Practical PETSc Tutorial

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CSCS Summer School, July 28, 2016

This Tutorial

- We will use PETSc as an extended example of working with a library
  - This is because I am familiar with it, and because its flexible design allows us to examine many things quickly
  - All libraries present limitations and annoyances, and no library is a silver bullet: PETSc is no exception
- We don't have time for a full tutorial on the library, unfortunately
- I have adapted the miniapp code to use PETSc so that you can see familiar concepts in a new framework
- The majority of the time will be spent experimenting with this code: libraries allow you to quickly leverage functionality that would be time-consuming to "roll yourself", and PETSc is an extreme example of this in that you can even do this experimentation at runtime
- Please ask questions at any time.

What is PETSc?

- Origins as one of the first success stories of MPI, a library for domain decomposition-based PDE solvers
- Extended to provide a full set of tools for solving large-scale discretized PDE in distributed-memory parallel environments
- Distributed linear algebra, linear solvers, preconditioners, nonlinear solvers, timesteppers, domain management tools, optimization tools (TAO), and associated utilities.
- Over 20 years of development, fully supported, based at Argonne National Lab
- Written in object-oriented C, with a Fortran interface [1]
- Forms the basis for many of the libraries we've seen in the previous lecture, especially higher-level PDE libraries

[1] and see `petsc4py`, which offers a Python interface

Why Use PETSc?

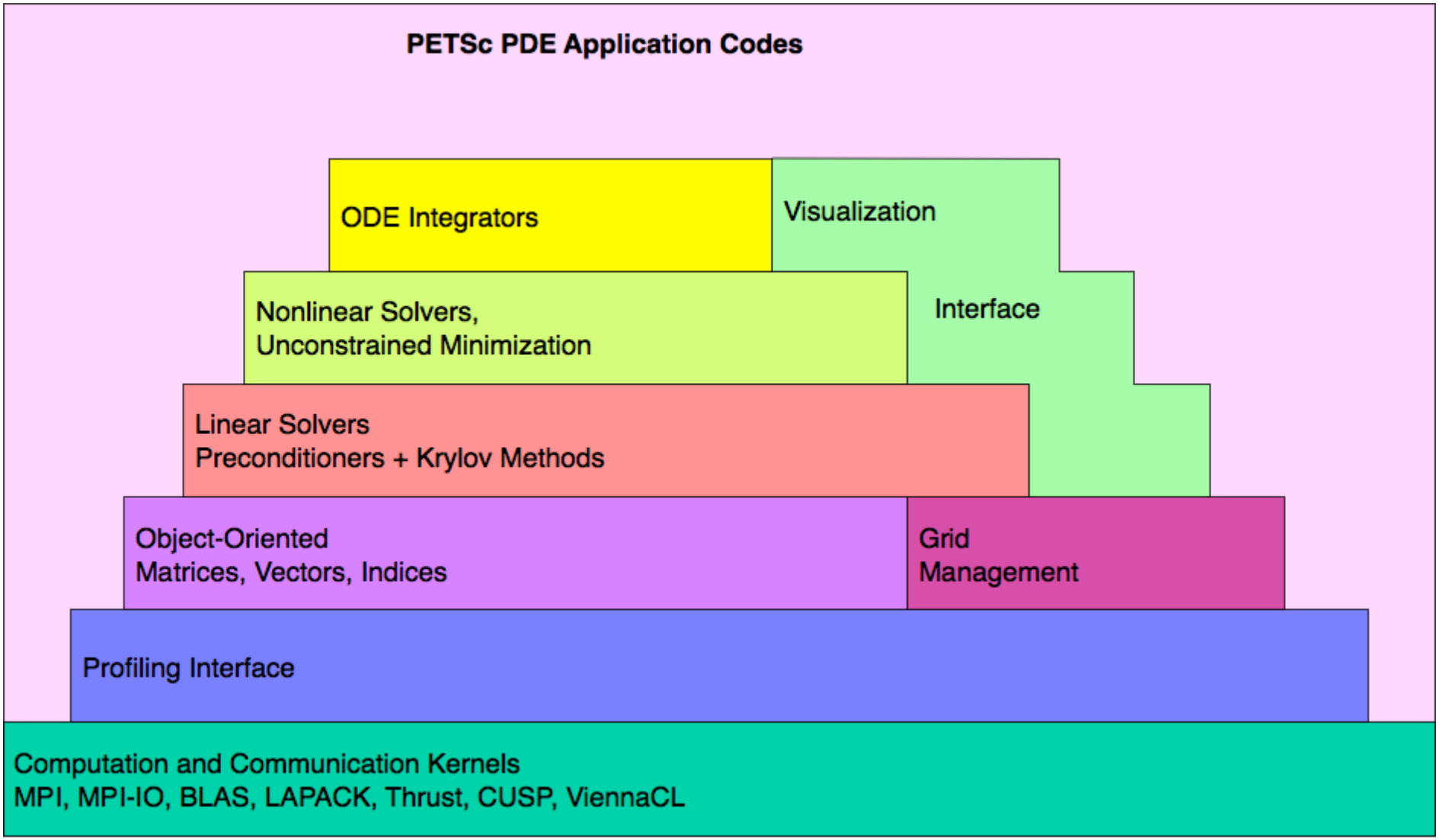
- Write robust, scalable MPI codes to solve PDE, without writing much MPI code yourself
- Use a combinatorial explosion of solvers, configurable at runtime
- Run your code essentially anywhere, from your laptop to Piz Daint
- Configure with a huge number of external packages (including external linear solvers)
- Excellent support and community

What's in a Name?

- **P**ortable
- **E**xtensible
- **T**oolkit for
- **S**cientific **c**omputation

An alternate acronym: the "**P**ortable, **E**xtensible **T**oolkit for **S**olver composition"

PETSc Components



PETSc Miniapp

- We will use the same PDE, Fischer's Equation in 2 dimensions

$$\frac{\partial s}{\partial t} = D\left(\frac{\partial^2 s}{\partial x^2} + \frac{\partial^2 s}{\partial y^2}\right) + Rs(1-s)$$

  discretized the same way on the same domain, a rectangle equipped with a regular grid, using standard finite differences / finite volumes.
- We will solve the same system, but using PETSc's abstractions
- We will leverage a powerful design component of PETSc, namely that it is **runtime configurable**, meaning that we can select from a huge number of solvers at runtime and quickly see how they perform
- We will write straightforward code which nevertheless will scale to large numbers of MPI processes (without us writing much MPI)

Porting to PETSc

As a short example, code which applies a finite difference Laplacian to a vector (similar, but not identical, to what we do to port the miniapp)

```
#include <petscdmda.h>
#include "ctx.h"

#undef __FUNCT__
#define __FUNCT__ "applyA"
PetscErrorCode applyA(Mat A, Vec in, Vec out)
{
  PetscErrorCode     ierr;
  Ctx                *ctx;
  const PetscScalar  **inarr;
  PetscScalar        val,**outarr;
  PetscInt           i,j,ixs,iys,ixm,iym,imin,imax,jmin,jmax,M,N;
  PetscBool          left,right,up,down;
  Vec                in_local;
  PetscReal          oneoverhy2,oneoverhx2;

  PetscFunctionBeginUser;

  ierr = MatShellGetContext(A, &ctx);CHKERRQ(ierr);
  M           = ctx->M;
  N           = ctx->N;
  in_local    = ctx->work_local[0];
  oneoverhy2  = 1.0/(ctx->hy*ctx->hy);
  oneoverhx2  = 1.0/(ctx->hx*ctx->hx);

  /* Scatter global-->local to have access to the required ghost values */
  ierr=DMGlobalToLocalBegin(ctx->da,in,INSERT_VALUES,in_local);CHKERRQ(ierr);
  ierr=DMGlobalToLocalEnd   (ctx->da,in,INSERT_VALUES,in_local);CHKERRQ(ierr);
```

Porting to PETSc (continued)

```
/* Get the boundaries of the local subdomain */
DMDAGetCorners(ctx->da, &ixs, &iys, 0, &ixm, &iym, 0);CHKERRQ(ierr);

/* Get access to the raw arrays (with ghosts).
   Note that PETSc allows these to be accessed with *global* indices */
DMDAVecGetArray(ctx->da,out,&outarr);CHKERRQ(ierr);
DMDAVecGetArrayRead(ctx->da,in_local,&inarr);CHKERRQ(ierr);

/* Determine active (global) boundaries */
up   = (iys       == 0); jmin = up   ? iys       + 1 : iys;
down = (iys + iym == N); jmax = down ? iys + iym - 1 : iys + iym;
left = (ixs       == 0); imin = left ? ixs       + 1 : ixs;
right= (ixs + ixm == M); imax = right? ixs + ixm - 1 : ixs + ixm;

/* Handle corners */
if(up && left){
  val=0;
  j=0; i=0;
  val+=inarr[j  ][i+1] *       (-oneoverhx2);
  val+=inarr[j+1][i  ] *       (-oneoverhy2);
  val+=inarr[j  ][i  ] * 2.0 * (oneoverhy2 + oneoverhx2);
  outarr[j][i]=val;
}
if(up && right){
  /* ... */
}
if(down && left){
  /* ... */
}
if(down && right){
  /* ... */
}
```

Porting to PETSc (continued)

```
/* Handle edges (excluding corners ) */
if (up){
  j=0;
  for (i=imin; i<imax; ++i) {
    val=0;
    val+=inarr[j  ][i-1] *       (-oneoverhx2);
    val+=inarr[j  ][i+1] *       (-oneoverhx2);
    val+=inarr[j+1][i  ] *       (-oneoverhy2);
    val+=inarr[j  ][i  ] * 2.0 * (oneoverhy2 + oneoverhx2);
    outarr[j][i]=val;
  }
}

if (down){
  /* ... */
}

if (left){
  /* ... */
}

if (right){
  /* ... */
}
```

Porting to PETSc (continued)

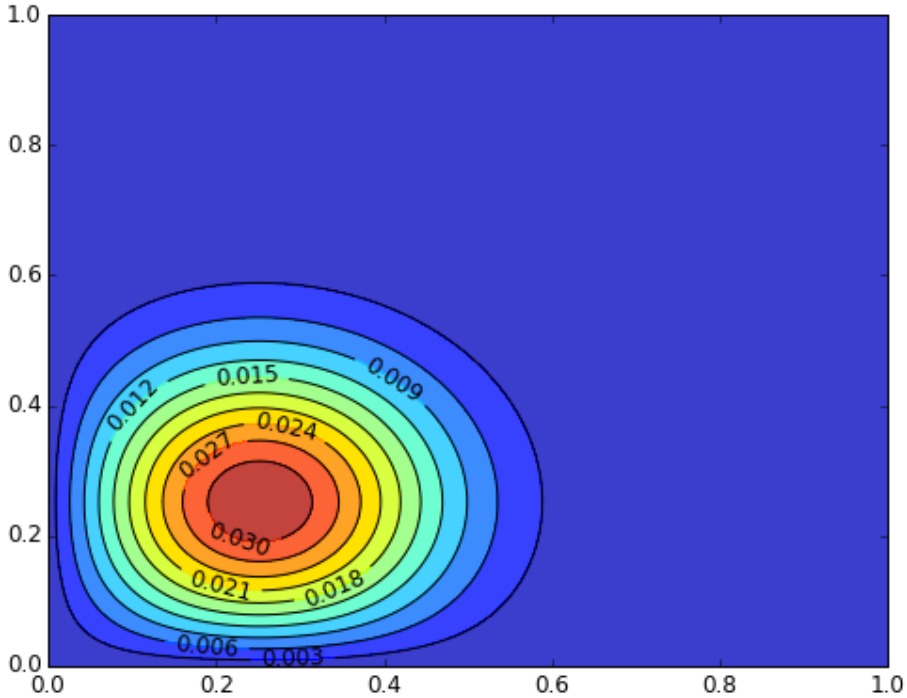
```
  /* Handle the interior points */
  for (j=jmin; j<jmax; ++j) {
    for (i=imin; i<imax; ++i) {
      val=0;
      val+=inarr[j-1][i  ] *      (-oneoverhy2);
      val+=inarr[j  ][i-1] *      (-oneoverhx2);
      val+=inarr[j  ][i+1] *      (-oneoverhx2);
      val+=inarr[j+1][i  ] *      (-oneoverhy2);
      val+=inarr[j  ][i  ] * 2.0 * (oneoverhy2 + oneoverhx2);
      outarr[j][i]=val;
    }
  }

  /* Revoke access to raw arrays */
  DMDAVecRestoreArray(ctx->da,out,&outarr);CHKERRQ(ierr);
  DMDAVecRestoreArrayRead(ctx->da,in_local,&inarr);CHKERRQ(ierr);

  PetscFunctionReturn(0);
}
```

Exercise 1: Run the Code

- In your course repository, navigate to `miniapp/petsc`
- Follow the instructions in `README.md`
- You should be able to produce an image like the one on the right



Aside: we are using the `cray-petsc` module, which frees us from having to configure and compile PETSc. If you would like to use additional external packages or a newer version of the library (the current version is 3.7.3, as opposed to 3.5.1 for `cray-petsc`), you can configure and build PETSc yourself. Also see the included `makefile.local` which is designed for more general systems.

Code Walkthrough: ODE Solver

- PETSc allows a "top-down" approach, so we begin by discussing how to adapt the miniapp to use PETSc ODE/DAE solver object, called `TS`
- The advantages of doing things this way include
  - The usual advantage of top-down design: having a clear view of the task, not implementing details until they are needed, etc.
  - Additional flexibility, as you can use PETSc's objects for more of the code
- Let's take a look at `main.c`

Exercise 2: Changing the ODE solver

- Run `./main -help` to see (many) possible command line options
- Experiment running the program
  - With different numbers of grid points
  - With different numbers of time steps
  - With different numbers of MPI processes
- Try the `-ts_view` and `-ts_monitor` options
- Try using different timesteppers, using `-ts_type`.
  - See the list of types in the manual or on the man page for `TSType` at http://www.mcs.anl.gov/petsc/petsc-current/docs/manualpages/TS/TSType.html
  - Not all will work immediately (some require you to provide more information about your system), but experiment with some standard choices like `rk`, `theta`, `ssp`, `bdf`, etc.

Code Walkthrough : Distributed Vectors, Array, and Linear Operators

- See `system.c`
- We will see how to assemble a Jacobian matrix
- PETSc also supports custom "matrix-free" operators [2], and can estimate the Jacobian for you using finite differences.

[2] See `MatShell`

Code Walkthrough : Viewing

- PETSc objects can be "viewed" in various ways
- This includes writing to the screen, to files, or even to network sockets
- See `dump.c`

Exercise 3: Parallel Preconditioners

- Use the `-assemble` option
- Using `-ts_view`, determine what the default preconditioner (`PC`) is for the linear solver (`KSP`)
- Use `-ksp_monitor` and describe what happens to the convergence as you strong scale (increase the number of MPI ranks for the same problem size)
- Experiment with another preconditioner, an additive Schwarz method, with `-pc_type asm`. Note that adding `-help` will now give you more options related to this preconditioner [3]

[3] The `-help` output can get long: try `./main -help -pc_type asm | grep asm`

Exercise 4: Bigger Time Steps

- Experiment with command line options to increase the time step to, say, 1
- Try to reduce the number of linear solver iterations by using a strong preconditioner like `-pc_type gamg`[4]

[4] This is algebraic multigrid

Performance Profiling

- `-log_summary`[5] provides a wealth of information, and is a necessary companion to allow quick interpertation of experiments with different solvers
- Includes
  - Time and flops
  - Call counts
  - Load balances
  - Cumulative memory usage (**Not** high-water mark)

[5] called `-log_view` in more recent versions of PETSc

Exercise 5: Algorithmic Experimentation

- Using only the command line options and `-log_summary`, see how much you can speed up the code
- Examine strong-scaling behavior (how does increasing the number of processes affect the solution time?

Exercise 6 (Bonus): Writing a matrix-free operator application

- Look at the documentation for MatShell,MatShellSetOperation(), etc. (See the man pages, linked exampes, and Section 3.3 of the manual)
- Using the example from earlier in the slides as an example, write a matrix-free operator which applies the Jacobian in the miniapp, and confirm that it gives the same results as using the assembled operator.

Continuing with PETSc

- See the manual and other documentation at
  www.mcs.anl.gov/petsc/documentation/index.html
- Learn how to use the mailing lists! See
  www.mcs.anl.gov/petsc/miscellaneous/mailing-lists.html.
  - Questions are answered quickly here
  - General questions : `petsc-users`
  - Developer topics (if planning to contribute) : `petsc-dev`
  - Private queries, bugs, installation problems : `petsc-maint`
  - For best results:
    1. Include the **entire** error message
    2. Include `configure.log` and `make.log` if sending a configure/install problem to `petsc-maint`
    3. The more specific, the better. If you can provide code to reproduce your problem, that is best.
    4. Note the archives
- Note the large number of examples (see links from the man pages)
- Up-and-coming resource: scicomp.stackexchange.com