Introduction to using PETSc for scientific computing

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Outline

1. Introduction
2. PETSc data structures and classes
3. Solving problems
4. Scaling of solutions

Outline

Source code for workshop examples

Exercise 1: Get example codes

Available in the git repository:

`https://github.com/kevinrichardgreen/petsc_westgrid_workshop`

Clone to the machine where you want to work:

```
$ ssh username@graham.computecanada.ca
$ git clone https://github.com/kevinrichardgreen/petsc_westgrid_workshop
```

The pdf of these slides is in there too.

During the workshop

- Stop me to ask for clarifications.
  - I'll do my best to help out / point you in the right direction.
  - I don't know everything $\in \Omega_{\mathrm{PETSc}}$, but
  - We can all learn from this!
- Take some notes. I say things that aren't necessarily written down here.

PETSc

https://www.mcs.anl.gov/petsc/

PETSc (|' petsi: |) stands for the Portable, Extensible Toolkit for Scientific computing.

It provides a suite of libraries for the numerical solution of partial differential equations (PDEs) and related problems.

Portable Extensible Toolkit for Scientific computing

- Architecture
  - tightly coupled (e.g. Cray, Blue Gene)
  - 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 (2-clause BSD license), open development
- 10^{12} unknowns, full-machine scalability on Top-10 systems
- Same code runs performantly on a laptop

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

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 best 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, Underworld, PFLOTRAN, MOOSE, Proteus, PyClaw, CHASTE
- Algorithm Developers (iterative methods and preconditioning)
- Package Developers
  - SLEPc, TAO, Deal.II, Libmesh, FEniCS, PETSc-FEM, MagPar, OOFEM, FreeCFD, OpenFVM, Nektar++
- Hundreds of tutorial-style examples
- Hyperlinked manual, examples, and manual pages for all routines
- Support from `petsc-maint@mcs.anl.gov`, `petsc-users@mcs.anl.gov`

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

PETSc installation

Installing on your own machine (see Appendix)

Installing on a cluster:

- Don't do it.
- Use pre-built install.
- Consult with computing staff if not available.

Enabling PETSc

PETSc requires a couple of environment variables to be set:

- `PETSC_DIR` - the top level directory of PETSc
- `PETSC_ARCH` - the *architecture* for which PETSc has been built

Allows multiple `ARCH` types built on a given system, which can easily be swapped for your specific application code.
ie., having a version configured with debugging flags enabled, and a version without.

Generally on a cluster, `PETSC_ARCH` is left empty, and only an optimized build is maintained.

On graham.computecanada.ca

PETSc is pre-built and has modules for multiple versions:

```
$ module load petsc/3.8.2
```

This sets up the required environment for compiling PETSc application programs.

The programs can then be run as any other MPI programs.

Testing your PETSc environment

Exercise 2: Testing PETSc env

```
$ module load petsc/3.8.2
$ cd petsc_westgrid_workshop/examples/test
$ make MPIVersion
```

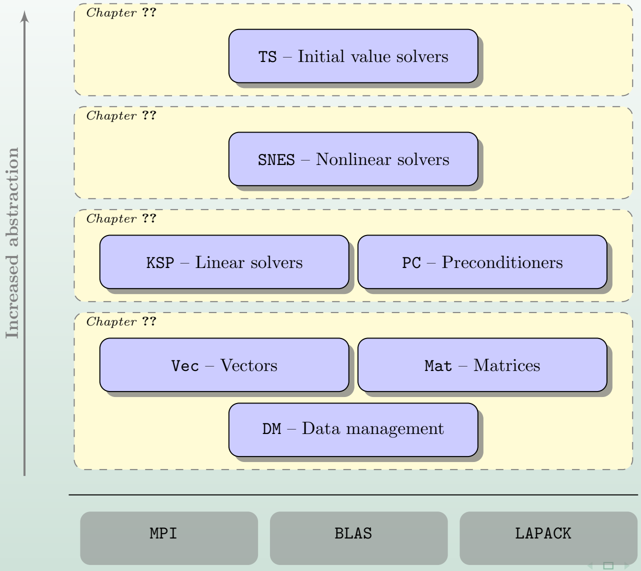
- Submit the executable as an MPI job using 8 cores, what kind of memory bandwidth does it show?
- Try submissions with 1, 8, 16, 32 cores.
- Try submissions with different numbers of nodes.

Outline

PETSc atomic data types

- `PetscInt`
  - defaults to 32bit integer
  - can be 64bit int if you're dealing with many unknowns (`--with-64-bit-indices`)
- `PetscScalar`
  - Primary type for your unknowns, depending on configuration can be:
    - Double precision real (default) or complex
    - Single precision
    - Quad precision
- `PetscReal`
  - Same precision as `PetscScalar`, but always real

PETSc hierarchy



Message passing interface (MPI)

Typically, user does not call MPI functions directly.

At most, `MPI_Comm_size()` and `MPI_Comm_rank()` should be used. All other MPI communication functions are wrapped within `PETSc` routines.

However, some degree of understanding how MPI works is needed to create `PETSc` code that can scale well.

MPI communicators in PETSc

- 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: *ie.*, `VecGetLocalSize()`, `MatSetValues()`
  - Logically Collective: *ie.*, `KSPSetType()`
    - checked when running in debug mode
  - Neighbor-wise Collective: `VecScatterBegin()`, `MatMult()`
    - Point-to-point communication between two processes
  - Collective: `VecNorm()`, `MatAssemblyBegin()`, `KSPCreate()`
    - Global communication, synchronous
- Deadlock if some process doesn't participate (e.g. wrong order)

PetscObject

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 command line
`SetUp()`	perform other initialization
`View()`	view the object
`Destroy()`	cleanup object allocation

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

Options

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]`

Vectors (`Vec`)

- Extension of arrays.
  - Parallel (global) representations
  - Serial (local) representations
- Think of them just like vectors in linear algebra.
- Used most often to store:
  - solution to your problem
  - residuals - nonlinear and linear
- Can be used to hold location dependent field data for the problem as well.
- Can extract data as arrays for manipulation.

Distributed `Vec`

Parallel vector stored on 3 processors, as an example

$$\mathbf{u}_{\text{global}} = \begin{bmatrix} u_0 \\ u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \\ u_6 \\ u_7 \end{bmatrix} \qquad \begin{cases} \mathbf{u}^{(0)}_{\text{local}} = \begin{bmatrix} u_0 & u_1 & u_2 & \mathbf{u}^{(0)\,T}_{\text{ghost}} \end{bmatrix}^T \\ \\ \mathbf{u}^{(1)}_{\text{local}} = \begin{bmatrix} u_3 & u_4 & u_5 & \mathbf{u}^{(1)\,T}_{\text{ghost}} \end{bmatrix}^T \\ \\ \mathbf{u}^{(2)}_{\text{local}} = \begin{bmatrix} u_6 & u_7 & \mathbf{u}^{(2)\,T}_{\text{ghost}} \end{bmatrix}^T \end{cases}$$

Vec operations

Man pages:
`http://www.mcs.anl.gov/petsc/petsc-current/docs/manualpages/Vec/index.html`

- Things you expect with vectors:
  - axpy, norms, dot products, etc.
- Explicit access to entries:
  - `VecGetArray()`, `VecRestoreArray()`
  - and their *read only* variants
- Parallel communication:
  - assembly, scatter, gather
- Examples: `petsc_westgrid_workshop/examples/vec/`

Vec exercise

Exercise 3: Basic vector routines

- Investigate the source code `examples/vec/ex1.c`, and the structure of its makefile.
- Set the vector size to 1000 using a command-line option.
- Investigate other options available to this program with the `-help` option.
- Can you get the program to output the line:
  `Total flops over all processors 32991.` ?

Matrices (Mat)

What are PETSc matrices?

- Linear operators on finite dimensional vector spaces.

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- Linear operators on finite dimensional vector spaces.
- 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, SuperLU, UMFPack, Hypre, Elemental

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Distributed Mat

Nonzero entries of a matrix stored on 3 processors.

$$\left[\begin{array}{ccc|ccc|cc}
1 & 2 & 0 & 3 & 0 & 0 & 4 & 0 \\
5 & 6 & 7 & 0 & 0 & 8 & 9 & 0 \\
0 & 10 & 11 & 12 & 0 & 0 & 13 & 14 \\
\hline
0 & 0 & 15 & 16 & 17 & 0 & 0 & 18 \\
19 & 0 & 0 & 20 & 21 & 22 & 23 & 0 \\
0 & 24 & 0 & 0 & 25 & 26 & 27 & 28 \\
\hline
0 & 29 & 0 & 0 & 0 & 30 & 31 & 32 \\
33 & 0 & 0 & 34 & 35 & 0 & 36 & 37
\end{array}\right]
\begin{array}{l}
\text{Proc 0} \\ \\ \text{Proc 1} \\ \\ \text{Proc 2}
\end{array}$$

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.

Important matrices

- Sparse (e.g. discretization of a PDE operator)
- Inverse of *anything* interesting $B = A^{-1}$
- Jacobian of a nonlinear function $Jy = \lim_{\epsilon \to 0} \frac{F(x+\epsilon y)-F(x)}{\epsilon}$
- Fourier transform $\mathcal{F}, \mathcal{F}^{-1}$
- Other fast transforms, e.g. Fast Multipole Method
- Low rank correction $B = A + uv^T$
- Schur complement $S = D - CA^{-1}B$
- Tensor product $A = \sum_e A_x^e \otimes A_y^e \otimes A_z^e$
- Linearization of a few steps of a time integration

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- These matrices are dense. Never form them.

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

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- None of these matrices "have entries"

How to 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
- `MatSetBlockSize(Mat, int bs)`
- `MatXAIJSetPreallocation(Mat,...)`
- `MatSetValues(Mat,...)`
  - `MatSetValuesLocal, MatSetValuesStencil`
  - `MatSetValuesBlocked`
- `MatAssemblyBegin/End`

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

Krylov solvers for $Au = b$

- Finding solutions in the Krylov subspace: $\{b, Ab, A^2b, A^3b, \dots\}$
- Convergence rate depends on the spectral properties of the matrix
  - Existence of small polynomials $p_n(A) < \epsilon$ where $p_n(0) = 1$.
  - condition number $\kappa(A) = \|A\|\|A^{-1}\| = \sigma_{\max}/\sigma_{\min}$
  - distribution of singular values, spectrum Λ, pseudospectrum Λ_ϵ

Krylov subspace problem (KSP)

- Solving linear systems:

$$Au = b$$

- Various *Krylov* methods:
    - GMRES (`gmres`)
    - Conjugate gradient (`cg`)
    - Biconjugate gradient - stabilized (`bcgs`)
    - etc
- Direct methods (external packages recommended):
    - LU factorization
    - Cholesky factorization

Quintessential Krylov example: GMRES

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

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

How to set up a linear solver

- `KSPCreate(MPI_Comm, KSP *)`
- `KSPSetOperators(KSP, Mat A, Mat A_p)`
- `KSPSetFromOptions(KSP)`
  - Can set all aspects of solver at runtime
- `KSPGetPC(KSP,PC *)`
  - Explicitly get the preconditioner to manipulate
  - can be set from command line if `KSPSetFromOptions` was used
- `KSPSolve(KSP,Vec b, Vec u)`

Preconditioning?

Definition (Preconditioner)

A *preconditioner* $\mathbf{P}$ is a method for constructing a matrix (just a linear function, not assembled!) $P^{-1} = \mathbf{P}(A, A_p)$ using a matrix A and extra information A_p, such that the spectrum of $P^{-1}A$ (or AP^{-1}) is well-behaved.

PC idea

Idea: improve the conditioning of the Krylov operator

- Left preconditioning

$$(P^{-1}A)u = P^{-1}b$$

$$\{P^{-1}b, (P^{-1}A)P^{-1}b, (P^{-1}A)^2P^{-1}b, \ldots\}$$

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$$\{P^{-1}b, (P^{-1}A)P^{-1}b, (P^{-1}A)^2P^{-1}b, \dots\}$$

- Right preconditioning

$$(AP^{-1})Pu = b$$

$$\{b, (AP^{-1})b, (AP^{-1})^2b, \dots\}$$

PC idea

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$$\{P^{-1}b, (P^{-1}A)P^{-1}b, (P^{-1}A)^2P^{-1}b, \dots\}$$

- Right preconditioning

$$(AP^{-1})Pu = b$$

$$\{b, (AP^{-1})b, (AP^{-1})^2b, \dots\}$$

- The product $P^{-1}A$ or AP^{-1} is *not* formed.

KSP exercise

Exercise 4: Simple linear solve

- Looking at the code in `examples/ksp/ex2.c`, determine:
  - Where the matrix values are set.
  - Where the solver type is set.
  - How the error is computed.
- What are the default `KSP` type and `PC` type?
  - *Don't forget about* `-help`
- Do defaults change for serial and parallel execution?
- Can you solve the system with LU factorization?

LU factorization

- Handled as a preconditioner.

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LU factorization

- Handled as a preconditioner.
- Logic: LU factorization with back/forward substitution is a *perfect* left preconditioner.
- PETSc only provides a serial LU preconditioner...
- But we can use external packages for parallel solves: MUMPS, SuperLU_dist

LU example

Exercise 5: Solve with LU factorization

- Use the options:
  `-pc_type lu -pc_factor_mat_solver_package mumps`
  to solve using LU factorization in parallel.
- Look at `-ksp_view` to see what info this gives you.

An alternative is to use
`-pc_factor_mat_solver_package superlu_dist`.

Structured nonlinear equation solver (SNES)

- Standard form of a nonlinear system

$$F(u) = 0$$

- Newton 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: $|u^{n+1} - u^*| \in \mathcal{O}\left(|u^n - u^*|^2\right)$
- *Quasi-Newton* methods can use a different $J(u)$

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Example: Nonlinear Poisson equation

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

How to set up a SNES I

- `SNESCreate(SNES *)`
- The SNES interface is based upon callback functions
  - `FormFunction(...)`, set by `SNESSetFunction()`
  - `FormJacobian(...)`, set by `SNESSetJacobian()`
- When PETSc needs to evaluate F and J,
  - Solver calls the **user's** function
  - User function gets application state through the `ctx` variable
    - cast to/from a void pointer (see upcoming exercise)
    - PETSc *never* sees application data
- `SNESSetFromOptions(SNES)`
  `SNESSolve(SNES,Vec b, Vec u)`

How to set up a SNES II

The user provided function which calculates the **nonlinear residual** has signature

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

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

How to set up a SNES III

Similar story for the function to evaluate Jacobian:

```
PetscErrorCode (*func)(SNES snes,Vec u,Mat J,
                      Mat Jpre,void *ctx)
```

`u`: The current solution

`J`: The Jacobian

`Jpre`: The Jacobian preconditioning matrix (possibly `J` itself)

`ctx`: The user context passed to `SNESSetFunction()`

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- `J`: The Jacobian
- `Jpre`: The Jacobian preconditioning matrix (possibly `J` itself)
- `ctx`: The user context passed to `SNESSetFunction()`
  - Use this to pass application information, e.g. physical constants

Alternatively, you can use

- a built-in sparse finite difference approximation (“coloring”)

SNES global strategies

Newton's method can diverge if not close to a solution.

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Line search (`newtonls`):

1. Update **direction** determined by linear solve in Newton method
2. Update **size** chosen by maximizing decrease in nonlinear residual in the update direction

SNES global strategies

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Line search (`newtonls`):

1. Update **direction** determined by linear solve in Newton method
2. Update **size** chosen by maximizing decrease in nonlinear residual in the update direction

Trust region (`newtontr`):

1. Trust region **size** chosen based on how well a local approximation matches F
2. Update **direction** chosen by maximizing the decrease in nonlinear residual within the trust region

SNES exercise

Exercise 6: Simple nonlinear solve

- Investigate the code in `examples/snes/ex2.c` (note this is a serial example!), determine:
  - How the residual is evaluated.
  - How the Jacobian is evaluated.
  - What is the monitor doing?
- What are the default methods employed?
- Can you get the program to output the reason for convergence?
- Can you monitor the linear system solves as well?

Timestepping (TS)

Typically applied to *method of lines* discretizations of PDEs.

- Additive Runge-Kutta IMEX methods

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

  - Stiff part in G.
  - Orders 2 through 5, embedded error estimates
  - Dense output, hot starts for Newton
  - Extensible adaptive controllers
  - Easy to register new methods: `TSARKIMEXRegister()`
- Other more simple methods available
- Single step interface so user can control their own time loop

Some TS methods

TSTHETA	Theta methods
TSALPHA	Alpha methods
TSRK	Runge-Kutta methods
TSARKIMEX	2-Additive Runge-Kutta methods
TSBDF	Backward differentiation methods
TSROSW	Rosenbrock-W methods
TSSSP	Strong stability methods (Total variation diminishing)
TSGL	General linear methods - multi-stage/multi-step
TSSUNDIALS	SUNDIALS (external) ode integrators

How to set up a TS I

- `TSCreate(TS *)`
- User provides functions for:
  - Explicit rhs - `TSSetRHSFunction()`
  - Implicit lhs - `TSSetIFunction()`, `TSSetIJacobian()`
- `TSSetFromOptions(TS)`
- `TSSolve(TS,Vec u)`

How to set up a TS II

Function signatures:

- `FormRHSFunction(ts,t,u,F,void *ctx);`
- `FormIFunction(ts,t,u,udot,G,void *ctx);`
- `FormIJacobian(ts,t,u,udot,alpha,J,J_p,void *ctx);`

How to set up a TS II

Function signatures:

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- `FormIFunction(ts,t,u,udot,G,void *ctx);`
- `FormIJacobian(ts,t,u,udot,alpha,J,J_p,void *ctx);`

Can also supply:

- `FormRHSJacobian(ts,t,u,F,J,J_p,void *ctx);`

to use fully implicit methods.

TS exercise

Exercise 7: Simple time integration

- Investigate the source code in `examples/ts/ex3.c`, determine:
  - What problem is being solved, and how is it discretized?
  - Is its formulation slightly different from `TS` as outlined in this document?
  - What is special about linear time integration problems?
- What types of time integration methods can you use, what is the default?
- Run the program with the backward Euler method, solving the linear system with LU factorization.

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Spatial discretization

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- its *ghost values*, bordering portions of u that are local to other processes

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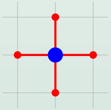
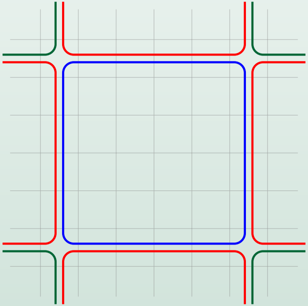
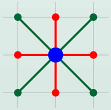
Example: logically rectangular grids



star-type stencil of width one





box-type stencil of width one

DMDA overview

Distribution **M**anager - **D**istributed **A**rrays

- handle allocation and communication requirements for logically rectangular grids.
- A subset of `DM`, which contains other formats (i.e., `DMPlex`, `DMFOREST`)
- Useful for finite difference and finite volume discretizations.

DMDA 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

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 (for Proc 0)

How to work with a DMDA I

Creation:

```
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

How to work with a DMDA II

Vectors and Matrices:

- 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!
- Can get arrays from either global or local vectors
  - `DMDAVecGetArray(DM,Vec,void *)`
  - `DMDAVecRestoreArray(DM,Vec,void *)`
- Matrices can be preallocated from DMDAs
  - `DMCreateMatrix(DM dm,Mat *mat)`

How to work with a DMDA III

Updating ghost values:

Two-step process, as with matrix assembly

- `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()`.

SNES and Jacobians

- May want to start off your problem solving by using a Finite differenced Jacobian approximation.
  - `-snes_fd`
- For data in a `DMDA`, coloring can be used to vastly speed up the finite differencing.
  - `-snes_fd_color`
- Using an analytic (coded) Jacobian will likely be the fastest.

FD Jacobian efficiency

Exercise 8: FD Jacobians

- Consider the code in `examples/snes/ex5.c` (This uses an analytical Jacobian)
- Run the code with the option `-da_refine 6`
    - What is this option doing?
- Compare run times when `-snes_fd` vs `-snes_fd_color` are used.

Convergence problems?

Why isn't `SNES` converging?

- Analytic Jacobians can be tricky to implement correctly for parallel code, your Jacobian may be wrong.
  - Check with `-snes_compare_explicit` and `-snes_mf_operator -pc_type lu`
- Linear system not solved accurately enough?
  - Try LU factorization
  - Try right preconditioning
  - Try `-ksp_true_residual`
- Singular Jacobian with inconsistent RHS
  - `MatNullSpace` can be used to set a known null space
- Really strong nonlinearity
  - `-snes_linesearch_monitor` to view behaviour of line search
  - Try `newtontr`

Debugging a Jacobian

Exercise 9: Output of `-snes_compare_explicit`

- Consider `exercises/snes/ex3.c`, in the `FormJacobian` function, investigate how the field arrays (`xx`) are obtained from the `DMDA`.
- Build and execute the code as is.
- Remove "`*xx[i]`" from line 467.
- Rebuild and execute the code. What happens to the solution?
- Use the command-line options:
  `-snes_compare_explicit -snes_max_it 1`
  - Which part indicates that the Jacobian is wrong?

Example codes

- PETSc has a wealth of example codes - exercises in this workshop have been taken directly from PETSc source.
- Generally located in `src/<classname>/example/tutorials` directories (see Appendix for obtaining source code).
- Hyperlinked in man pages, for example
  - http://www.mcs.anl.gov/petsc/petsc-current/docs/manualpages/TS/TSSolve.html
  - http://www.mcs.anl.gov/petsc/petsc-current/docs/manualpages/DM/DMDACreate3d.html

Nonlinear example: 3D Bratu problem

Bratu equation in 3D (`examples/snes/ex14.c`):

$$-\nabla^2 u - \lambda e^u = 0$$

$$(x, y, z) \in [0, 1]^3$$

$$u = 0 \text{ on boundary}$$

PDE TS example problem

Reaction diffusion problem in 2D (`examples/ts/ex5.c`):

$$
\begin{aligned}
u_t &= D_1 \nabla^2 u - uv^2 + \gamma(1-u) \\
v_t &= D_2 \nabla^2 + uv^2 - (\gamma + \kappa) v
\end{aligned}
$$

$$(x, y) \in [0, 1]^2$$

Periodic boundary conditions in all directions.

Outline

PETSc logging features

- Use `-log_view` 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
  - *ie.*, in Function or Jacobian assembly
  - flops within PETSc recorded automatically

Reading -log_view

- Look out for this:

```
##########################################################
#                                                        #
#                       WARNING!!!                       #
#                                                        #
#   This code was compiled with a debugging option,      #
#   To get timing results run ./configure                #
#   using --with-debugging=no, the performance will      #
#   be generally two or three times faster.              #
#                                                        #
##########################################################
```

- Get 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_view` when asking performance questions on the mailing lists

Reading -log_view II

```
------------------------------------------------------------------------------------------------------------------------
Event                Count      Time (sec)     Flops                             --- Global ---  --- Stage ---   Total
                   Max Ratio  Max     Ratio   Max  Ratio  Mess   Avg len Reduct  %T %F %M %L %R  %T %F %M %L %R Mflop/s
------------------------------------------------------------------------------------------------------------------------

--- Event Stage 0: Main Stage

SNESSolve              1 1.0 3.6435e+01 1.0 6.75e+10 1.0 0.0e+00 0.0e+00 0.0e+00100100  0  0  0 100100  0  0  0  1852
SNESFunctionEval       4 1.0 1.4375e-02 1.0 6.52e+06 1.0 0.0e+00 0.0e+00 0.0e+00  0  0  0  0  0   0  0  0  0  0   454
SNESJacobianEval       3 1.0 7.3466e-02 1.0 0.00e+00 0.0 0.0e+00 0.0e+00 0.0e+00  0  0  0  0  0   0  0  0  0  0     0
SNESLineSearch         3 1.0 1.7947e-02 1.0 1.38e+07 1.0 0.0e+00 0.0e+00 0.0e+00  0  0  0  0  0   0  0  0  0  0   768
VecDot                 3 1.0 4.9686e-04 1.0 8.89e+05 1.0 0.0e+00 0.0e+00 0.0e+00  0  0  0  0  0   0  0  0  0  0  1790
VecMDot             5319 1.0 7.9103e+00 1.0 2.44e+10 1.0 0.0e+00 0.0e+00 0.0e+00 22 36  0  0  0  22 36  0  0  0  3079
VecNorm             5505 1.0 8.8808e-01 1.0 1.63e+09 1.0 0.0e+00 0.0e+00 0.0e+00  2  2  0  0  0   2  2  0  0  0  1838
VecScale            5498 1.0 5.7987e-01 1.0 8.15e+08 1.0 0.0e+00 0.0e+00 0.0e+00  2  1  0  0  0   2  1  0  0  0  1405
VecCopy              185 1.0 3.4122e-02 1.0 0.00e+00 0.0 0.0e+00 0.0e+00 0.0e+00  0  0  0  0  0   0  0  0  0  0     0
VecSet               223 1.0 3.0877e-02 1.0 0.00e+00 0.0 0.0e+00 0.0e+00 0.0e+00  0  0  0  0  0   0  0  0  0  0     0
VecAXPY              355 1.0 6.0618e-02 1.0 1.05e+08 1.0 0.0e+00 0.0e+00 0.0e+00  0  0  0  0  0   0  0  0  0  0  1736
VecWAXPY               3 1.0 6.5303e-04 1.0 4.45e+05 1.0 0.0e+00 0.0e+00 0.0e+00  0  0  0  0  0   0  0  0  0  0   681
VecMAXPY            5498 1.0 9.9785e+00 1.0 2.59e+10 1.0 0.0e+00 0.0e+00 0.0e+00 27 38  0  0  0  27 38  0  0  0  2599
VecScatterBegin        7 1.0 1.0543e-03 1.0 0.00e+00 0.0 0.0e+00 0.0e+00 0.0e+00  0  0  0  0  0   0  0  0  0  0     0
VecReduceArith         6 1.0 9.5391e-04 1.0 1.78e+06 1.0 0.0e+00 0.0e+00 0.0e+00  0  0  0  0  0   0  0  0  0  0  1865
VecReduceComm          3 1.0 2.8610e-06 1.0 0.00e+00 0.0 0.0e+00 0.0e+00 0.0e+00  0  0  0  0  0   0  0  0  0  0     0
VecNormalize        5498 1.0 1.4746e+00 1.0 2.44e+09 1.0 0.0e+00 0.0e+00 0.0e+00  4  4  0  0  0   4  4  0  0  0  1658
MatMult             5498 1.0 6.2141e+00 1.0 7.32e+09 1.0 0.0e+00 0.0e+00 0.0e+00 17 11  0  0  0  17 11  0  0  0  1178
MatSolve            5498 1.0 1.0525e+01 1.0 7.32e+09 1.0 0.0e+00 0.0e+00 0.0e+00 29 11  0  0  0  29 11  0  0  0   695
MatLUFactorNum         3 1.0 2.2453e-02 1.0 4.83e+06 1.0 0.0e+00 0.0e+00 0.0e+00  0  0  0  0  0   0  0  0  0  0   215
MatILUFactorSym        1 1.0 5.4770e-03 1.0 0.00e+00 0.0 0.0e+00 0.0e+00 0.0e+00  0  0  0  0  0   0  0  0  0  0     0
MatAssemblyBegin       4 1.0 1.9073e-06 1.0 0.00e+00 0.0 0.0e+00 0.0e+00 0.0e+00  0  0  0  0  0   0  0  0  0  0     0
MatAssemblyEnd         4 1.0 7.3540e-03 1.0 0.00e+00 0.0 0.0e+00 0.0e+00 0.0e+00  0  0  0  0  0   0  0  0  0  0     0
```

Predicting resource usage - time

Made a little easier thanks to PETSc's extensive, minimally intrusive logging and profiling.

However, there are still many things that need to be observed to predict scaling in time

- Number of iterations may increase when problem is refined, which can lead to
  - Restarts (slows convergence rate greatly)
  - Loss of orthogonality (breaks convergence completely)
- Extra communication required for more stable algorithms:
  - Classical vs modified Gram–Schmidt
  - Increased iterations when only changing the number of processors

Time scaling

Exercise 10: 2D Bratu scaling

- Source code: `examples/snes/ex5.c`.
- Run with `-snes_monitor -ksp_monitor`.
- Observe number of `KSP` iterations for `da_refine` factors of 3,4,5.
- Estimate `KSP` iteration count for a refinement factor of 6.
- How close were you?

Summary

- PETSc can give you a fully scriptable process for experimenting with the large scale solution of PDE models.
- Plenty of existing examples to use as a starting point for what you want to accomplish.
- Don't be afraid to ask for help/clarification: `petsc-users@mcs.anl.gov`
  - But at least show that you've made some effort to understand the manual and/or example codes!

Appendix

5 References

6 Personal installation

For Further Reading I

- PETSc website: `http://www.mcs.anl.gov/petsc/`
  - pdf manual
  - man pages
  - talks/workshop pdfs
- Jed Brown: `http://jedbrown.org`
  - talks/workshop pdfs
  - PETSc and general scientific computing topics

Appendix

Obtaining PETSc source code

- Specific releases, zipped tarballs
  `http://www.mcs.anl.gov/petsc/download/`
- Git repository [preferred]
  `https://github.com/petsc/petsc`

Why is Git preferred?

- Public development repository, you can get *any* development version.
- All releases are just tags: eg. v3.7.6
- Easily rollback changes and releases.

Unpacking PETSc

Clone from repository:

```
git clone https://github.com/petsc/petsc
git checkout v3.8.2
```

OR

Unpack the archive:

```
tar xzf petsc.tar.gz
```

Configuring PETSc

- Set environment variable `$PETSC_DIR` to the installation root directory
- Choose a value for `PETSC_ARCH` (perhaps `c-debug` for a standard debug build)
- Run the configuration utility
  - `$PETSC_DIR/configure [--help]`
- May require additional dependencies
  - Read the output message if the configure fails, should tell you why, and suggest configure options to help

(Can be done under Cygwin in Windows)

External libraries

External libraries can be downloaded during the configuration phase.

For example, MUMPS and SuperLU_dist can be obtained with

```
--download-mumps --download-scalapack
```

and

```
--download-superlu_dist --download-metis --download-parmetis
```

respectively.

Buidling PETSc

After successful configure, run

```
$ make
$ make test
$ make streams
```