The Portable Extensible Toolkit for Scientific computing

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ATPESC 2013-08-02

Thanks to Jed Brown and Matt Knepley for the slides

Outline

1. Introduction
2. Objects - Building Blocks of the Code
3. Options Database - Controling the Code
4. Core PETSc Components and Algorithms Primer
   - Time integration
   - Nonlinear solvers: SNES
   - Linear Algebra background/theory
   - Structured grid distribution: DMDA
   - Profiling
   - Matrix Redux

Follow Up; Getting Help

- http://www.mcs.anl.gov/petsc
- Public questions: `petsc-users@mcs.anl.gov`, archived
- Private questions: `petsc-maint@mcs.anl.gov`, not archived
- Today, speak with
  - me
  - Satish Balay
  - Jed Brown
  - Lois McInnes

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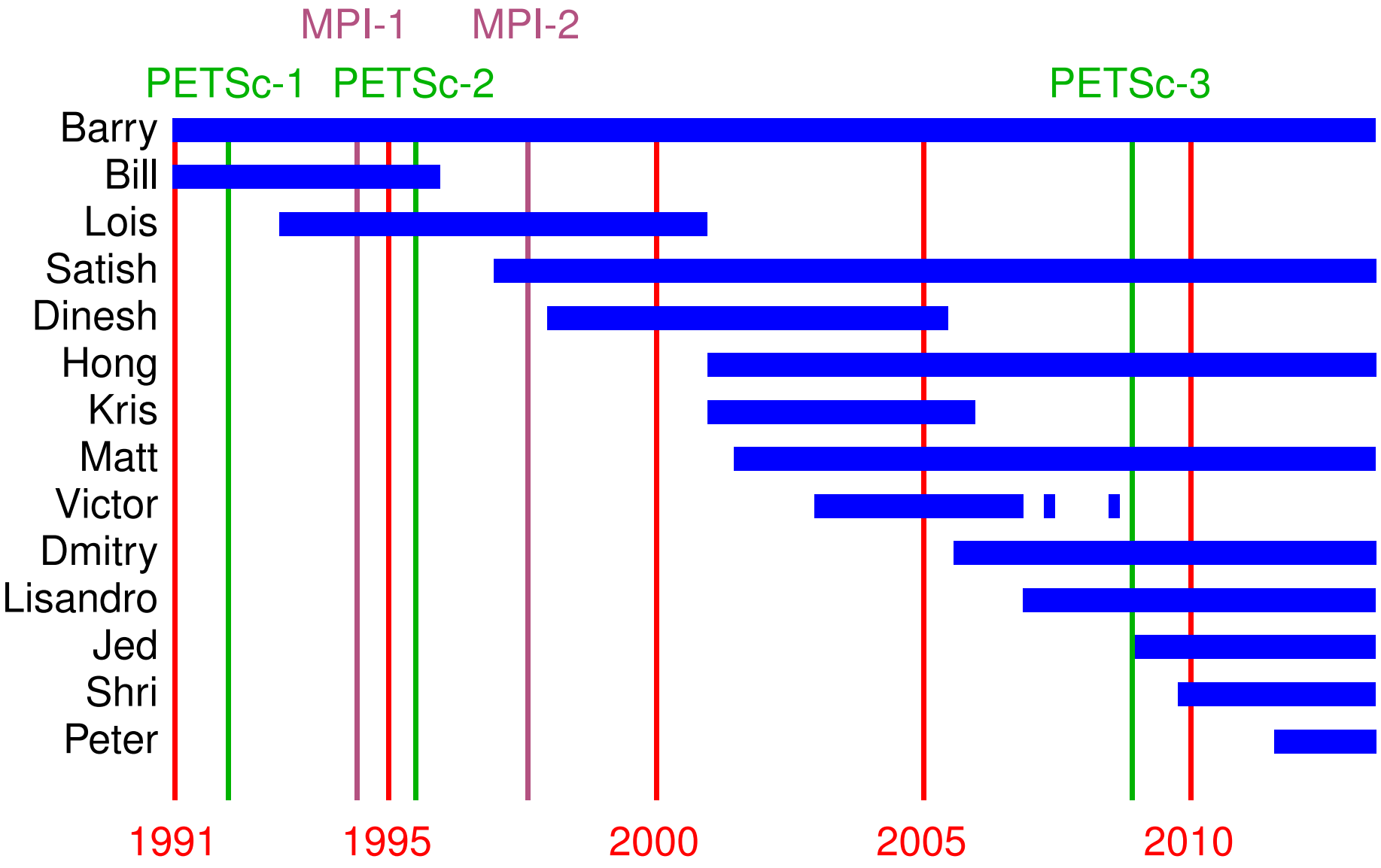
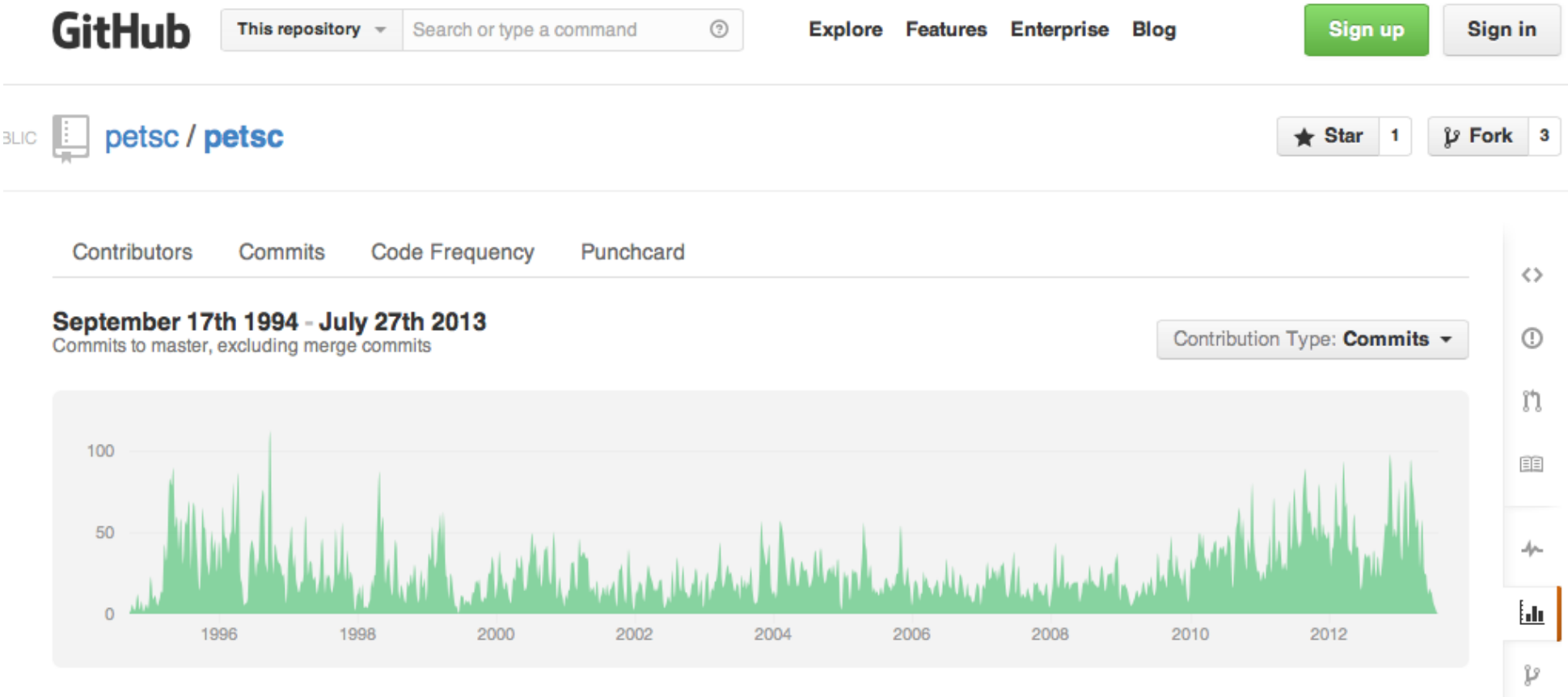

MPI-1
MPI-2
PETSc-1
PETSc-2
PETSc-3
Barry
Bill
Lois
Satish
Dinesh
Hong
Kris
Matt
Victor
Dmitry
Lisandro
Jed
Shri
Peter
1991
1995
2000
2005
2010

Commits to the PETSc Repository



Portable Extensible Toolkit for Scientific computing

- Architecture
  - tightly coupled (e.g. XT5, BG/P, Earth Simulator)
  - loosely coupled such as network of workstations
  - GPU clusters (many vector and sparse matrix kernels)
- Operating systems (Linux, Mac, Windows, BSD, proprietary Unix)
- Any compiler
- Real/complex, single/double/quad precision, 32/64-bit int
- Usable from C, C++, Fortran 77/90, Python, and MATLAB
- Free to everyone (BSD-style license), open development
- 500B unknowns, 75% weak scalability on Jaguar (225k cores) and Jugene (295k cores)
- Same code runs performantly on a laptop
- ~~No~~ iPhone support

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Portable **Extensible** Toolkit for Scientific computing

Philosophy: Everything has a plugin architecture

- Vectors, Matrices, Coloring/ordering/partitioning algorithms
- Preconditioners, Krylov accelerators
- Nonlinear solvers, Time integrators
- Spatial discretizations/topology*

Example

Vendor 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

Algorithms, (parallel) debugging aids, low-overhead profiling

Composability

Try new algorithms by choosing from product space and composing existing algorithms (multilevel, domain decomposition, splitting).

Experimentation

- It is not possible to pick the solver a priori.
  What will deliver best/competitive performance for a given physics, discretization, architecture, and problem size?
- PETSc's response: expose an algebra of composition so new solvers can be created at runtime.
- Important to keep solvers decoupled from physics and discretization because we also experiment with those.

Portable Extensible Toolkit for **Scientific computing**

- Computational Scientists
  - PyLith (CIG), Underworld (Monash), Magma Dynamics (LDEO, Columbia), PFLOTRAN (DOE), SHARP/UNIC (DOE)
- Algorithm Developers (iterative methods and preconditioning)
- Package Developers
  - SLEPc, TAO, Deal.II, Libmesh, FEniCS, PETSc-FEM, MagPar, OOFEM, FreeCFD, OpenFVM
- Funding
  - Department of Energy
    - SciDAC, ASCR ISICLES, MICS Program, INL Reactor Program
  - National Science Foundation
    - CIG, CISE, Multidisciplinary Challenge Program
- Hundreds of tutorial-style examples
- Hyperlinked manual, examples, and manual pages for all routines
- Support from `petsc-maint@mcs.anl.gov`

The Role of PETSc

Developing parallel, nontrivial PDE solvers that deliver high performance is still difficult and requires months (or even years) of concentrated effort.

PETSc is a toolkit that can ease these difficulties and reduce the development time, but it is not a black-box PDE solver, nor a silver bullet.

— Barry Smith

Better To Use than PETSc

Use the package with the highest level of abstraction that uses PETSc

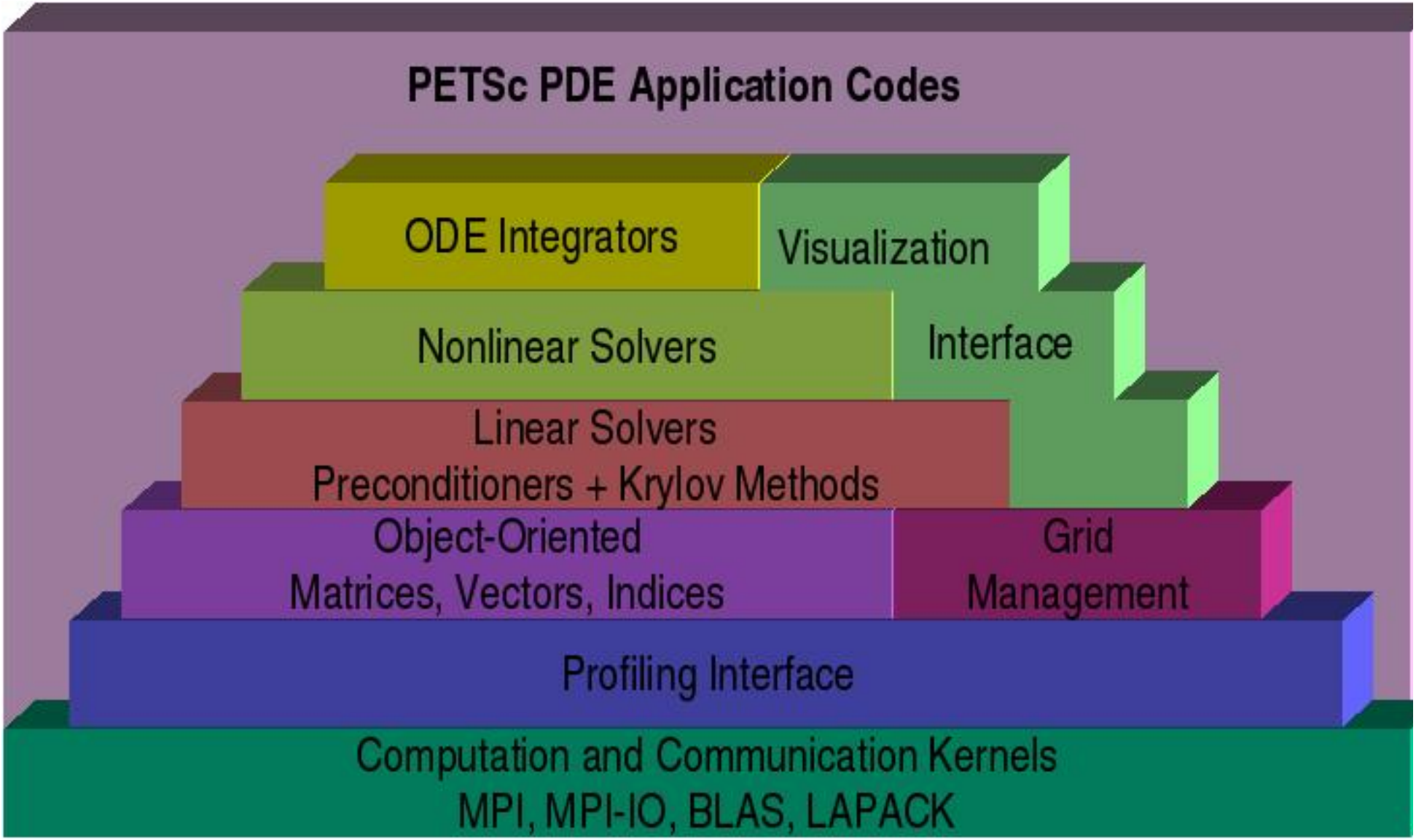
- Eigenvalues - SLEPc,
- Optimizationation (with PDE constraints) - TAO
- Finite Elements - Deal.II, Libmesh, FEniCS, PETSc-FEM, OOFEM,
- Finite Elements and Multiphysics - MOOSE
- Finite Volumes - FreeCFD, OpenFVM
- Micromagnetics - MagPar

Advice from Bill Gropp

You want to think about how you decompose your data structures, how you think about them globally. [...] If you were building a house, you'd start with a set of blueprints that give you a picture of what the whole house looks like. You wouldn't start with a bunch of tiles and say. "Well I'll put this tile down on the ground, and then I'll find a tile to go next to it." But all too many people try to build their parallel programs by creating the smallest possible tiles and then trying to have the structure of their code emerge from the chaos of all these little pieces. You have to have an organizing principle if you're going to survive making your code parallel.

(`http://www.rce-cast.com/Podcast/rce-28-mpich2.html`)

PETSc Structure



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MPI communicators

- Opaque object, defines process group and synchronization channel
- PETSc objects need an `MPI_Comm` in their constructor
  - `PETSC_COMM_SELF` for serial objects
  - `PETSC_COMM_WORLD` common, but not required
- Can split communicators, spawn processes on new communicators, etc
- Operations are one of
  - Not Collective: `VecGetLocalSize(), MatSetValues()`
  - Logically Collective: `KSPSetType(), PCMGSetCycleType()`
    - checked when running in debug mode
  - Neighbor-wise Collective: `VecScatterBegin(), MatMult()`
    - Point-to-point communication between two processes
    - Neighbor collectives in upcoming MPI-3
  - Collective: `VecNorm(), MatAssemblyBegin(), KSPCreate()`
    - Global communication, synchronous
    - Non-blocking collectives in upcoming MPI-3
- Deadlock if some process doesn't participate (e.g. wrong order)

Objects

```
Mat A;
PetscInt m,n,M,N;
MatCreate(comm,&A);
MatSetSizes(A,m,n,M,N);        /* or PETSC_DECIDE */
MatSetOptionsPrefix(A,"foo_");
MatSetFromOptions(A);
/* Use A */
MatView(A,PETSC_VIEWER_DRAW_WORLD);
MatDestroy(A);
```

- `Mat` is an opaque object (pointer to incomplete type)
  - Assignment, comparison, etc, are cheap
- What's up with this "Options" stuff?
  - Allows the type to be determined at runtime: `-foo_mat_type sbaij`
  - Inversion of Control similar to "service locator", related to "dependency injection"
  - Other options (performance and semantics) can be changed at runtime under `-foo_mat_`

Basic `PetscObject` Usage

Every object in PETSc supports a basic interface

Function	Operation
`Create()`	create the object
`Get/SetName()`	name the object
`Get/SetType()`	set the implementation type
`Get/SetOptionsPrefix()`	set the prefix for all options
`SetFromOptions()`	customize object from the command line
`SetUp()`	preform other initialization
`View()`	view the object
`Destroy()`	cleanup object allocation

Also, all objects support the `-help` option.

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Ways to set options

- Command line
- Filename in the third argument of `PetscInitialize()`
- `~/.petscrc`
- `$PWD/.petscrc`
- `$PWD/petscrc`
- `PetscOptionsInsertFile()`
- `PetscOptionsInsertString()`
- `PETSC_OPTIONS` environment variable
- command line option `-options_file [file]`

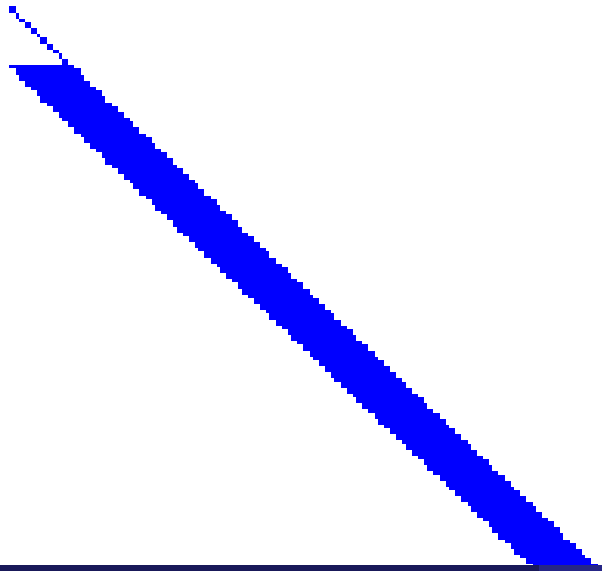
Try it out

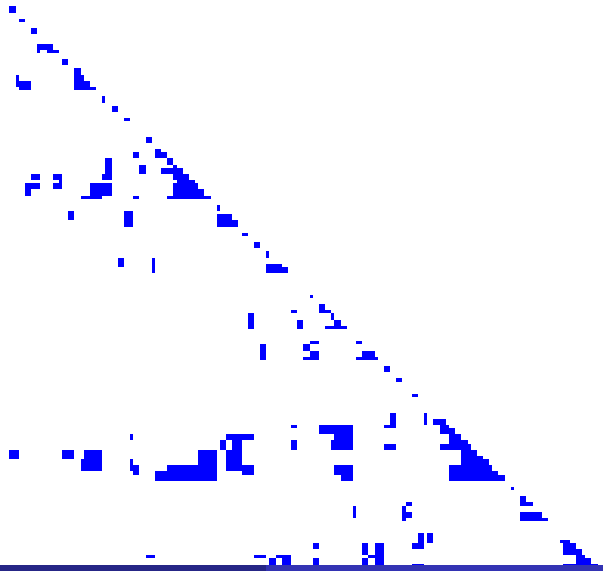
```
$ cd $PETSC_DIR/src/snes/examples/tutorials && make ex5
```

- `$ ./ex5 -da_grid_x 10 -da_grid_y 10 -par 6.7 -snes_monitor -{ksp,snes}_converged_reason -snes_view`
- `$ ./ex5 -da_grid_x 10 -da_grid_y 10 -par 6.7 -snes_monitor -{ksp,snes}_converged_reason -snes_view -mat_view_draw -draw_pause 0.5`
- `$ ./ex5 -da_grid_x 10 -da_grid_y 10 -par 6.7 -snes_monitor -{ksp,snes}_converged_reason -snes_view -mat_view_draw -draw_pause 0.5 -pc_type lu -pc_factor_mat_ordering_type natural`
- Use `-help` to find other ordering types

Sample output

```
0 SNES Function norm 1.139460779565e+00
Linear solve converged due to CONVERGED_RTOL iterations 1
1 SNES Function norm 4.144493702305e-02
Linear solve converged due to CONVERGED_RTOL iterations 1
2 SNES Function norm 6.309075568032e-03
Linear solve converged due to CONVERGED_RTOL iterations 1
3 SNES Function norm 3.359792279909e-04
Linear solve converged due to CONVERGED_RTOL iterations 1
4 SNES Function norm 1.198827244256e-06
Linear solve converged due to CONVERGED_RTOL iterations 1
```





Sample output (SNES and KSP)

```
SNES Object: 1 MPI processes
  type: ls
    line search variant: CUBIC
    alpha=1.000000000000e-04, maxstep=1.000000000000e+08, minlambd
    damping factor=1.000000000000e+00
  maximum iterations=50, maximum function evaluations=10000
  tolerances: relative=1e-08, absolute=1e-50, solution=1e-08
  total number of linear solver iterations=5
  total number of function evaluations=6
  KSP Object:   1 MPI processes
    type: gmres
      GMRES: restart=30, using Classical (unmodified) Gram-Schmidt
      GMRES: happy breakdown tolerance 1e-30
    maximum iterations=10000, initial guess is zero
    tolerances:  relative=1e-05, absolute=1e-50, divergence=10000
    left preconditioning
    using PRECONDITIONED norm type for convergence test
```

Sample output (PC and Mat)

```
PC Object:   1 MPI processes
  type: lu
    LU: out-of-place factorization
    tolerance for zero pivot 2.22045e-14
    matrix ordering: nd
    factor fill ratio given 5, needed 2.95217
      Factored matrix follows:
        Matrix Object:           1 MPI processes
          type: seqaij
          rows=100, cols=100
          package used to perform factorization: petsc
          total: nonzeros=1358, allocated nonzeros=1358
          total number of mallocs used during MatSetValues calls
            not using I-node routines
  linear system matrix = precond matrix:
  Matrix Object:     1 MPI processes
    type: seqaij
    rows=100, cols=100
    total: nonzeros=460, allocated nonzeros=460
    total number of mallocs used during MatSetValues calls =0
      not using I-node routines
```

In parallel

- `$ mpiexec -n 4 ./ex5 -da_grid_x 10 -da_grid_y 10 -par 6.7 -snes_monitor -{ksp,snes}_converged_reason -snes_view -sub_pc_type lu`
- How does the performance change as you
  - vary the number of processes (up to 32 or 64)?
  - increase the problem size?
  - use an inexact subdomain solve?
  - try an overlapping method: `-pc_type asm -pc_asm_overlap 2`
  - simulate a big machine: `-pc_asm_blocks 512`
  - change the Krylov method: `-ksp_type ibcgs`
  - use algebraic multigrid: `-pc_type hypre`
  - use smoothed aggregation multigrid: `-pc_type ml`

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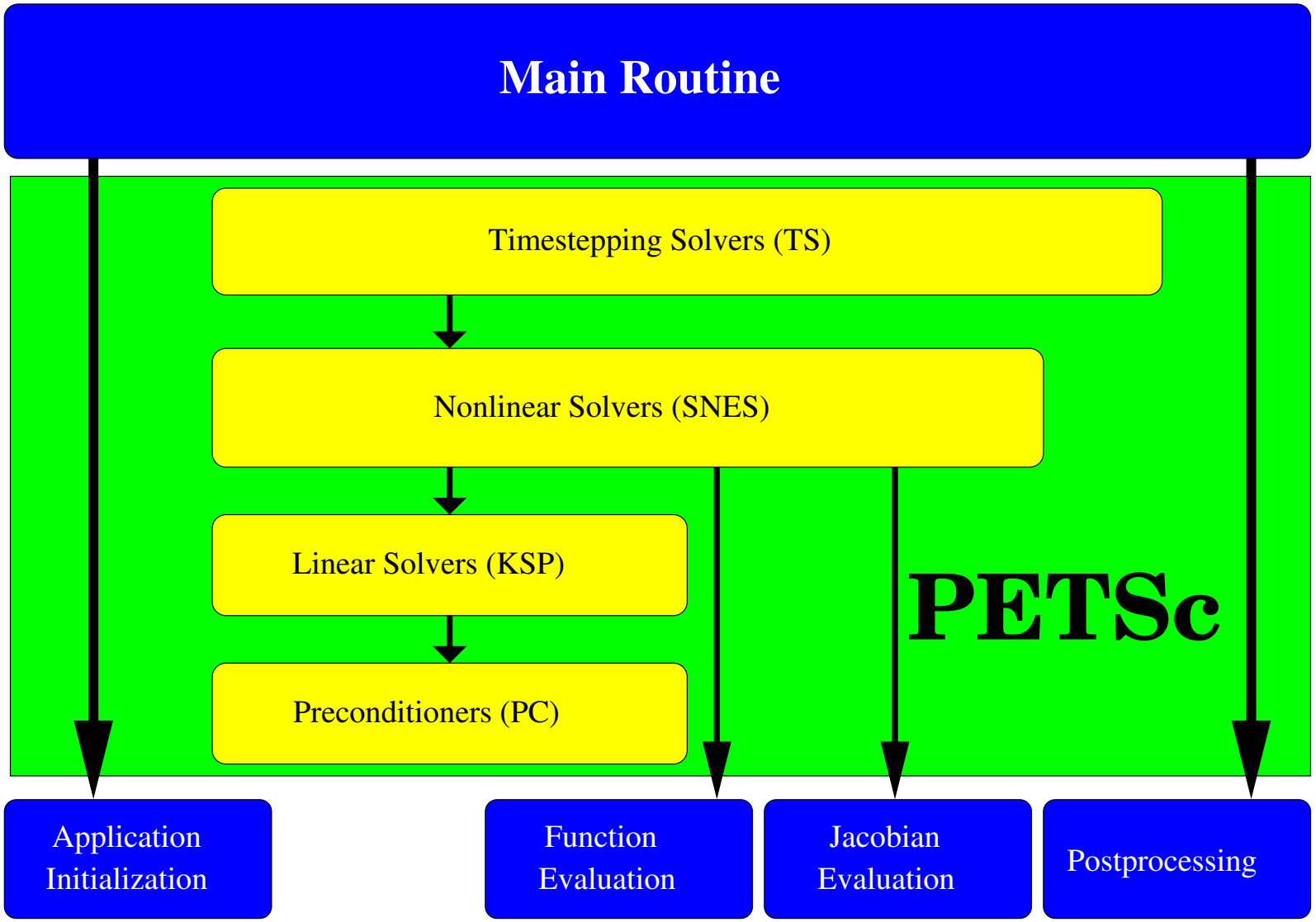
IMEX time integration in PETSc

- 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);`
  - L-stable DIRK for stiff part G
  - Choice of explicit method, e.g. SSP
  - 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()`
- Eliminated many interface quirks in PETSc 3.3
- Single step interface so user can have own time loop

Flow Control for a PETSc Application



Some TS methods

TSSSPRK104 10-stage, fourth order, low-storage, optimal explicit SSP Runge-Kutta $c_{\text{eff}} = 0.6$ (Ketcheson 2008)

TSARKIMEX2E second order, one explicit and two implicit stages, L-stable, optimal (Constantinescu)

TSARKIMEX3 (and 4 and 5), L-stable (Kennedy and Carpenter, 2003)

TSROSWRA3PW three stage, third order, for index-1 PDAE, A-stable, $R(\infty) = 0.73$, second order strongly A-stable embedded method (Rang and Angermann, 2005)

TSROSWRA34PW2 four stage, third order, L-stable, for index 1 PDAE, second order strongly A-stable embedded method (Rang and Angermann, 2005)

TSROSWLLSSP3P4S2C four stage, third order, L-stable implicit, SSP explicit, L-stable embedded method (Constantinescu)

TS Examples

- 1D nonlinear hyperbolic conservation laws
  - `src/ts/examples/tutorials/ex9.c`
  - `./ex9 -da_grid_x 100 -initial 1 -physics shallow -limit minmod -ts_ssp_type rks2 -ts_ssp_nstages 8 -ts_monitor_solution`
- Stiff linear advection-reaction test problem
  - `src/ts/examples/tutorials/ex22.c`
  - `./ex22 -da_grid_x 200 -ts_monitor_solution -ts_type rosw -ts_rosw_type ra34pw2 -ts_adapt_monitor`
- 1D Brusselator (reaction-diffusion)
  - `src/ts/examples/tutorials/ex25.c`
  - `./ex25 -da_grid_x 40 -ts_monitor_solution -ts_type rosw -ts_rosw_type 2p -ts_adapt_monitor`

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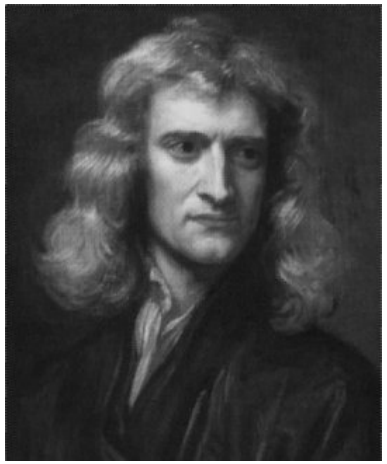
Newton iteration: workhorse of SNES



- Standard form of a nonlinear system

$$F(u) = 0$$

- Iteration

$$\begin{aligned} \text{Solve:} \quad & J(u)w = -F(u) \\ \text{Update:} \quad & u^+ \leftarrow u + w \end{aligned}$$

- Quadratically convergent near a root: $\left|u^{n+1} - u^*\right| \in \mathscr{O}\left(\left|u^n - u^*\right|^2\right)$
- Picard is the same operation with a different $J(u)$

Example (Nonlinear Poisson)

$$\begin{aligned} F(u) = 0 \quad &\sim \quad -\nabla\cdot\left[(1+u^2)\nabla u\right] - f = 0 \\ J(u)w \quad &\sim \quad -\nabla\cdot\left[(1+u^2)\nabla w + 2uw\nabla u\right] \end{aligned}$$

SNES Paradigm

The SNES interface is based upon callback functions

- `FormFunction()`, set by `SNESSetFunction()`
- `FormJacobian()`, set by `SNESSetJacobian()`

When PETSc needs to evaluate the nonlinear residual $F(x)$,

- Solver calls the **user's** function
- User function gets application state through the `ctx` variable
  - PETSc never sees application data

SNES Function

The user provided function which calculates the nonlinear residual has signature

```
PetscErrorCode (*func)(SNES snes,Vec x,Vec r,void *ctx)
```

- `x`: The current solution
- `r`: The residual
- `ctx`: The user context passed to `SNESSetFunction()`
  - Use this to pass application information, e.g. physical constants

SNES Jacobian

The user provided function which calculates the Jacobian has signature

```
PetscErrorCode (*func)(SNES snes,Vec x,Mat *J,Mat *M,
                       MatStructure *flag,void *ctx)
```

- `x`: The current solution
- `J`: The Jacobian
- `M`: The Jacobian preconditioning matrix (possibly J itself)
- `ctx`: The user context passed to `SNESSetFunction()`
  - Use this to pass application information, e.g. physical constants
- Possible `MatStructure` values are:
  - SAME_NONZERO_PATTERN
  - DIFFERENT_NONZERO_PATTERN

Alternatively, you can use

- a builtin sparse finite difference approximation ("coloring")
- automatic differentiation (ADIC/ADIFOR)

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Matrices

Definition (Matrix)

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

Definition (Forming a matrix)

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

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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.

Important matrices

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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 $\kappa(A) = \|A\| \left\|A^{-1}\right\| = \sigma_{\max}/\sigma_{\min}$
  - 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 nth iteration requires at most $\mathscr{O}(mn)$

GMRES

Brute force minimization of residual in $\{b, Ab, A^2b, \dots\}$

1. Use Arnoldi to orthogonalize the nth subspace, producing

$$AQ_n = Q_{n+1}H_n$$

2. Minimize residual in this space by solving the overdetermined system

$$H_n y_n = e_1^{(n+1)}$$

using QR-decomposition, updated cheaply at each iteration.

Properties

- Converges in n steps for all right hand sides if there exists a polynomial of degree n such that $\|p_n(A)\| < tol$ and $p_n(0) = 1$.
- Residual is monotonically decreasing, robust in practice
- Restarted variants are used to bound memory requirements

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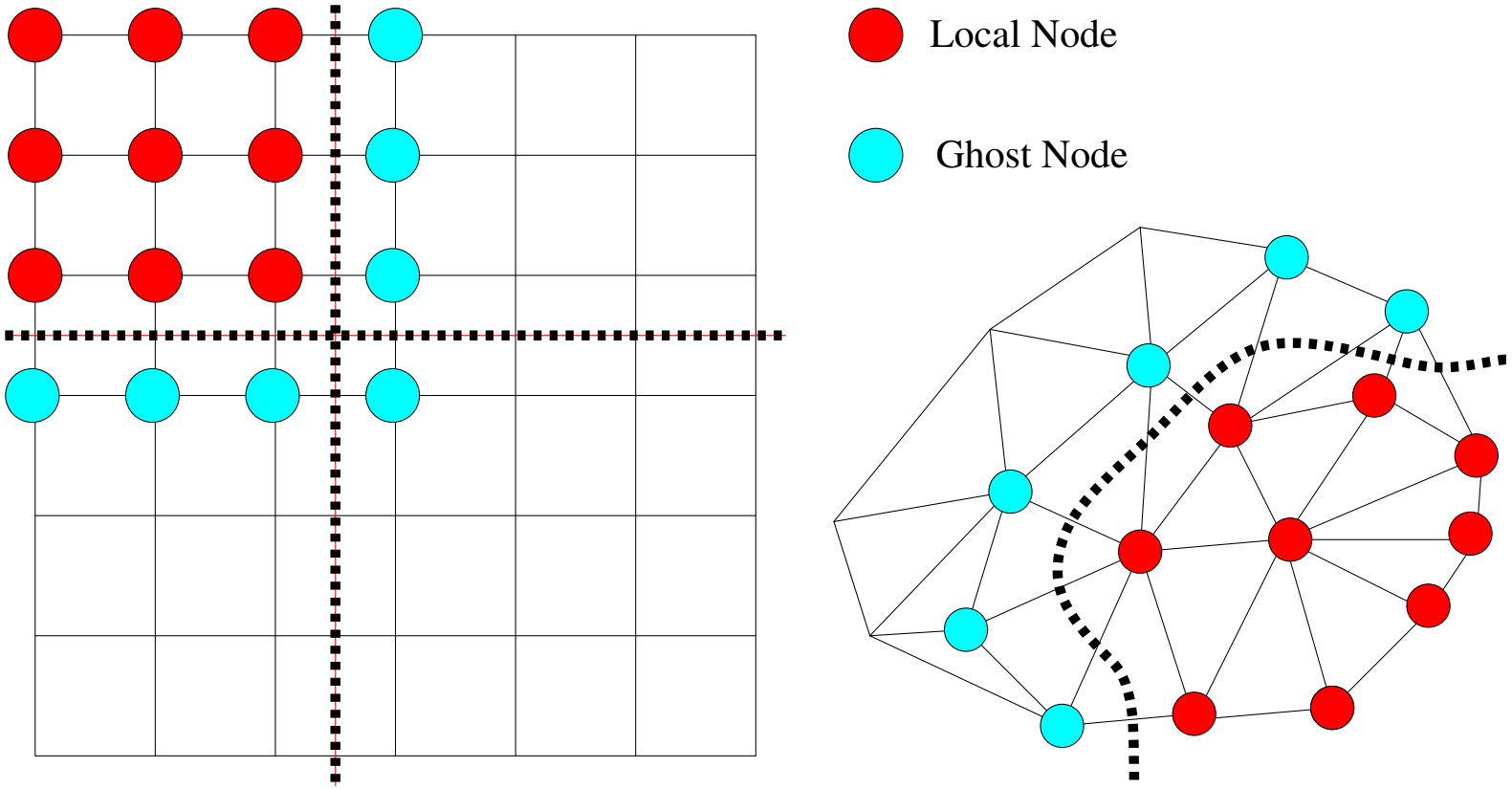
Distributed Array

- Interface for topologically structured grids
- Defines (topological part of) a finite-dimensional function space
  - Get an element from this space: `DMCreateGlobalVector()`
- Provides parallel layout
- Refinement and coarsening
  - `DMRefineHierarchy()`
- Ghost value coherence
  - `DMGlobalToLocalBegin()`
- Matrix preallocation:
  - `DMCreateMatrix()` (formerly `DMGetMatrix()`)

Ghost Values

To evaluate a local function $f(x)$, each process requires

- its local portion of the vector x
- its ghost values, bordering portions of x owned by neighboring processes



DMDA Global Numberings

Proc 2			Proc 3	
25	26	27	28	29
20	21	22	23	24
15	16	17	18	19
10	11	12	13	14
5	6	7	8	9
0	1	2	3	4
Proc 0			Proc 1	

Natural numbering

Proc 2			Proc 3	
21	22	23	28	29
18	19	20	26	27
15	16	17	24	25
6	7	8	13	14
3	4	5	11	12
0	1	2	9	10
Proc 0			Proc 1	

PETSc numbering

DMDA Global vs. Local Numbering

- **Global**: Each vertex has a unique id belongs on a unique process
- **Local**: Numbering includes vertices from neighboring processes
  - These are called ghost vertices

Proc 2			Proc 3	
X	X	X	X	X
X	X	X	X	X
12	13	14	15	X
8	9	10	11	X
4	5	6	7	X
0	1	2	3	X
Proc 0			Proc 1	

Local numbering

Proc 2			Proc 3	
21	22	23	28	29
18	19	20	26	27
15	16	17	24	25
6	7	8	13	14
3	4	5	11	12
0	1	2	9	10
Proc 0			Proc 1	

Global numbering

DM Vectors

- The DM object contains only layout (topology) information
  - All field data is contained in PETSc `Vec`s
- Global vectors are parallel
  - Each process stores a unique local portion
  - `DMCreateGlobalVector(DM dm, Vec *gvec)`
- Local vectors are sequential (and usually temporary)
  - Each process stores its local portion plus ghost values
  - `DMCreateLocalVector(DM dm, Vec *lvec)`
  - includes ghost values!
- Coordinate vectors store the mesh geometry
  - `DMDAGetCoordinates(DM dm, Vec *coords)`
  - Can be manipulated with their own DMDA
    `DMDAGetCoordinateDA(DM dm,DM *cda)`

Updating Ghosts

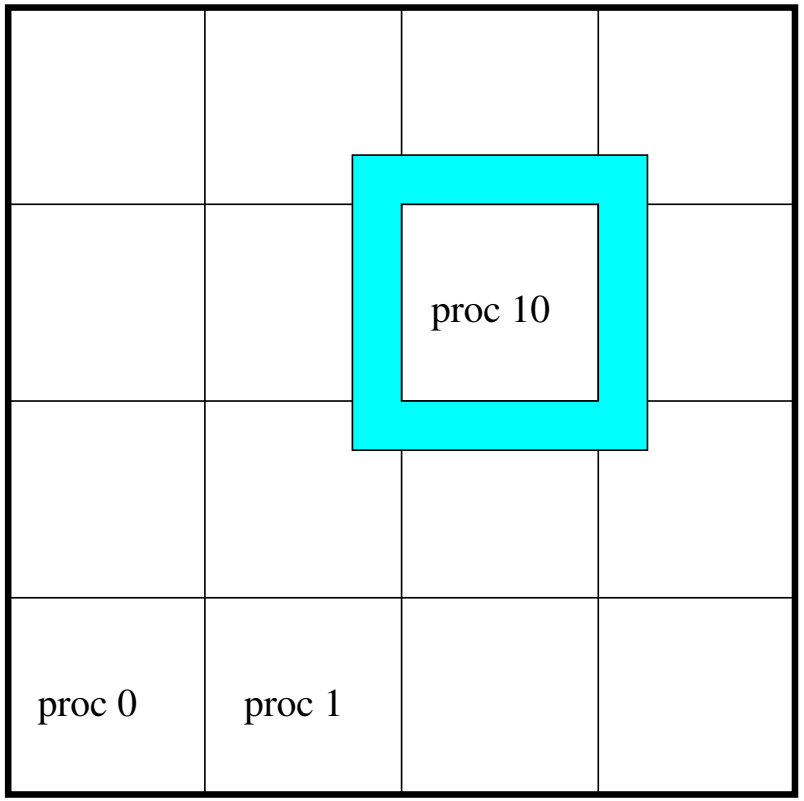
Two-step process enables overlapping computation and communication

- `DMGlobalToLocalBegin(dm, gvec, mode, lvec)`
  - `gvec` provides the data
  - `mode` is either `INSERT_VALUES` or `ADD_VALUES`
  - `lvec` holds the local and ghost values
- `DMGlobalToLocalEnd(dm, gvec, mode, lvec)`
  - Finishes the communication

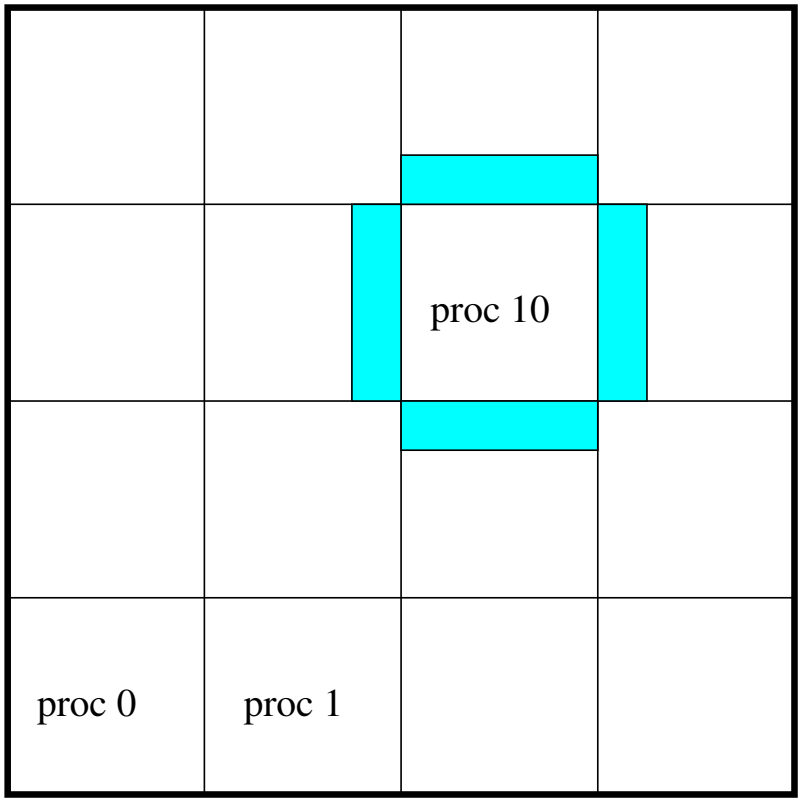
The process can be reversed with `DMLocalToGlobalBegin()` and `DMLocalToGlobalEnd()`.

DMDA Stencils

Both the box stencil and star stencil are available.



Box Stencil



Star Stencil

Creating a DMDA

```
DMDACreate2d(comm, xbdy, ybdy, type, M, N, m, n,
             dof, s, lm[], ln[], DA *da)
```

- `xbdy,ybdy`: Specifies periodicity or ghost cells
  - `DMDA_BOUNDARY_NONE`, `DMDA_BOUNDARY_GHOSTED`, `DMDA_BOUNDARY_MIRROR`, `DMDA_BOUNDARY_PERIODIC`
- `type`: Specifies stencil
  - `DMDA_STENCIL_BOX` or `DMDA_STENCIL_STAR`
- `M,N`: Number of grid points in x/y-direction
- `m,n`: Number of processes in x/y-direction
- `dof`: Degrees of freedom per node
- `s`: The stencil width
- `lm,ln`: Alternative array of local sizes
  - Use `PETSC_NULL` for the default

Working with the local form

Wouldn't it be nice if we could just write our code for the natural numbering?

- Yes, that's what `DMDAVecGetArray()` is for.
- Also, DMDA offers local callback functions
  - `FormFunctionLocal()`, set by `DMDASetLocalFunction()`
  - `FormJacobianLocal()`, set by `DMDASetLocalJacobian()`
- When PETSc needs to evaluate the nonlinear residual $F(x)$,
  - Each process evaluates the local residual
  - PETSc assembles the global residual automatically
    - Uses `DMLocalToGlobal()` method

DA Local Function

The user provided function which calculates the nonlinear residual in 2D has signature

```
PetscErrorCode (*lfunc)(DMDALocalInfo *info,
          Field **x, Field **r, void *ctx)
```

- `info`: All layout and numbering information
- `x`: The current solution
  - Notice that it is a multidimensional array
- `r`: The residual
- `ctx`: The user context passed to `DMSetApplicationContext()` or to SNES

The local DMDA function is activated by calling

```
SNESSetDM(snes,dm) SNESSetFunction(snes, r,
          SNESDAFormFunction, ctx)
```

Bratu Residual Evaluation

$$-\Delta u - \lambda e^u = 0$$

```
BratuResidualLocal(DMDALocalInfo *info,Field **x,Field **f,
                   UserCtx *user)
{
  /* Not Shown: Handle boundaries */
  /* Compute over the interior points */
  for(j = info->ys; j < info->ys+info->ym; j++) {
    for(i = info->xs; i < info->xs+info->xm; i++) {
      u       = x[j][i];
      u_xx    = (2.0*u - x[j][i-1] - x[j][i+1])*hydhx;
      u_yy    = (2.0*u - x[j-1][i] - x[j+1][i])*hxdhy;
      f[j][i] = u_xx + u_yy - hx*hy*lambda*exp(u);
    }
  }
}
```

$PETSC_DIR/src/snes/examples/tutorials/ex5.c

Other DMs

- DMPlex - sophisticated dimension independent management of unstructured meshes as a CW complex
- DMMoab - interface to the MOAB unstructured mesh library

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   - Nonlinear solvers: SNES
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   - Structured grid distribution: DMDA
   - Profiling
   - Matrix Redux

Profiling

- Use `-log_summary` for a performance profile
  - Event timing
  - Event flops
  - Memory usage
  - MPI messages
- Call `PetscLogStagePush()` and `PetscLogStagePop()`
  - User can add new stages
- Call `PetscLogEventBegin()` and `PetscLogEventEnd()`
  - User can add new events
- Call `PetscLogFlops()` to include your flops

Reading -log_summary

-

```
                          Max       Max/Min        Avg      Total
Time (sec):           1.548e+02     1.00122   1.547e+02
Objects:              1.028e+03     1.00000   1.028e+03
Flops:                1.519e+10     1.01953   1.505e+10  1.204e+11
Flops/sec:            9.814e+07     1.01829   9.727e+07  7.782e+08
MPI Messages:         8.854e+03     1.00556   8.819e+03  7.055e+04
MPI Message Lengths:  1.936e+08     1.00950   2.185e+04  1.541e+09
MPI Reductions:       2.799e+03     1.00000
```

- Also a summary per stage
- Memory usage per stage (based on when it was allocated)
- Time, messages, reductions, balance, flops per event per stage
- Always send `-log_summary` when asking performance questions on mailing list

Reading -log_summary

```
Event                Count      Time (sec)     Flops                             --- Global ---  -
                   Max Ratio  Max     Ratio   Max  Ratio  Mess   Avg len Reduct  %T %F %M %L %R  %
------------------------------------------------------------------------------------------------------
--- Event Stage 1: Full solve
VecDot                43 1.0 4.8879e-02 8.3 1.77e+06 1.0 0.0e+00 0.0e+00 4.3e+01  0  0  0  0  0
VecMDot             1747 1.0 1.3021e+00 4.6 8.16e+07 1.0 0.0e+00 0.0e+00 1.7e+03  0  1  0  0 14
VecNorm             3972 1.0 1.5460e+00 2.5 8.48e+07 1.0 0.0e+00 0.0e+00 4.0e+03  0  1  0  0 31
VecScale            3261 1.0 1.6703e-01 1.0 3.38e+07 1.0 0.0e+00 0.0e+00 0.0e+00  0  0  0  0  0
VecScatterBegin     4503 1.0 4.0440e-01 1.0 0.00e+00 0.0 6.1e+07 2.0e+03 0.0e+00  0  0 50 26  0
VecScatterEnd       4503 1.0 2.8207e+00 6.4 0.00e+00 0.0 0.0e+00 0.0e+00 0.0e+00  0  0  0  0  0
MatMult             3001 1.0 3.2634e+01 1.1 3.68e+09 1.1 4.9e+07 2.3e+03 0.0e+00 11 22 40 24  0  2
MatMultAdd           604 1.0 6.0195e-01 1.0 5.66e+07 1.0 3.7e+06 1.3e+02 0.0e+00  0  0  3  0  0
MatMultTranspose     676 1.0 1.3220e+00 1.6 6.50e+07 1.0 4.2e+06 1.4e+02 0.0e+00  0  0  3  0  0
MatSolve            3020 1.0 2.5957e+01 1.0 3.25e+09 1.0 0.0e+00 0.0e+00 0.0e+00  9 21  0  0  0  1
MatCholFctrSym         3 1.0 2.8324e-04 1.0 0.00e+00 0.0 0.0e+00 0.0e+00 0.0e+00  0  0  0  0  0
MatCholFctrNum        69 1.0 5.7241e+00 1.0 6.75e+08 1.0 0.0e+00 0.0e+00 0.0e+00  2  4  0  0  0
MatAssemblyBegin     119 1.0 2.8250e+00 1.5 0.00e+00 0.0 2.1e+06 5.4e+04 3.1e+02  1  0  2 24  2
MatAssemblyEnd       119 1.0 1.9689e+00 1.4 0.00e+00 0.0 2.8e+05 1.3e+03 6.8e+01  1  0  0  0  1
SNESSolve              4 1.0 1.4302e+02 1.0 8.11e+09 1.0 6.3e+07 3.8e+03 6.3e+03 51 50 52 50 50  9
SNESLineSearch        43 1.0 1.5116e+01 1.0 1.05e+08 1.1 2.4e+06 3.6e+03 1.8e+02  5  1  2  2  1  1
SNESFunctionEval      55 1.0 1.4930e+01 1.0 0.00e+00 0.0 1.8e+06 3.3e+03 8.0e+00  5  0  1  1  0  1
SNESJacobianEval      43 1.0 3.7077e+01 1.0 7.77e+06 1.0 4.3e+06 2.6e+04 3.0e+02 13  0  4 24  2  2
KSPGMRESOrthog      1747 1.0 1.5737e+00 2.9 1.63e+08 1.0 0.0e+00 0.0e+00 1.7e+03  1  1  0  0 14
KSPSetup             224 1.0 2.1040e-02 1.0 0.00e+00 0.0 0.0e+00 0.0e+00 3.0e+01  0  0  0  0  0
KSPSolve              43 1.0 8.9988e+01 1.0 7.99e+09 1.0 5.6e+07 2.0e+03 5.8e+03 32 49 46 24 46  6
PCSetUp              112 1.0 1.7354e+01 1.0 6.75e+08 1.0 0.0e+00 0.0e+00 8.7e+01  6  4  0  0  1  1
PCSetUpOnBlocks     1208 1.0 5.8182e+00 1.0 6.75e+08 1.0 0.0e+00 0.0e+00 8.7e+01  2  4  0  0  1
PCApply              276 1.0 7.1497e+01 1.0 7.14e+09 1.0 5.2e+07 1.8e+03 5.1e+03 25 44 42 20 41  4
```

Communication Costs

- Reductions: usually part of Krylov method, latency limited
  - `VecDot`
  - `VecMDot`
  - `VecNorm`
  - `MatAssemblyBegin`
  - Change algorithm (e.g. IBCGS)
- Point-to-point (nearest neighbor), latency or bandwidth
  - `VecScatter`
  - `MatMult`
  - `PCApply`
  - `MatAssembly`
  - `SNESFunctionEval`
  - `SNESJacobianEval`
  - Compute subdomain boundary fluxes redundantly
  - Ghost exchange for all fields at once
  - Better partition

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Matrices, redux

What are PETSc matrices?

- Linear operators on finite dimensional vector spaces. (snarky)
- Fundamental objects for storing stiffness matrices and Jacobians
- Each process locally owns a contiguous set of rows
- Supports many data types
  - AIJ, Block AIJ, Symmetric AIJ, Block Diagonal, etc.
- Supports structures for many packages
  - MUMPS, Spooles, SuperLU, UMFPack, Hypre

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How do I create matrices?

- `MatCreate(MPI_Comm, Mat *)`
- `MatSetSizes(Mat, int m, int n, int M, int N)`
- `MatSetType(Mat, MatType typeName)`
- `MatSetFromOptions(Mat)`
  - Can set the type at runtime
- `MatMPIBAIJSetPreallocation(Mat,...)`
  - important for assembly performance, more tomorrow
- `MatSetBlockSize(Mat, int bs)`
  - for vector problems
- `MatSetValues(Mat,...)`
  - **MUST** be used, but does automatic communication
  - `MatSetValuesLocal(),MatSetValuesStencil()`
  - `MatSetValuesBlocked()`

Matrix Polymorphism

The PETSc `Mat` has a single user interface,

- Matrix assembly
  - `MatSetValues()`
- Matrix-vector multiplication
  - `MatMult()`
- Matrix viewing
  - `MatView()`

but multiple underlying implementations.

- AIJ, Block AIJ, Symmetric Block AIJ,
- Dense, Elemental
- Matrix-Free
- etc.

A matrix is defined by its interface, not by its data structure.

Matrix Assembly

- A three step process
  - Each process sets or adds values
  - Begin communication to send values to the correct process
  - Complete the communication
- `MatSetValues(Mat A, m, rows[], n, cols[], values[], mode)`
  - `mode` is either INSERT_VALUES or ADD_VALUES
  - Logically dense block of values
- Two phase assembly allows overlap of communication and computation
  - `MatAssemblyBegin(Mat m, type)`
  - `MatAssemblyEnd(Mat m, type)`
  - `type` is either MAT_FLUSH_ASSEMBLY or MAT_FINAL_ASSEMBLY
- For vector problems

```
MatSetValuesBlocked(Mat A, m, rows[],
        n, cols[], values[], mode)
```

- The same assembly code can build matrices of different format
  - choose format at run-time.

Matrix Assembly

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```

- The same assembly code can build matrices of different format
  - choose format at run-time.

One Way to Set the Elements of a Matrix

Simple 3-point stencil for 1D Laplacian

```
v[0] = -1.0; v[1] = 2.0; v[2] = -1.0;
if (rank == 0) {
  for(row = 0;  row < N; row++) {
    cols[0] = row-1; cols[1] = row; cols[2] = row+1;
    if (row == 0) {
      MatSetValues(A,1,&row,2,&cols[1],&v[1],INSERT_VALUES)
    } else if (row == N-1) {
      MatSetValues(A,1,&row,2,cols,v,INSERT_VALUES);
    } else {
      MatSetValues(A,1,&row,3,cols,v,INSERT_VALUES);
    }
  }
}
MatAssemblyBegin(A,MAT_FINAL_ASSEMBLY);
MatAssemblyEnd(A,MAT_FINAL_ASSEMBLY);
```

A Better Way to Set the Elements of a Matrix

Simple 3-point stencil for 1D Laplacian

```
v[0] = -1.0; v[1] = 2.0; v[2] = -1.0;
for(row = start;  row < end; row++) {
  cols[0] = row-1; cols[1] = row; cols[2] = row+1;
  if (row == 0) {
    MatSetValues(A,1,&row,2,&cols[1],&v[1],INSERT_VALUES);
  } else if (row == N-1) {
    MatSetValues(A,1,&row,2,cols,v,INSERT_VALUES);
  } else {
    MatSetValues(A,1,&row,3,cols,v,INSERT_VALUES);
  }
}
MatAssemblyBegin(A, MAT_FINAL_ASSEMBLY);
MatAssemblyEnd(A, MAT_FINAL_ASSEMBLY);
```

Why Are PETSc Matrices That Way?

- No one data structure is appropriate for all problems
  - Blocked and diagonal formats provide significant performance benefits
  - PETSc has many formats and makes it easy to add new data structures
- Assembly is difficult enough without worrying about partitioning
  - PETSc provides parallel assembly routines
  - Achieving high performance still requires making most operations local
  - However, programs can be incrementally developed.
  - `MatPartitioning` and `MatOrdering` can help
- Matrix decomposition in contiguous chunks is simple
  - Makes interoperation with other codes easier
  - For other ordering, PETSc provides “Application Orderings” (AO)

Preliminary Conclusions

PETSc can help you

- solve algebraic and DAE problems in your application area
- rapidly develop efficient parallel code, can start from examples
- develop new solution methods and data structures
- debug and analyze performance
- advice on software design, solution algorithms, and performance
  - Public questions: `petsc-users@mcs.anl.gov`, archived
  - Private questions: `petsc-maint@mcs.anl.gov`, not archived

You can help PETSc

- report bugs and inconsistencies, or if you think there is a better way
- tell us if the documentation is inconsistent or unclear
- consider developing new algebraic methods as plugins, contribute if your idea works

Outline

5 Application Integration

6 Performance and Scalability

Memory hierarchy

Application Integration

- Be willing to experiment with algorithms
  - No optimality without interplay between physics and algorithmics
- Adopt flexible, extensible programming
  - Algorithms and data structures not hardwired
- Be willing to play with the real code
  - Toy models have limited usefulness
  - But make test cases that run quickly
- If possible, profile before integration
  - Automatic in PETSc

Incorporating PETSc into existing codes

- PETSc does not seize `main()`, does not control output
- Propogates errors from underlying packages, flexible error handling
- Nothing special about `MPI_COMM_WORLD`
- Can wrap existing data structures/algorithms
  - `MatShell`, `PCShell`, full implementations
  - `VecCreateMPIWithArray()`
  - `MatCreateSeqAIJWithArrays()`
  - Use an existing semi-implicit solver as a preconditioner
  - Usually worthwhile to use native PETSc data structures unless you have a good reason not to
- Uniform interfaces across languages
  - C, C++, Fortran 77/90, Python, MATLAB
- Do not have to use high level interfaces (e.g. SNES, TS, DM)
  - but PETSc can offer more if you do, like MFFD and SNES Test

Integration Stages

- Version Control
  - It is impossible to overemphasize
- Initialization
  - Linking to PETSc
- Profiling
  - Profile before changing
  - Also incorporate command line processing
- Linear Algebra
  - First PETSc data structures
- Solvers
  - Very easy after linear algebra is integrated

Initialization

- Call `PetscInitialize()`
  - Setup static data and services
  - Setup MPI if it is not already
  - Can set `PETSC_COMM_WORLD` to use your communicator (can always use subcommunicators for each object)
- Call `PetscFinalize()`
  - Calculates logging summary
  - Can check for leaks/unused options
  - Shutdown and release resources
- Can only initialize PETSc once

Matrix Memory Preallocation

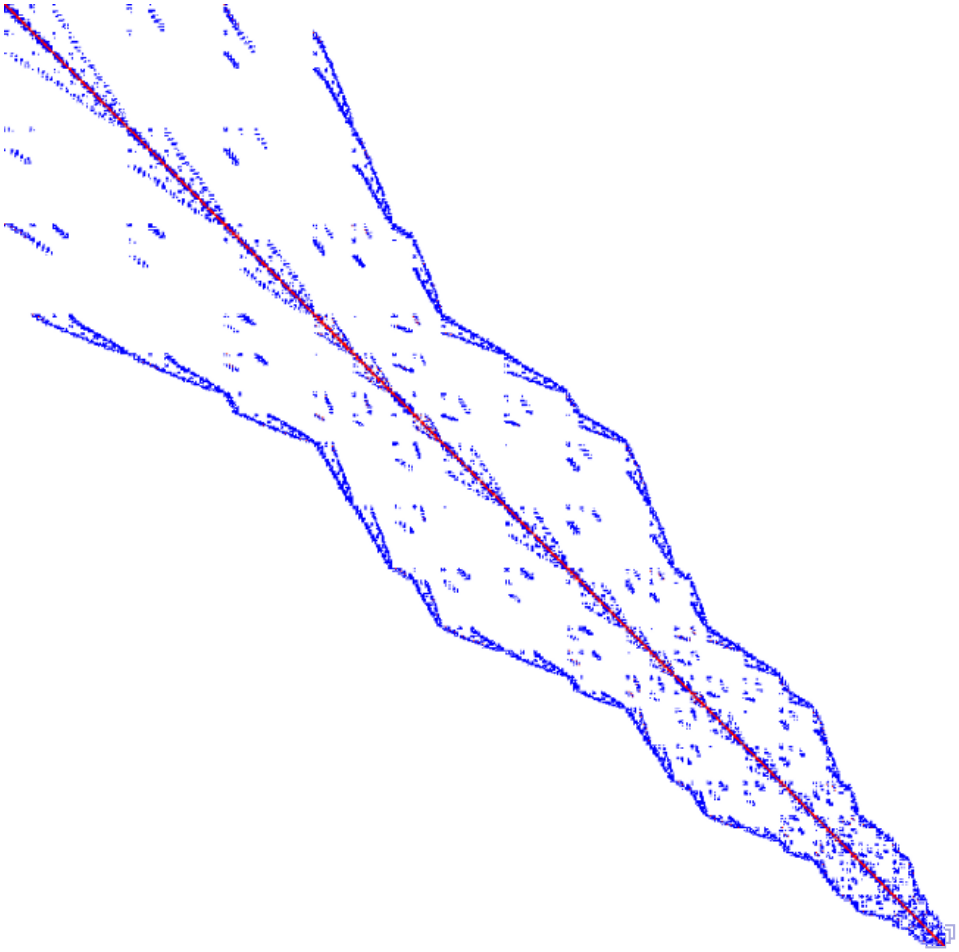
- PETSc sparse matrices are dynamic data structures
  - can add additional nonzeros freely
- Dynamically adding many nonzeros
  - requires additional memory allocations
  - requires copies
  - can kill performance
- Memory preallocation provides
  - the freedom of dynamic data structures
  - good performance
- Easiest solution is to replicate the assembly code
  - Remove computation, but preserve the indexing code
  - Store set of columns for each row
- Call preallocation routines for all datatypes
  - `MatSeqAIJSetPreallocation()`
  - `MatMPIBAIJSetPreallocation()`
  - Only the relevant data will be used

Sequential Sparse Matrices

```
MatSeqAIJSetPreallocation(Mat A, int nz, int nnz[])
```

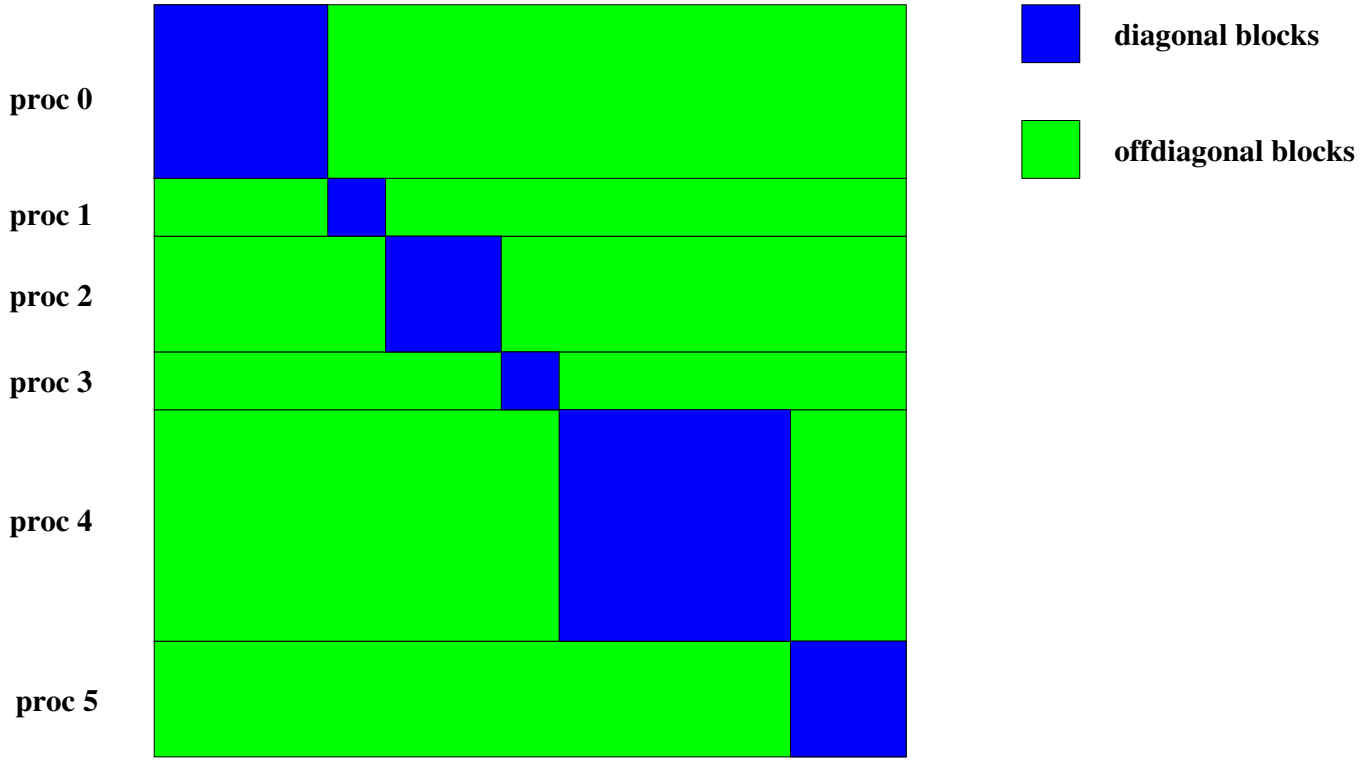
nz: expected number of nonzeros in any row

nnz(i): expected number of nonzeros in row i



Parallel Sparse Matrix

- Each process locally owns a submatrix of contiguous global rows
- Each submatrix consists of diagonal and off-diagonal parts



- `MatGetOwnershipRange(Mat A,int *start,int *end)`

`start:` first locally owned row of global matrix

`end-1:` last locally owned row of global matrix

Parallel Sparse Matrices

```
MatMPIAIJSetPreallocation(Mat A, int dnz, int
dnnz[],
        int onz, int onnz[])
```

dnz: expected number of nonzeros in any row in the diagonal block

dnnz(i): expected number of nonzeros in row i in the diagonal block

onz: expected number of nonzeros in any row in the offdiagonal portion

onnz(i): expected number of nonzeros in row i in the offdiagonal portion

Verifying Preallocation

- Use runtime options
  `-mat_new_nonzero_location_err`
  `-mat_new_nonzero_allocation_err`
- Use runtime option `-info`
- Output:
  `[proc #] Matrix size: %d X %d; storage space: %d unneeded, %d used`
  `[proc #] Number of mallocs during MatSetValues( ) is %d`

```
[merlin] mpirun ex2 -log_info
[0]MatAssemblyEnd_SeqAIJ:Matrix size: 56 X 56; storage space:
[0]   310 unneeded, 250 used
[0]MatAssemblyEnd_SeqAIJ:Number of mallocs during MatSetValues() is 0
[0]MatAssemblyEnd_SeqAIJ:Most nonzeros in any row is 5
[0]Mat_AIJ_CheckInode: Found 56 nodes out of 56 rows. Not using Inode routine
[0]Mat_AIJ_CheckInode: Found 56 nodes out of 56 rows. Not using Inode routine
Norm of error 0.000156044 iterations 6
[0]PetscFinalize:PETSc successfully ended!
```

Block and symmetric formats

- BAIJ
  - Like AIJ, but uses static block size
  - Preallocation is like AIJ, but just one index per block
- SBAIJ
  - Only stores upper triangular part
  - Preallocation needs number of nonzeros in upper triangular parts of on- and off-diagonal blocks
- `MatSetValuesBlocked()`
  - Better performance with blocked formats
  - Also works with scalar formats, if `MatSetBlockSize()` was called
  - Variants `MatSetValuesBlockedLocal()`, `MatSetValuesBlockedStencil()`
  - Change matrix format at runtime, don't need to touch assembly code

Linear Solvers

Krylov Methods

- Using PETSc linear algebra, just add:
  - `KSPSetOperators(KSP ksp, Mat A, Mat M, MatStructure flag)`
  - `KSPSolve(KSP ksp, Vec b, Vec x)`
- Can access subobjects
  - `KSPGetPC(KSP ksp, PC *pc)`
- Preconditioners must obey PETSc interface
  - Basically just the KSP interface
- Can change solver dynamically from the command line, `-ksp_type`

Nonlinear Solvers

Newton and Picard Methods

- Using PETSc linear algebra, just add:
  - `SNESSetFunction(SNES snes, Vec r, residualFunc, void *ctx)`
  - `SNESSetJacobian(SNES snes, Mat A, Mat M, jacFunc, void *ctx)`
  - `SNESSolve(SNES snes, Vec b, Vec x)`
- Can access subobjects
  - `SNESGetKSP(SNES snes, KSP *ksp)`
- Can customize subobjects from the cmd line
  - Set the subdomain preconditioner to ILU with `-sub_pc_type ilu`

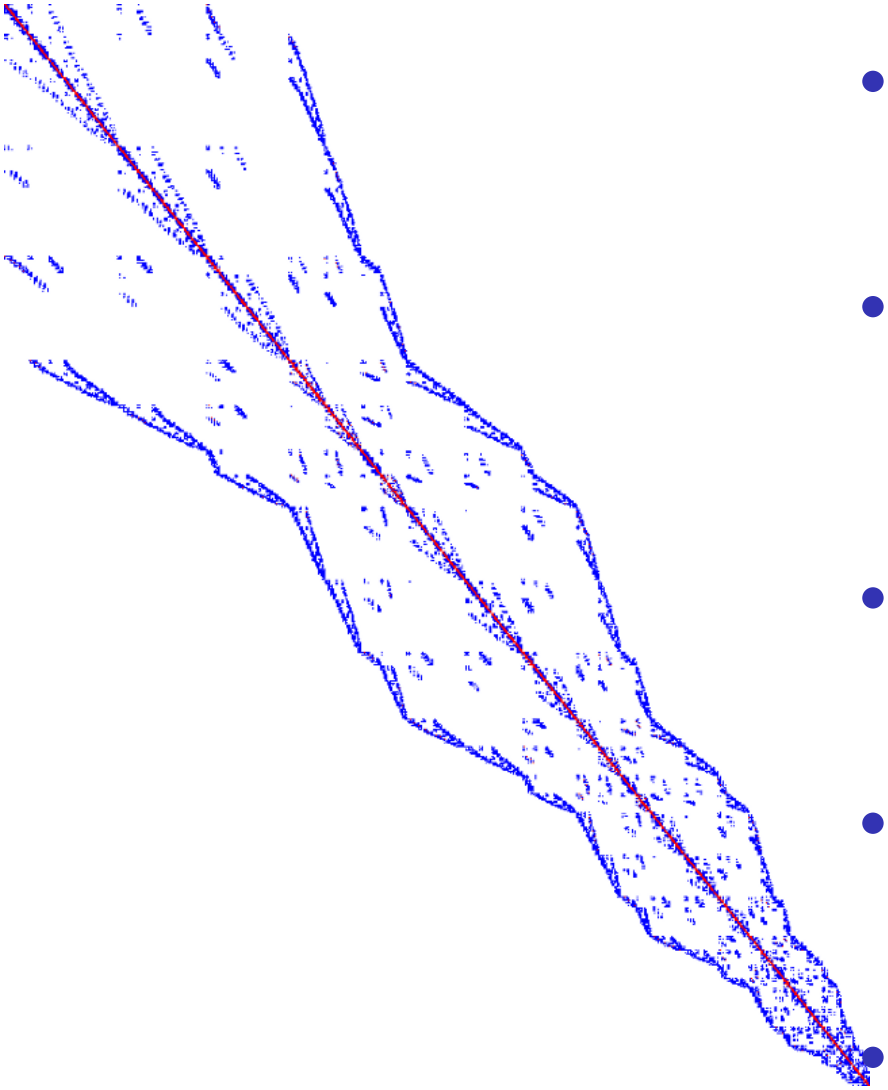
Outline

5 Application Integration

6 Performance and Scalability

Memory hierarchy

Bottlenecks of (Jacobian-free) Newton-Krylov

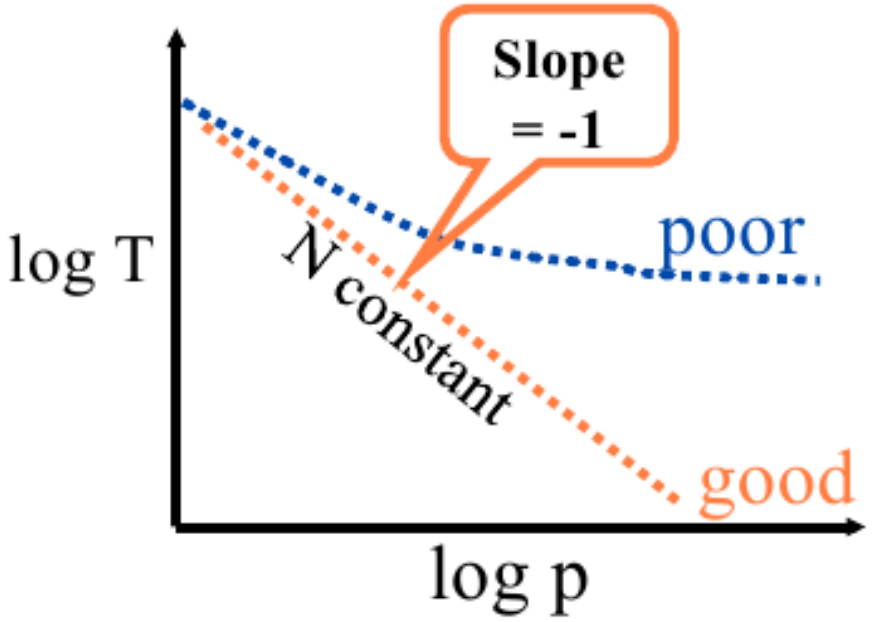


- Matrix assembly
  - integration/fluxes: FPU
  - insertion: memory/branching
- Preconditioner setup
  - coarse level operators
  - overlapping subdomains
  - (incomplete) factorization
- Preconditioner application
  - triangular solves/relaxation: memory
  - coarse levels: network latency
- Matrix multiplication
  - Sparse storage: memory
  - Matrix-free: FPU
- Globalization

Scalability definitions

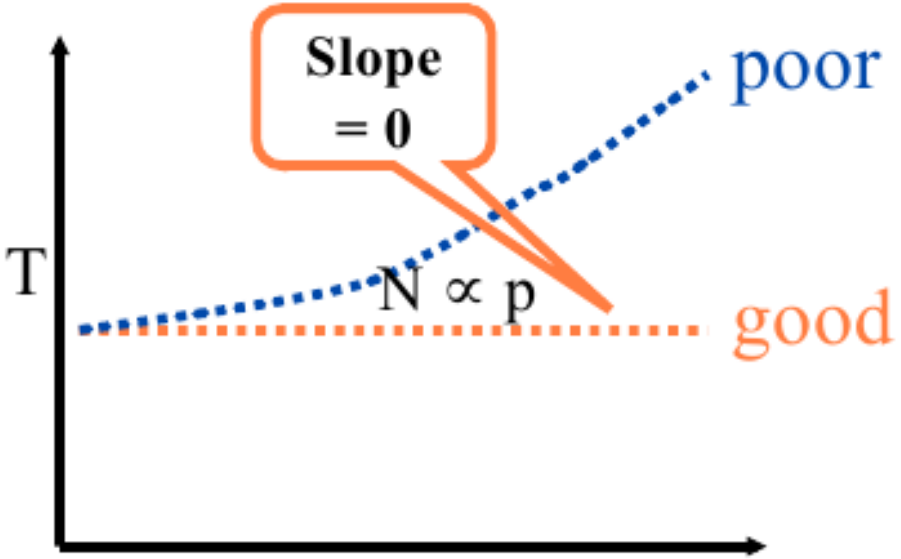
Strong scalability

- Fixed problem size
- execution time T inversely proportional to number of processors p



Weak scalability

- Fixed problem size per processor
- execution time constant as problem size increases



Scalability Warning

The easiest way to make software scalable is to make it sequentially inefficient. (Gropp 1999)

- We really want efficient software
- Need a performance model
  - memory bandwidth and latency
  - algorithmically critical operations (e.g. dot products, scatters)
  - floating point unit
- Scalability shows marginal benefit of adding more cores, nothing more
- Constants hidden in the choice of algorithm
- Constants hidden in implementation

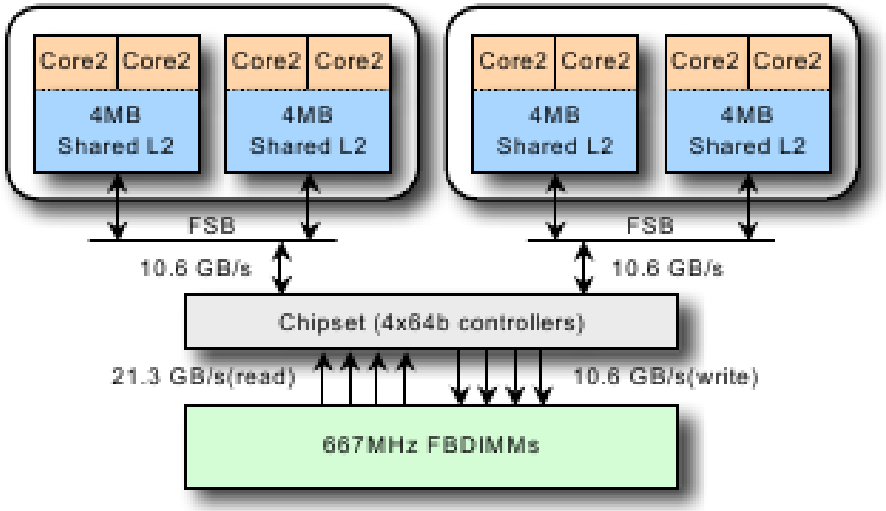
Outline

5 Application Integration

6 Performance and Scalability

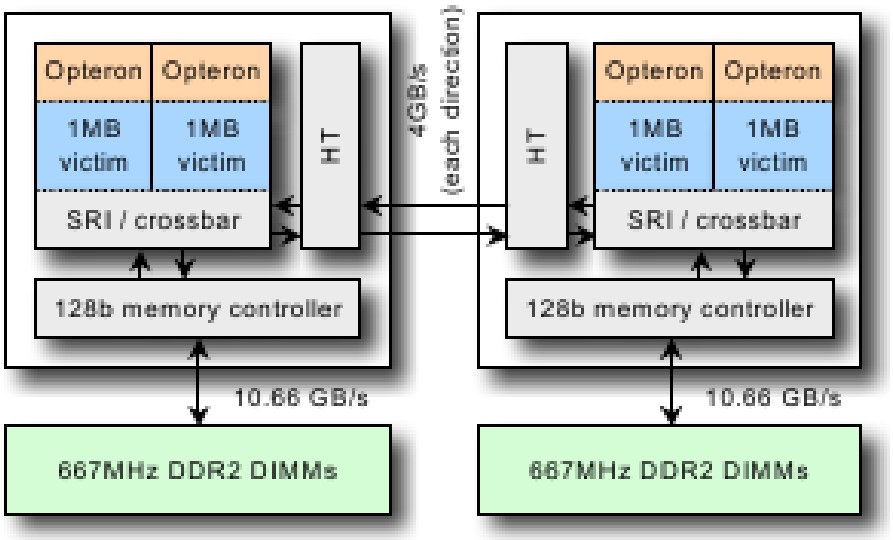
Memory hierarchy

Intel Clowertown



- 75 Gflop/s
- 21 GB/s bandwidth
- thread + instruction level parallelism
- vector instructions (SSE)

AMD Opteron



- 17 Gflop/s
- 21 GB/s bandwidth
- thread + instruction level parallelism
- vector instructions (SSE)

Hardware capabilities

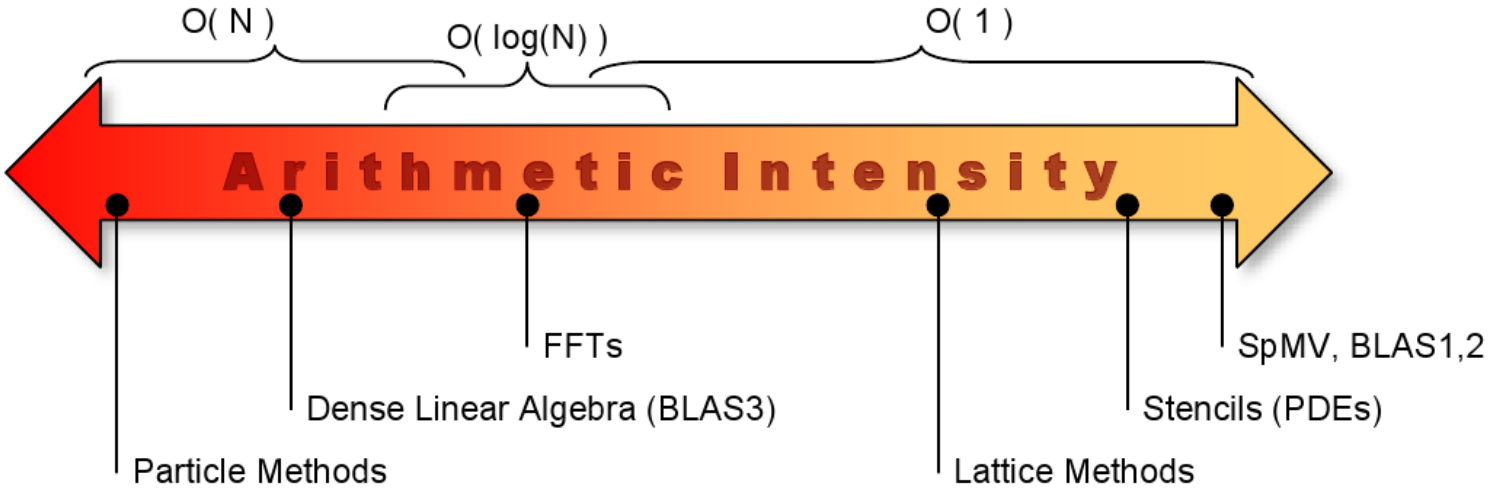
Floating point unit

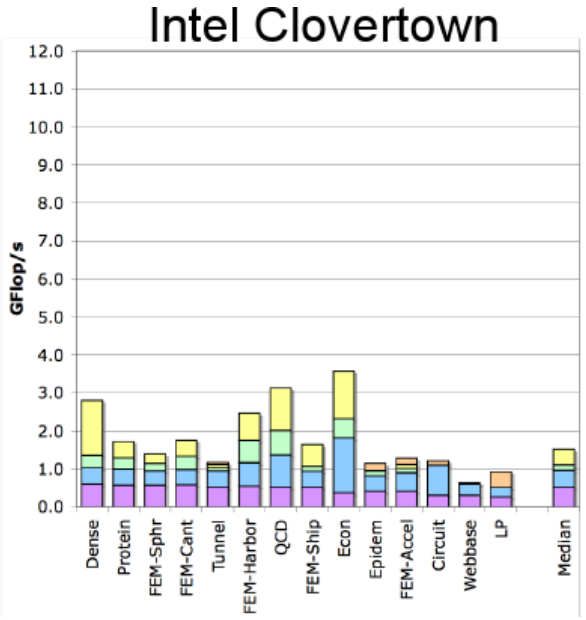
Recent Intel: each core can issue

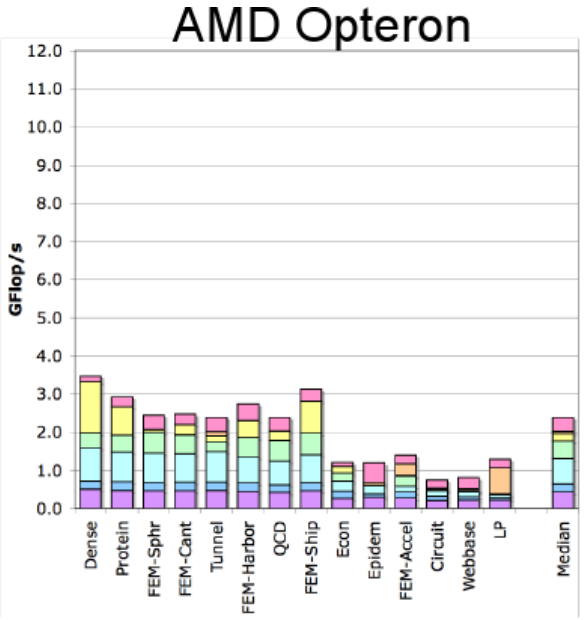
- 1 packed add (latency 3)
- 1 packed mult (latency 5)
- One can include an aligned read
- Out of Order execution
- Peak: 10 Gflop/s (`double`)

Memory

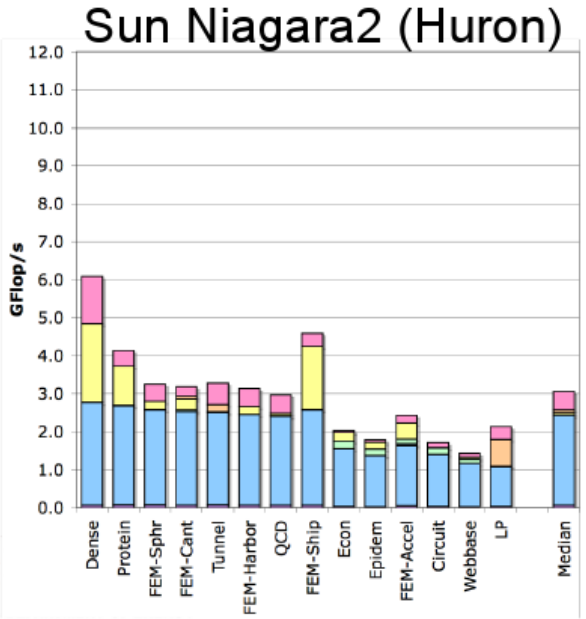
- $\sim$ 250 cycle latency
- 5.3 GB/s bandwidth
- 1 `double` load / 3.7 cycles
- Pay by the cache line (32/64 B)
- L2 cache: $\sim$ 10 cycle latency

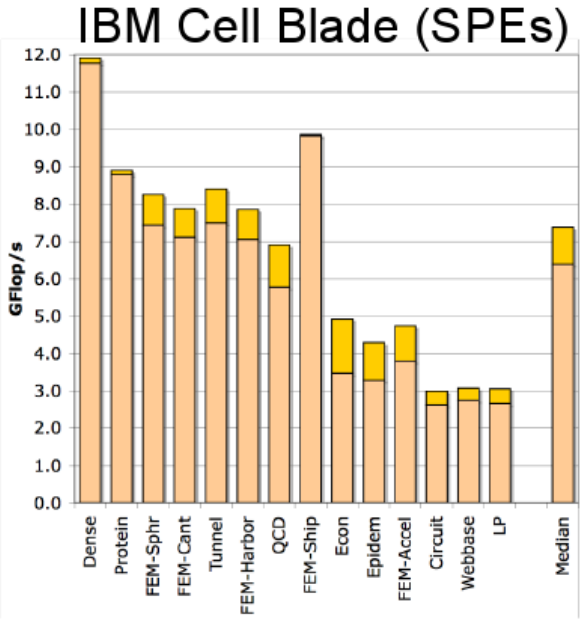






- Model faster cores by commenting out the inner kernel calls, but still performing all DMAs
- Enabled 1x1 BCOO
- ~16% improvement





- +better Cell implementation
- +More DIMMs(opteron), +FW fix, array padding(N2), etc...
- +Cache/TLB Blocking
- +Compression
- +SW Prefetching
- +NUMA/Affinity
- Naïve Pthreads
- Naïve

(Oliker et al. Multi-core Optimization of Sparse Matrix Vector Multiplication, 2008)

Sparse Mat-Vec performance model

Compressed Sparse Row format (AIJ)

For $m \times n$ matrix with N nonzeros

- ai row starts, length $m+1$
- aj column indices, length N, range $[0, n-1)$
- aa nonzero entries, length N, scalar values

$y \leftarrow y + Ax$

```
for (i=0; i<m; i++)
  for (j=ai[i]; j<ai[i+1]; j++)
    y[i] += aa[j] * x[aj[j]];
```

- One add and one multiply per inner loop
- Scalar `aa[j]` and integer `aj[j]` only used once
- Must load `aj[j]` to read from `x`, may not reuse cache well

Memory Bandwidth

- Stream Triad benchmark (GB/s): $w \leftarrow \alpha x + y$

Threads per Node	Cray XT5		BlueGene/P	
	Total	Per Core	Total	Per Core
1	8448	8448	2266	2266
2	10112	5056	4529	2264
4	10715	2679	8903	2226
6	10482	1747	-	-

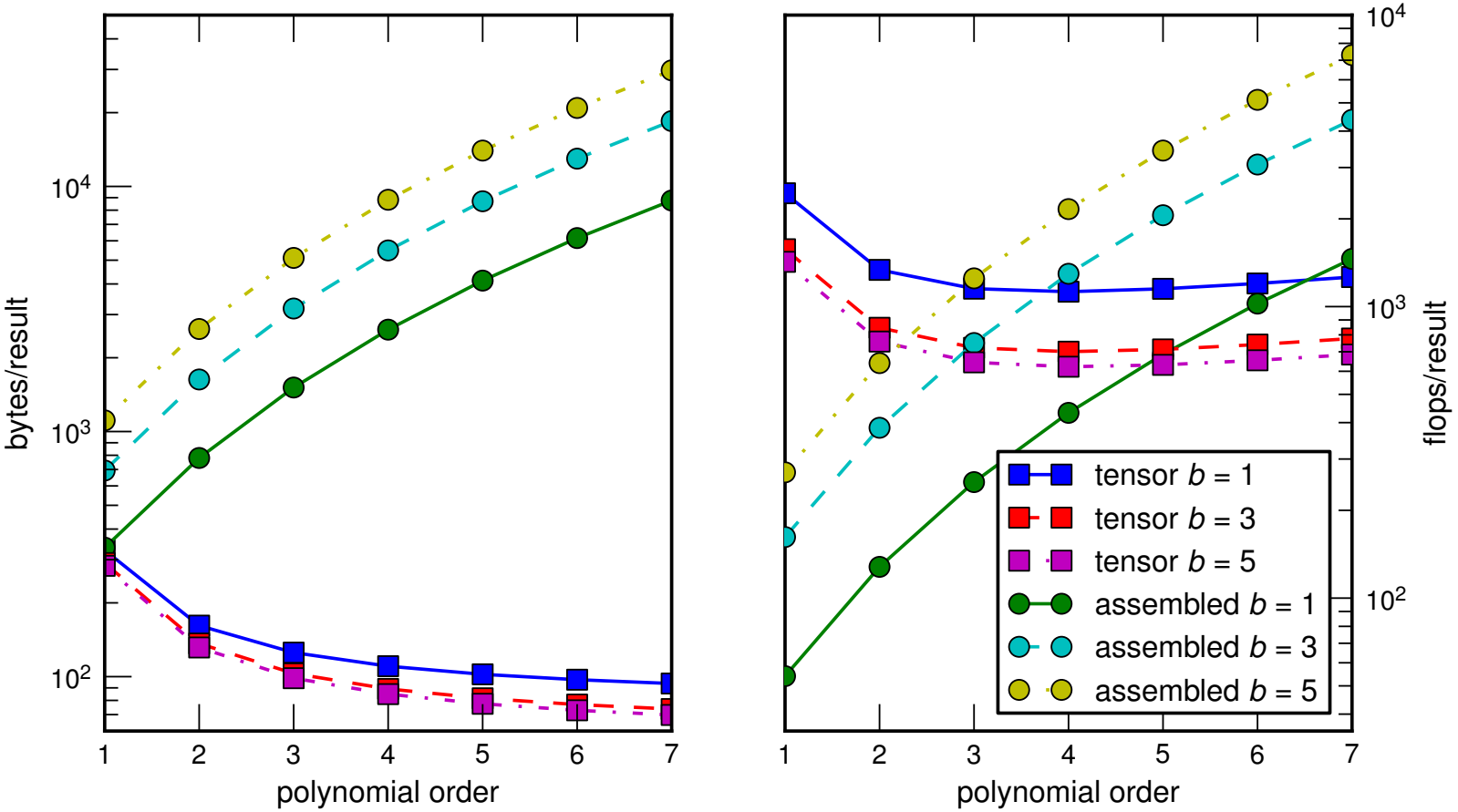
- Sparse matrix-vector product: 6 bytes per flop

Machine	Peak MFlop/s per core	Bandwidth (GB/s)		Ideal MFlop/s
		Required	Measured	
Blue Gene/P	3,400	20.4	2.2	367
XT5	10,400	62.4	1.7	292

Optimizing Sparse Mat-Vec

- Order unknows so that vector reuses cache (Reverse Cuthill-McKee)
  - Optimal: $\frac{(2\text{ flops})(\text{bandwidth})}{\texttt{sizeof(Scalar)+sizeof(Int)}}$
  - Usually improves strength of ILU and SOR
- Coalesce indices for adjacent rows with same nonzero pattern (Inodes)
  - Optimal: $\frac{(2\text{ flops})(\text{bandwidth})}{\texttt{sizeof(Scalar)+sizeof(Int)}/i}$
  - Can do block SOR (much stronger than scalar SOR)
  - Default in PETSc, turn off with `-mat_no_inode`
  - Requires ordering unknowns so that fields are interlaced, this is (much) better for memory use anyway
- Use explicit blocking, hold one index per block (BAIJ format)
  - Optimal: $\frac{(2\text{ flops})(\text{bandwidth})}{\texttt{sizeof(Scalar)+sizeof(Int)}/b^2}$
  - Block SOR and factorization
  - Symbolic factorization works with blocks (much cheaper)
  - Very regular memory access, unrolled dense kernels
  - Faster insertion: `MatSetValuesBlocked()`

Performance of assembled versus unassembled



- Arithmetic intensity for Q_p elements
  - $\leq \frac{1}{4}$ (assembled), ≈ 10 (unassembled), ≈ 4 (hardware)
- store Jacobian information at Quass quadrature points, can use AD

Optimizing unassembled Mat-Vec

- High order spatial discretizations do more work per node
  - Dense tensor product kernel (like small BLAS3)
  - Cubic (Q_3) elements in 3D can achieve $> 70\%$ of peak FPU (compare to $< 5\%$ for assembled operators on multicore)
  - Can store Jacobian information at quadrature points (usually pays off for Q_2 and higher in 3D)
  - Spectral, WENO, DG, FD
  - Often still need an assembled operator for preconditioning
- Boundary element methods
  - Dense kernels
  - Fast Multipole Method (FMM)
- Preconditioning requires more effort
  - Useful have code to assemble matrices: try out new methods quickly

Optimizing unassembled Mat-Vec

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  - Dense kernels
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- Preconditioning requires more effort
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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

Outline

7. Representative examples and algorithms
   - Hydrostatic Ice
   - Driven cavity
8. Hard problems
9. Recent developments in PETSc
   - Improved multiphysics support
   - Variational inequalities

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Hydrostatic equations for ice sheet flow

- Valid when $w_x \ll u_z$, independent of basal friction (Schoof&Hindmarsh 2010)
- Eliminate p and w from Stokes by incompressibility:
  3D elliptic system for $u = (u, v)$

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

$$\eta(\theta, \gamma) = \frac{B(\theta)}{2} (\gamma_0 + \gamma)^{\frac{1-\mathfrak{n}}{2\mathfrak{n}}}, \qquad \mathfrak{n} \approx 3$$

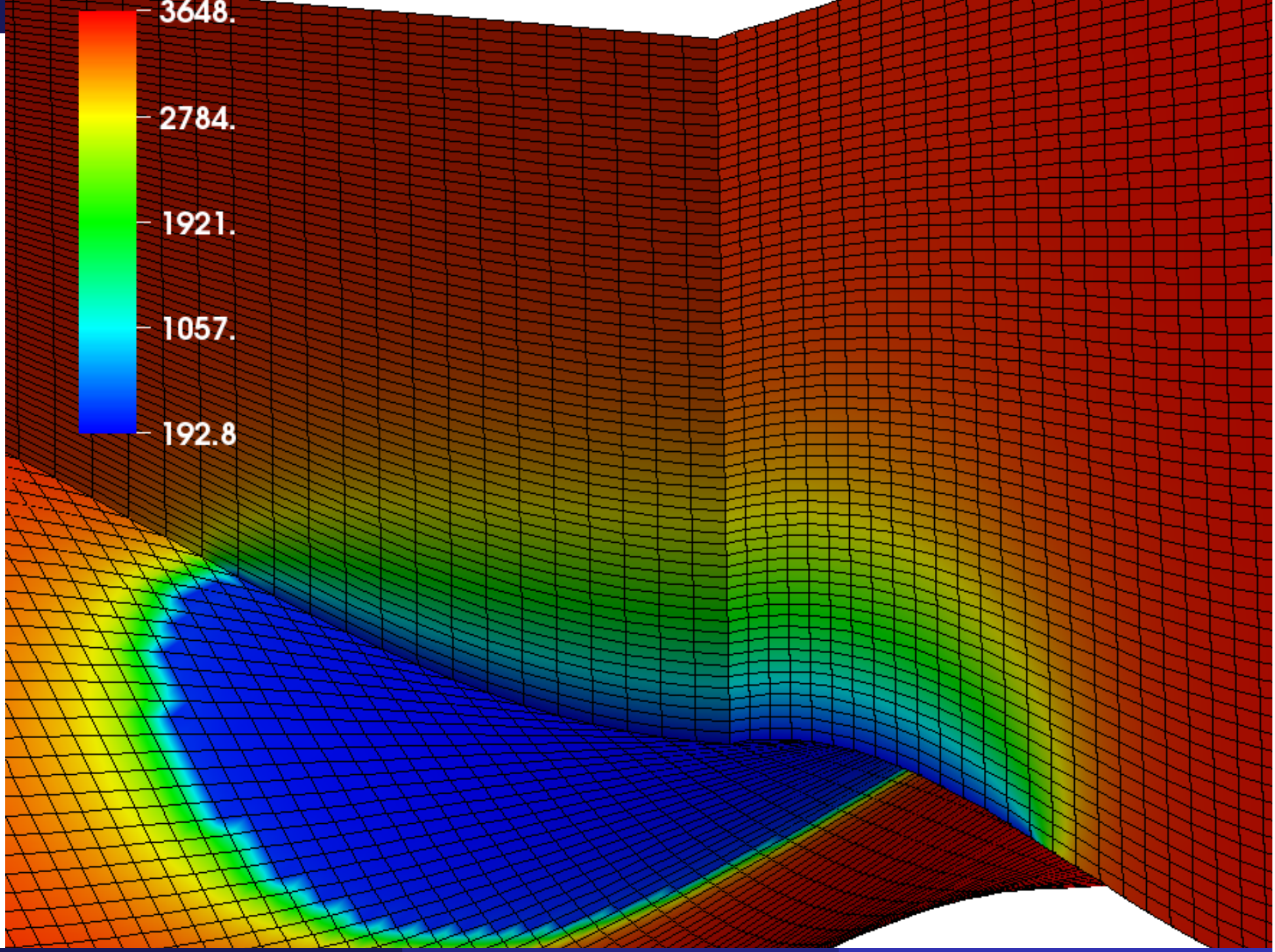
$$\gamma = u_x^2 + v_y^2 + u_x v_y + \frac{1}{4}(u_y + v_x)^2 + \frac{1}{4} u_z^2 + \frac{1}{4} v_z^2$$

and slip boundary $\sigma \cdot n = \beta^2 u$ where

$$\beta^2(\gamma_b) = \beta_0^2 (\varepsilon_b^2 + \gamma_b)^{\frac{\mathfrak{m}-1}{2}}, \qquad 0 < \mathfrak{m} \leq 1$$

$$\gamma_b = \frac{1}{2}(u^2 + v^2)$$

- Q_1 FEM with Newton-Krylov-Multigrid solver in PETSc:
  `src/snes/examples/tutorials/ex48.c`


3648.
2784.
1921.
1057.
192.8

Some Multigrid Options

- `-snes_grid_sequence`: [0]
  Solve nonlinear problems on coarse grids to get initial guess
- `-pc_mg_galerkin`: [FALSE]
  Use Galerkin process to compute coarser operators
- `-pc_mg_type`: [FULL]
  (choose one of) MULTIPLICATIVE ADDITIVE FULL KASKADE
- `-mg_coarse_{ksp,pc}_*`
  control the coarse-level solver
- `-mg_levels_{ksp,pc}_*`
  control the smoothers on levels
- `-mg_levels_3_{ksp,pc}_*`
  control the smoother on specific level
- These also work with ML's algebraic multigrid.

What is this doing?

- `mpiexec -n 4 ./ex48 -M 16 -P 2 -da_refine_hierarchy_x 1,8,8 -da_refine_hierarchy_y 2,1,1 -da_refine_hierarchy_z 2,1,1 -snes_grid_sequence 1 -log_summary -ksp_converged_reason -ksp_gmres_modifiedgramschmidt -ksp_monitor -ksp_rtol 1e-2 -pc_mg_type multiplicative -mg_coarse_pc_type lu -mg_levels_0_pc_type lu -mg_coarse_pc_factor_mat_solver_package mumps -mg_levels_0_pc_factor_mat_solver_package mumps -mg_levels_1_sub_pc_type cholesky -snes_converged_reason -snes_monitor -snes_stol 1e-12 -thi_L 80e3 -thi_alpha 0.05 -thi_friction_m 0.3 -thi_hom x -thi_nlevels 4`
- What happens if you remove `-snes_grid_sequence`?
- What about solving with block Jacobi, ASM, or algebraic multigrid?

Outline

7. Representative examples and algorithms
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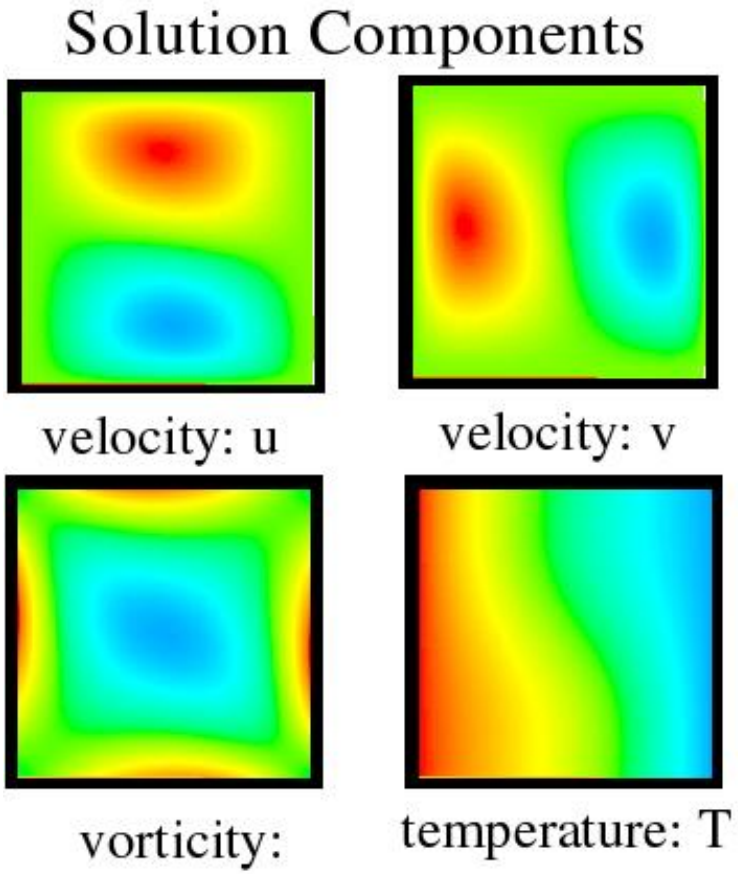
SNES Example

Driven Cavity



- Velocity-vorticity formulation
- Flow driven by lid and/or bouyancy
- Logically regular grid
  - Parallelized with `DMDA`
- Finite difference discretization
- Authored by David Keyes

`src/snes/examples/tutorials/ex19.c`

SNES Example

Driven Cavity Application Context

```
/* Collocated at each node */
typedef struct {
  PetscScalar u,v,omega,temp;
} Field;

typedef struct {
        /* physical parameters */
   PassiveReal lidvelocity,prandtl,grashof;
        /* color plots of the solution */
   PetscTruth  draw_contours;
} AppCtx;
```

SNES Example

```
DrivenCavityFunction(SNES snes, Vec X, Vec F, void *ptr) {
  AppCtx         *user = (AppCtx *) ptr;
  /* local starting and ending grid points */
  PetscInt        istart, iend, jstart, jend;
  PetscScalar     *f;              /* local vector data */
  PetscReal       grashof = user->grashof;
  PetscReal       prandtl = user->prandtl;
  PetscErrorCode ierr;

  /* Code to communicate nonlocal ghost point data */
  VecGetArray(F, &f);

  /* Loop over local part and assemble into f[idxloc] */
  /* .... */

  VecRestoreArray(F, &f);
  return 0;
}
```

SNES Example with local evaluation

```
PetscErrorCode DrivenCavityFuncLocal(DMDALocalInfo *info,
                    Field **x,Field **f,void *ctx) {
  /* Handle boundaries ... */
  /* Compute over the interior points */
  for(j = info->ys; j < info->ys+info->ym; j++) {
    for(i = info->xs; i < info->xs+info->xm; i++) {
      /* convective coefficients for upwinding ... */
      /* U velocity */
      u          = x[j][i].u;
      uxx        = (2.0*u - x[j][i-1].u - x[j][i+1].u)*hydhx;
      uyy        = (2.0*u - x[j-1][i].u - x[j+1][i].u)*hxdhy;
      f[j][i].u  = uxx + uyy - .5*(x[j+1][i].omega-x[j-1][i].omega
      /* V velocity, Omega ... */
      /* Temperature */
      u            = x[j][i].temp;
      uxx          = (2.0*u - x[j][i-1].temp - x[j][i+1].temp)*hy
      uyy          = (2.0*u - x[j-1][i].temp - x[j+1][i].temp)*hx
      f[j][i].temp =  uxx + uyy + prandtl
        * (  (vxp*(u - x[j][i-1].temp) + vxm*(x[j][i+1].temp - u))
           + (vyp*(u - x[j-1][i].temp) + vym*(x[j+1][i].temp - u))
```

Running the driven cavity

- `./ex19 -lidvelocity 100 -grashof 1e2 -da_grid_x 16 -da_grid_y 16 -snes_monitor -snes_view -da_refine 2`
- `./ex19 -lidvelocity 100 -grashof 1e4 -da_grid_x 16 -da_grid_y 16 -snes_monitor -snes_view -da_refine 2`
- `./ex19 -lidvelocity 100 -grashof 1e5 -da_grid_x 16 -da_grid_y 16 -snes_monitor -snes_view -da_refine 2 -pc_type lu`
- Uh oh, we have convergence problems
- Does `-snes_grid_sequence` help?

Running the driven cavity

- `./ex19 -lidvelocity 100 -grashof 1e2 -da_grid_x 16 -da_grid_y 16 -snes_monitor -snes_view -da_refine 2`

```
lid velocity = 100, prandtl # = 1, grashof # = 1000
0 SNES Function norm 7.682893957872e+02
1 SNES Function norm 6.574700998832e+02
2 SNES Function norm 5.285205210713e+02
3 SNES Function norm 3.770968117421e+02
4 SNES Function norm 3.030010490879e+02
5 SNES Function norm 2.655764576535e+00
6 SNES Function norm 6.208275817215e-03
7 SNES Function norm 1.191107243692e-07
Number of SNES iterations = 7
```

- `./ex19 -lidvelocity 100 -grashof 1e4 -da_grid_x 16 -da_grid_y 16 -snes_monitor -snes_view -da_refine 2`
- `./ex19 -lidvelocity 100 -grashof 1e5 -da_grid_x 16 -da_grid_y 16 -snes_monitor -snes_view -da_refine 2 -pc_type lu`
- Uh oh, we have convergence problems
- Does `-snes_grid_sequence` help?

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- `./ex19 -lidvelocity 100 -grashof 1e2 -da_grid_x 16 -da_grid_y 16 -snes_monitor -snes_view -da_refine 2`
- `./ex19 -lidvelocity 100 -grashof 1e4 -da_grid_x 16 -da_grid_y 16 -snes_monitor -snes_view -da_refine 2`

```
lid velocity = 100, prandtl # = 1, grashof # = 10000
0 SNES Function norm 7.854040793765e+02
1 SNES Function norm 6.630545177472e+02
2 SNES Function norm 5.195829874590e+02
3 SNES Function norm 3.608696664876e+02
4 SNES Function norm 2.458925075918e+02
5 SNES Function norm 1.811699413098e+00
6 SNES Function norm 4.688284580389e-03
7 SNES Function norm 4.417003604737e-08
Number of SNES iterations = 7
```

- `./ex19 -lidvelocity 100 -grashof 1e5 -da_grid_x 16 -da_grid_y 16 -snes_monitor -snes_view -da_refine 2 -pc_type lu`
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- `./ex19 -lidvelocity 100 -grashof 1e5 -da_grid_x 16 -da_grid_y 16 -snes_monitor -snes_view -da_refine 2 -pc_type lu`

```
lid velocity = 100, prandtl # = 1, grashof # = 100000
0 SNES Function norm 1.809960438828e+03
1 SNES Function norm 1.678372489097e+03
2 SNES Function norm 1.643759853387e+03
3 SNES Function norm 1.559341161485e+03
4 SNES Function norm 1.557604282019e+03
5 SNES Function norm 1.510711246849e+03
6 SNES Function norm 1.500472491343e+03
7 SNES Function norm 1.498930951680e+03
8 SNES Function norm 1.498440256659e+03
...
```

- Uh oh, we have convergence problems
- Does `-snes_grid_sequence` help?

Running the driven cavity

- `./ex19 -lidvelocity 100 -grashof 1e2 -da_grid_x 16 -da_grid_y 16 -snes_monitor -snes_view -da_refine 2`
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- Uh oh, we have convergence problems
- Does `-snes_grid_sequence` help?

Why isn't SNES converging?

- The Jacobian is wrong (maybe only in parallel)
  - Check with `-snes_type test` and `-snes_mf_operator -pc_type lu`
- The linear system is not solved accurately enough
  - Check with `-pc_type lu`
  - Check `-ksp_monitor_true_residual`, try right preconditioning
- The Jacobian is singular with inconsistent right side
  - Use `MatNullSpace` to inform the `KSP` of a known null space
  - Use a different Krylov method or preconditioner
- The nonlinearity is just really strong
  - Run with `-info` or `-snes_ls_monitor` (petsc-dev) to see line search
  - Try using trust region instead of line search `-snes_type tr`
  - Try grid sequencing if possible
  - Use a continuation

Globalizing the lid-driven cavity

- Pseudotransient continuation continuation (Ψtc)
  - Do linearly implicit backward-Euler steps, driven by steady-state residual
  - Residual-based adaptive controller retains quadratic convergence in terminal phase
- Implemented in `src/ts/examples/tutorials/ex26.c`
- `$ ./ex26 -ts_type pseudo -lidvelocity 100 -grashof 1e5 -da_grid_x 16 -da_grid_y 16 -ts_monitor`
- Make the method nonlinearly implicit: `-snes_type ls -snes_monitor`
  - Compare required number of linear iterations
- Try error-based adaptivity: `-ts_type rosw`
- Try increasing `-lidvelocity`, `-grashof`, and problem size
- Coffey, Kelley, and Keyes, Pseudotransient continuation and differential algebraic equations, SIAM J. Sci. Comp, 2003.

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- `$ ./ex26 -ts_type pseudo -lidvelocity 100 -grashof 1e5 -da_grid_x 16 -da_grid_y 16 -ts_monitor`

```
16x16 grid, lid velocity = 100, prandtl # = 1, grashof # = 100000
0 TS dt 0.03125 time 0
1 TS dt 0.034375 time 0.034375
2 TS dt 0.0398544 time 0.0742294
3 TS dt 0.0446815 time 0.118911
4 TS dt 0.0501182 time 0.169029
...
24 TS dt 3.30306 time 11.2182
25 TS dt 8.24513 time 19.4634
26 TS dt 28.1903 time 47.6537
27 TS dt 371.986 time 419.64
28 TS dt 379837 time 380257
29 TS dt 3.01247e+10 time 3.01251e+10
30 TS dt 6.80049e+14 time 6.80079e+14

CONVERGED_TIME at time 6.80079e+14 after 30 steps
```

- Make the method nonlinearly implicit: `-snes_type ls -snes_monitor`
  - Compare required number of linear iterations

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- Implemented in `src/ts/examples/tutorials/ex26.c`
- `$ ./ex26 -ts_type pseudo -lidvelocity 100 -grashof 1e5 -da_grid_x 16 -da_grid_y 16 -ts_monitor`
- Make the method nonlinearly implicit: `-snes_type ls -snes_monitor`
  - Compare required number of linear iterations
- Try error-based adaptivity: `-ts_type rosw`
- Try increasing `-lidvelocity`, `-grashof`, and problem size
- Coffey, Kelley, and Keyes, Pseudotransient continuation and differential algebraic equations, SIAM J. Sci. Comp, 2003.

Nonlinear multigrid (full approximation scheme)

- V-cycle structure, but use nonlinear relaxation and skip the matrices
- `./ex19 -da_refine 4 -snes_monitor -snes_type nrichardson -npc_fas_levels_snes_type gs -npc_fas_levels_snes_gs_sweeps 3 -npc_snes_type fas -npc_fas_levels_snes_type gs -npc_snes_max_it 1 -npc_snes_fas_smoothup 6 -npc_snes_fas_smoothdown 6 -lidvelocity 100 -grashof 4e4`
- `./ex19 -da_refine 4 -snes_monitor -snes_type ngmres -npc_fas_levels_snes_type gs -npc_fas_levels_snes_gs_sweeps 3 -npc_snes_type fas -npc_fas_levels_snes_type gs -npc_snes_max_it 1 -npc_snes_fas_smoothup 6 -npc_snes_fas_smoothdown 6 -lidvelocity 100 -grashof 4e4`

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```
lid velocity = 100, prandtl # = 1, grashof # = 40000
0 SNES Function norm 1.065744184802e+03
1 SNES Function norm 5.213040454436e+02
2 SNES Function norm 6.416412722900e+01
3 SNES Function norm 1.052500804577e+01
4 SNES Function norm 2.520004680363e+00
5 SNES Function norm 1.183548447702e+00
6 SNES Function norm 2.074605179017e-01
7 SNES Function norm 6.782387771395e-02
8 SNES Function norm 1.421602038667e-02
9 SNES Function norm 9.849816743803e-03
10 SNES Function norm 4.168854365044e-03
11 SNES Function norm 4.392925390996e-04
12 SNES Function norm 1.433224993633e-04
13 SNES Function norm 1.074357347213e-04
14 SNES Function norm 6.107933844115e-05
15 SNES Function norm 1.509756087413e-05
16 SNES Function norm 3.478180386598e-06

Number of SNES iterations = 16
```

- `./ex19 -da_refine 4 -snes_monitor -snes_type ngmres -npc_fas_levels_snes_type gs -npc_fas_levels_snes_gs_sweeps 3 -npc_snes_type fas -npc_fas_levels_snes_type gs`

Nonlinear multigrid (full approximation scheme)

- V-cycle structure, but use nonlinear relaxation and skip the matrices
- `./ex19 -da_refine 4 -snes_monitor -snes_type nrichardson -npc_fas_levels_snes_type gs -npc_fas_levels_snes_gs_sweeps 3 -npc_snes_type fas -npc_fas_levels_snes_type gs -npc_snes_max_it 1 -npc_snes_fas_smoothup 6 -npc_snes_fas_smoothdown 6 -lidvelocity 100 -grashof 4e4`
- `./ex19 -da_refine 4 -snes_monitor -snes_type ngmres -npc_fas_levels_snes_type gs -npc_fas_levels_snes_gs_sweeps 3 -npc_snes_type fas -npc_fas_levels_snes_type gs -npc_snes_max_it 1 -npc_snes_fas_smoothup 6 -npc_snes_fas_smoothdown 6 -lidvelocity 100 -grashof 4e4`

```
lid velocity = 100, prandtl # = 1, grashof # = 40000
0 SNES Function norm 1.065744184802e+03
1 SNES Function norm 9.413549877567e+01
2 SNES Function norm 2.117533223215e+01
3 SNES Function norm 5.858983768704e+00
4 SNES Function norm 7.303010571089e-01
5 SNES Function norm 1.585498982242e-01
6 SNES Function norm 2.963278257962e-02
7 SNES Function norm 1.152790487670e-02
8 SNES Function norm 2.092161787185e-03
9 SNES Function norm 3.129419807458e-04
10 SNES Function norm 3.503421154426e-05
11 SNES Function norm 2.898344063176e-06

Number of SNES iterations = 11
```

Outline

7 Representative examples and algorithms
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- Driven cavity

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- Improved multiphysics support
- Variational inequalities

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

Coupled approach to multiphysics

- Smooth all components together
  - Block SOR is the most popular
  - Block ILU sometimes more robust (e.g. transport/anisotropy)
  - Vanka field-split smoothers or for saddle-point problems
  - Distributive relaxation
- Scaling between fields is critical
- Indefiniteness
  - Make smoothers and interpolants respect inf-sup condition
  - Difficult to handle anisotropy
  - Exotic interpolants for Helmholtz
- Transport
  - Define smoother in terms of first-order upwind discretization (*h*-ellipticity)
  - Evaluate residuals using high-order discretization
  - Use Schur field-split: “parabolize” at top level or for smoother on levels
- Multigrid inside field-split or field-split inside multigrid
- Open research area, hard to write modular software

"Physics-based" preconditioners (semi-implicit method)

Shallow water with stiff gravity wave

h is hydrostatic pressure, u is velocity, $\sqrt{gh}$ is fast wave speed

$$h_t - (uh)_x = 0$$
$$(uh)_t + (u^2 h + \frac{1}{2} g h^2)_x = 0$$

Semi-implicit method

Suppress spatial discretization, discretize in time, implicitly for the terms contributing to the gravity wave

$$\frac{h^{n+1} - h^n}{\Delta t} + (uh)_x^{n+1} = 0$$
$$\frac{(uh)^{n+1} - (uh)^n}{\Delta t} + (u^2 h)_x^n + g(h^n h^{n+1})_x = 0$$

Rearrange, eliminating $(uh)^{n+1}$

$$\frac{h^{n+1} - h^n}{\Delta t} - \Delta t (g h^n h_x^{n+1})_x = -(\text{known})^n$$

Delta form

- Preconditioner should work like the Newton step: $-F(x) \mapsto \delta x$
- Recast semi-implicit method in delta form

$$\frac{\delta h}{\Delta t} + (\delta uh)_x = -F_0, \quad \frac{\delta uh}{\Delta t} + gh^n(\delta h)_x = -F_1, \quad \widehat{J} = \begin{pmatrix} \frac{1}{\Delta t} & \nabla\cdot \\ gh^n\nabla & \frac{1}{\Delta t} \end{pmatrix}$$

- Eliminate δuh

$$\frac{\delta h}{\Delta t} - \Delta t(gh^n(\delta h)_x)_x = -F_0 + (\Delta t F_1)_x, \quad S \sim \frac{1}{\Delta t} - g\Delta t\nabla\cdot h^n\nabla$$

- Solve for δh, then evaluate

$$\delta uh = -\Delta t\left[gh^n(\delta h)_x - F_1\right]$$

- Fully implicit solver
  - Is nonlinearly consistent (no splitting error)
  - Implementation used same code as semi-implicit method
  - Efficient bifurcation analysis, steady-state analysis, data assimilation
- IMEX methods can also be high order, only need "stiff part" $\widehat{J}$

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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

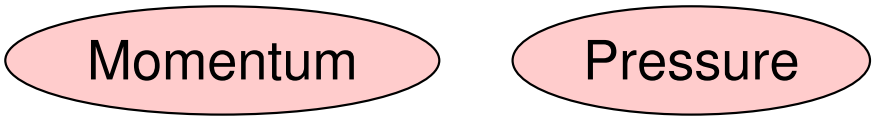
Split

- 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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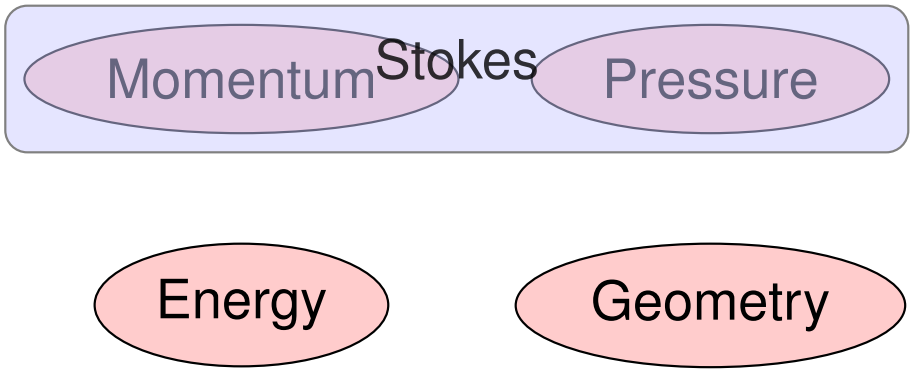

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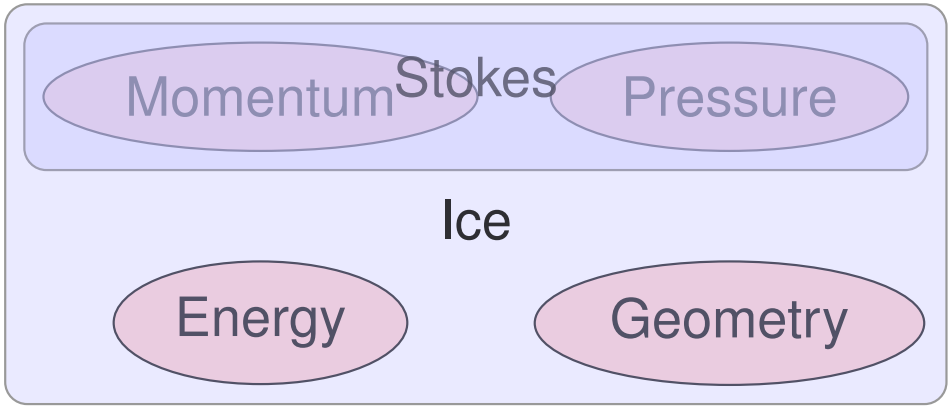

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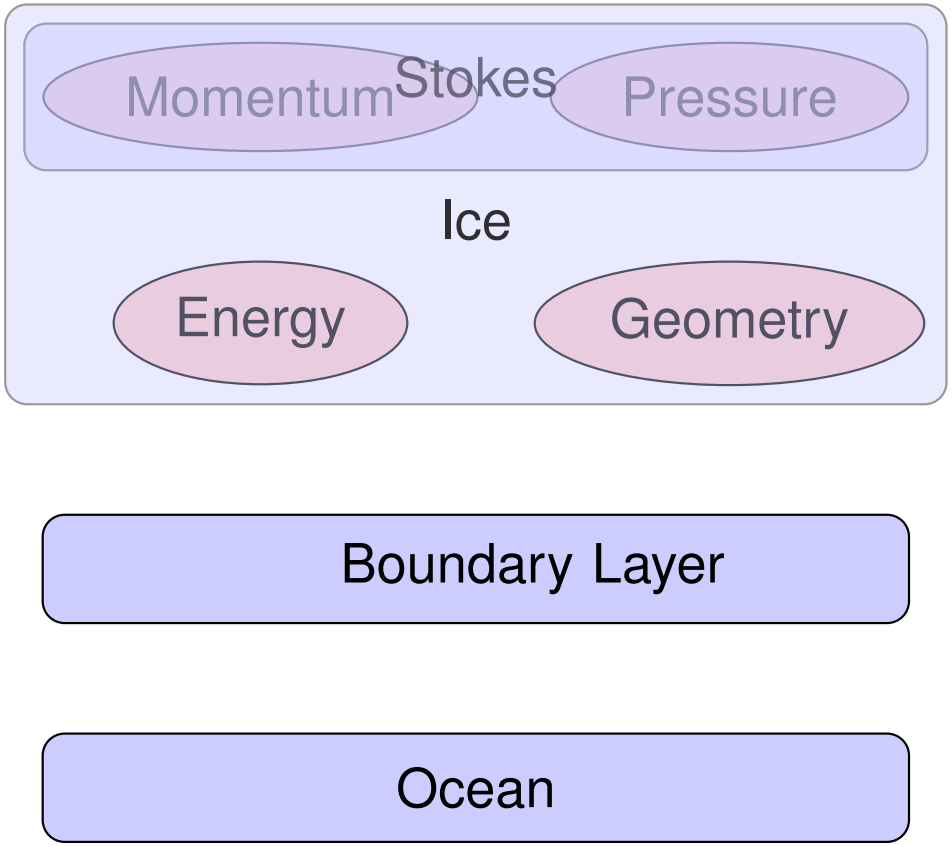

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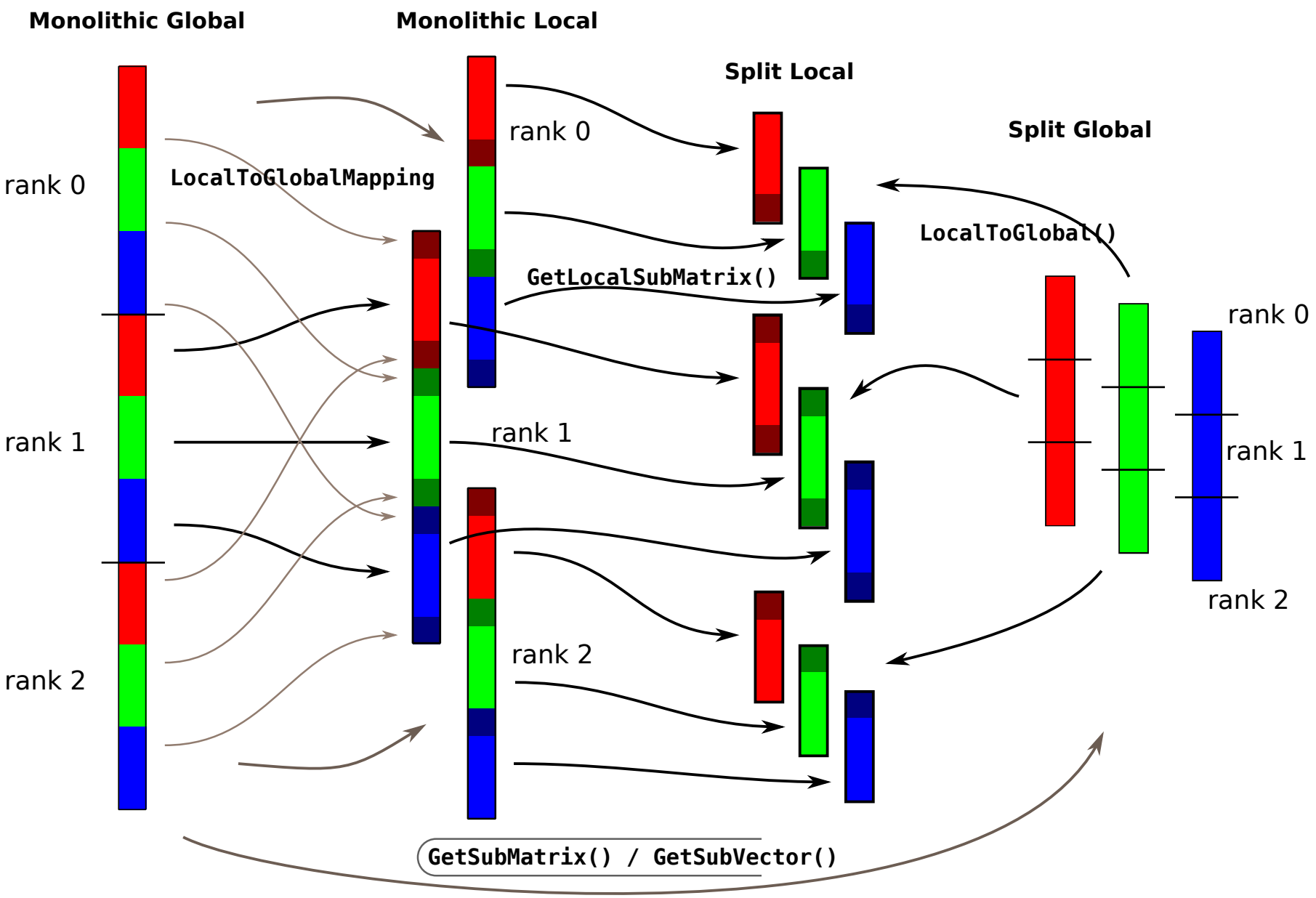

Work in Split Local space, matrix data structures reside in any space.

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);
  DMDAGetLocalInfo(dau,&infou);
  DMDAGetLocalInfo(dak,&infok);
  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 g
  FormFunctionLocal_K(user,&infok,u,k,fk); // k residual with u g
  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 phy
  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 phy
  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

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Variational Inequalities

- Supports inequality and box constraints on solution variables.
- Solution methods
  - Semismooth Newton
    - reformulate problem as a non-smooth system, Newton on subdifferential
    - Newton step solves diagonally perturbed systems
  - Active set
    - similar linear algebra to solving PDE
    - solve in reduced space by eliminating constrained variables
    - or enforce constraints by Lagrange multipliers
    - sometimes slower convergence or “bouncing”
- composes with multigrid and field-split
- demonstrated optimality for phase-field problems with millions of degrees of freedom

References

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