Time integration with PETSc

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Outline

Outline

Source code for example problems

All example codes from these lectures are available in the

```
Course Materials / PETSc / Examples
```

directory on Blackboard.
The (updated) pdf of these slides is also available on Blackboard.

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
- 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 (instructions to follow)

Installing on a cluster:

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

Obtaining PETSc source code

- Specific releases, zipped tarballs
  `http://www.mcs.anl.gov/petsc/download/`
- Git repository [preferred]
  `https://bitbucket.org/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://bitbucket.org/petsc/petsc.git
$ git checkout v3.7.6
```

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

External libraries

External libraries can be downloaded during the configuration phase.

For example, MUMPS and SuperLU_dist (efficient algorithms for direct solving of linear systems) 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
```

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.

Using PETSc on plato.usask.ca

I've built a version of PETScfor use throughout these lectures. Add the following to your ~/.bashrc file:

```
source /home/krg958/petsc/math314.env
```

This sets up the required environment for compiling PETSc application programs. The programs can then be run as any other MPI programs. eg. with the Slurm job scheduler (template given with examples):

```
$ sbatch submit_template.slurm
```

More info about submitting jobs on plato can be found here
It is important that you edit at least the following for each submission:

- executable name
- maximum runtime
- maximum RAM

Installing yourself

Exercise 1: Personal installation

Install PETSc `v3.7.6` on a machine you use regularly. Set it up with the following properties

- configured with MUMPS with debugging symbols
- `PETSC_ARCH=MUMPS-debug`

Install a second version with

- configured with MUMPS and no debugging symbols
- `PETSC_ARCH=MUMPS-opt`

Testing your PETSc environment

Exercise 2: Testing memory bandwidth of your system

With `PETSC_DIR` and `PETSC_ARCH` set appropriately for your current system:

- Build the `MPIVersion.c` example code.
- Run the `MPIVersion` executable. What kind of memory bandwidth does it show? What does *memory bandwidth* mean?
- Try running with 1, 2, 4, 8, 16, 32 cores.

Recall that running jobs on a cluster should be done by submission with the appropriate job scheduler.

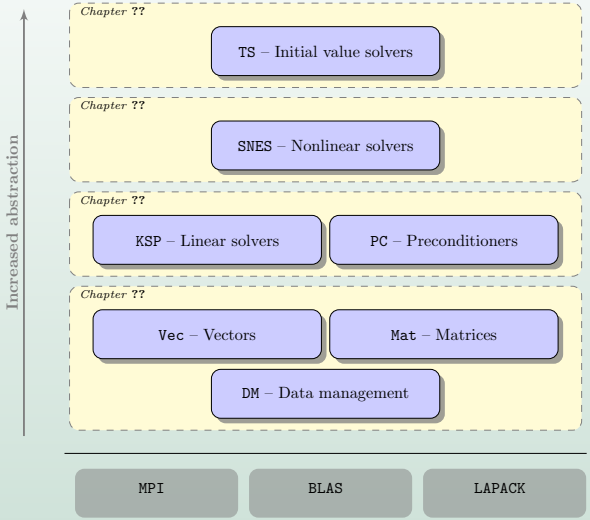
Outline

PETSc data types

Examples.

- `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



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

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

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

Matrices (Mat)

What are PETSc matrices?

- Linear operators on finite dimensional vector spaces.

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- 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.

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

Proc 0

Proc 1

Proc 2

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.

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?

Iterative 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

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

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

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

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- Right preconditioning

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

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

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- Right preconditioning

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

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

LU factorization

- Handled as a preconditioner.

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LU factorization

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- 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

Vec exercise

Exercise 3: Basic vector routines

- Investigate the source code `examples/Lecture_02/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.` ?

KSP direct solver exercise

Exercise 4: Simple linear solve

- Looking at the code in `examples/Lecture_02/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`

Exercise 5: Solve with LU factorization

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

Message passing interface (MPI)

Typically, user does not call MPI functions directly.

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

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)

Outline

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 $J(u)$

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()`
  - 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:

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PetscErrorCode (*func)(SNES snes,Vec u,Mat J,
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- `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

Timestepping (TS)

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

PETSc permits 2 forms for initial value problems

1. Standard ODE IVP form:
$$\dot{u} = F(t, u)$$
2. DAE and IMEX methods:
$$G(t, u, \dot{u}) = F(t, u)$$
$$J_\alpha = \alpha G_{\dot{u}} + G_u$$

Single `Step` interface so user can control their own time loop, or one-shot `Solve` to produce a solution at some desired final time.

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:

- `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);`

Can also supply:

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

to use fully implicit methods.

SNES exercise

Exercise 6: Simple nonlinear solve

- Investigate the code in `examples/Lecture_03/ex1.c` (note this is a serial example!), determine:
  - How the residual is evaluated.
  - How the Jacobian is evaluated.
- 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?

TS exercise

Exercise 7: DAE benchmark problems for TS

- Investigate the source code in `examples/Lecture_03/ex8.c`, determine:
  - What problems are being solved?
  - How do you select a problem from command line?
- What types of time integration methods can you use, what is the default? (`-ts_view`)
- Run the program with LU factorization for the linear system solves.

Outline

ODE TS example problem

Forced, damped oscillator:

$$m\ddot{x} + c\dot{x} + kx = f(t),\ x(0) = x_0,\ \dot{x}(0) = 0$$

written as a first order system

$$\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{f}(t),$$

with

$$\mathbf{x} = \begin{bmatrix} x \\ \dot{x} \end{bmatrix},\ \mathbf{A} = \begin{bmatrix} 0 & 1 \\ -k/m & -c/m \end{bmatrix},\ \mathbf{f} = \begin{bmatrix} 0 \\ f(t)/m \end{bmatrix}$$

Feeling out the code

Build the example:
`cd examples/Lecture_04 && make fdo1`

Start by discovering defaults and available options:
`./fdo1 -help -ts_view > options_and_defaults`

User provided option to output solution during time integration:
`-monitor_solution`

(Can be easily visualized with your tool of choice, ie., gnuplot)

Problem struct

Problem specific data stored in one of these.

```
typedef struct _Parameters Parameters;
struct _Parameters {
  PetscReal   m,c,k;   // eqn parameters
  PetscScalar F,omega; // forcing parameters
  PetscScalar x0,xp0;  // initial conditions
};
```

Created in main program as

```
  Parameters* params;
  ierr = PetscMalloc(sizeof(Parameters),&params);CHKERRQ(ierr);
```

Problem cli options

In main program,

```
ierr = PetscOptionsBegin(PETSC_COMM_WORLD,NULL,"Title","Man");CHKERRQ(ierr);
{
  /* ... */
}
ierr = PetscOptionsEnd();CHKERRQ(ierr);
```

nicely annotates the `-help` with your problem-specific options.

Set defaults and get cli options in this region, ie.,

```
params->m = 1;
ierr      = PetscOptionsReal("-m","Mass parameter","",params->m, &(params->m),NULL);CHKERRQ
```

Problem function evaluation

```
#undef __FUNCT__
#define __FUNCT__ "RHSFunction"
static PetscErrorCode RHSFunction(TS ts,PetscReal t,Vec X,Vec F,void *ctx)
{
  PetscErrorCode    ierr;
  Parameters*       params = (Parameters*)(ctx);
  PetscScalar       *f;
  const PetscScalar *x;

  PetscFunctionBeginUser;
  ierr = VecGetArrayRead(X,&x);CHKERRQ(ierr);
  ierr = VecGetArray(F,&f);CHKERRQ(ierr);
  f[0] = x[1];
  f[1] = (-params->k*x[0] - params->c*x[1] + params->c*forcing_function(t,params)) / params
  ierr = VecRestoreArrayRead(X,&x);CHKERRQ(ierr);
  ierr = VecRestoreArray(F,&f);CHKERRQ(ierr);
  PetscFunctionReturn(0);
}
```

Problem Jacobian evaluation

Similar to function evaluation.

```
#undef __FUNCT__
#define __FUNCT__ "RHSJacobian"
static PetscErrorCode RHSJacobian(TS ts,PetscReal t,Vec X,Mat A,Mat B,void *ctx)
{
  PetscErrorCode    ierr;
  Parameters*       params = (Parameters*)(ctx);
  PetscInt          rowcol[] = {0,1};
  PetscScalar       J[2][2];
  const PetscScalar *x;

  PetscFunctionBeginUser;
  /* ... */
  PetscFunctionReturn(0);
}
```

TS setup

Getting everything into a TS object.

```
ierr = TSCreate(PETSC_COMM_WORLD,&ts);CHKERRQ(ierr);
ierr = TSSetProblemType(ts,TS_LINEAR);CHKERRQ(ierr);
ierr = TSSetRHSFunction(ts,NULL,RHSFunction,params);CHKERRQ(ierr);
ierr = TSSetRHSJacobian(ts,A,A,RHSJacobian,params);CHKERRQ(ierr);
ierr = TSSetDuration(ts,maxsteps,final_time);CHKERRQ(ierr);
ierr = TSSetExactFinalTime(ts,TS_EXACTFINALTIME_STEPOVER);CHKERRQ(ierr);
ierr = TSSetMaxStepRejections(ts,10);CHKERRQ(ierr);
```

ODE examples

For running examples, use $c = 10001,\ k = 10000$.

Exercise 8: Code modification

Modify the `fdo1.c` example code to the following:

- The default method is BDF3.
- BDF adaptivity is on by default.
- The custom monitor function outputs the stepsize at each time step.

ODE examples

Exercise 9: Adaptive step sizes

Solving the `fdo` problem with `-ts_type bdf -ts_order 3`:

- Adjust the relative and absolute tolerances for the adaptation, note how this affects the time step sizes.
- Set the relative and absolute tolerances to be 10 times tighter for the derivative $\dot{x}$ than for the position x. (This has to be done within the code!)

Outline

DMDA overview

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

- handle allocation and communication requirements for logically rectangular grids.
- A subset of DM, which is generally more complicated to set up.
- Useful for finite difference and finite volume discretizations.

Can be used to easily set up the sparsity structure of a Jacobian.

How to work with a DMDA

Creation:

```
DMDACreate1d(comm, xbdy, M, dof, s, lm[], DA *da)
```

`xbdy`: Specifies periodicity or ghost cells

- `DMDA_BOUNDARY_NONE`, `DMDA_BOUNDARY_GHOSTED`, `DMDA_BOUNDARY_MIRROR`, `DMDA_BOUNDARY_PERIODIC`

`M`: Number of grid points in x/y-direction

`dof`: Degrees of freedom per node

`s`: The stencil width

`lm`: Array of local sizes

- Use `PETSC_NULL` for the default

Useful DMDA options

Assuming a DMDA has been setup in your application code:

`-da_refine N`: Uniformly refine the DMDA `N` times.
`-da_grid_x N`: Sets the number of grid points in the x dimension to `N`. (Similar command for multiple dimensions)

SNES and DMDA working together

An SNES can have a DMDA associated with it:

```
PetscErrorCode  SNESSetDM(SNES snes,DM dmda)
```

Changes the interface (slightly) to SNES:

```
PetscErrorCode DMDASNESSetFunctionLocal(DM dm,InsertMode imode,
    PetscErrorCode (*func)(DMDALocalInfo*,void*,void*,void*),
    void *ctx)

PetscErrorCode DMDASNESSetJacobianLocal(DM dm,
    PetscErrorCode (*func)(DMDALocalInfo*,void*,Mat,Mat,void*),
    void *ctx)
```

Useful SNES options

With an SNES setup in the application code:

`-snes_type XXX`: Sets the type of the SNES to XXX.
`-snes_Xtol TOL`: Sets a tolerance to TOL
`-snes_max_it N`: Sets maximum iterations to N
`-snes_max_funcs N`: Sets the maximum number of residual evaluations to N

Get more exhaustive list using:
```
./executable -help | grep snes
```

Nonlinear example: 1D Bratu problem

Bratu equation in 1D:

$$-u_{xx} - \lambda e^u = 0$$

$$x \in [0, 1]$$

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

Solved with a uniform mesh in `examples/Lecture_05/bratu_1d.c`
Solved with a non-uniform mesh in `examples/Lecture_05/bratu_1d_nonuniform.c`

Linear example: 2nd order BVP in 1D

$$\epsilon u_{xx} + (1+\epsilon)u_x + u = 0$$

$$x \in [0,1]$$

$$u(0) = 0,\ u(1) = 1$$

Has the exact solution

$$u(x) = \frac{e^{-x} - e^{-x/\epsilon}}{e^{-1} - e^{-1/\epsilon}}$$

Solved with a non-uniform mesh in `examples/Lecture_05/bvp1.c`

BVP exercies I

Exercise 10: Bratu

There are actually 2 solutions to the 1D Bratu equation for $\lambda < 3.51$. By modifying the initial conditions, can you find the 2nd solution?

Exercise 11: 2nd order BVP

Shrinking the ϵ parameter in the `bvp1.c` example produces a very steep gradient at the left boundary (commonly called a *boundary layer*).

- Is there any point when a uniform mesh completely breaks down in handling this problem?
- How does the size of this *boundary layer* seem to scale with the parameter ϵ?

BVP exercises II

Exercise 12: Code modification

- Modify the `bvp1.c` example code to include a comparison of the numerical solution with the exact solution.
- Show that the error converges with second order accuracy. What does this mean in the context of nonuniform mesh?

Outline