problems possible
  - Already many tools to make easy problems elegant
  - Ease of extending (versus DSLs/compilers)
- Strong-scaling necessity: ruthlessly shorten critical path
  - $2\times$ increase in resolution requires at least $2\times$ more steps
  - At fixed turn-around time, need twice as many steps/second
  - Algorithmic optimality is crucial