Practical PETSc Tutorial

Patrick Sanan
patrick.sanan@[usi.ch,erdw.ethz.ch]

USI Lugano / ETH Zürich

CSCS Summer School, July 27, 2017

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 a library for parallel domain decomposition-based PDE solvers
- One of the first success stories of MPI
- 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]
- Critical component of 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?

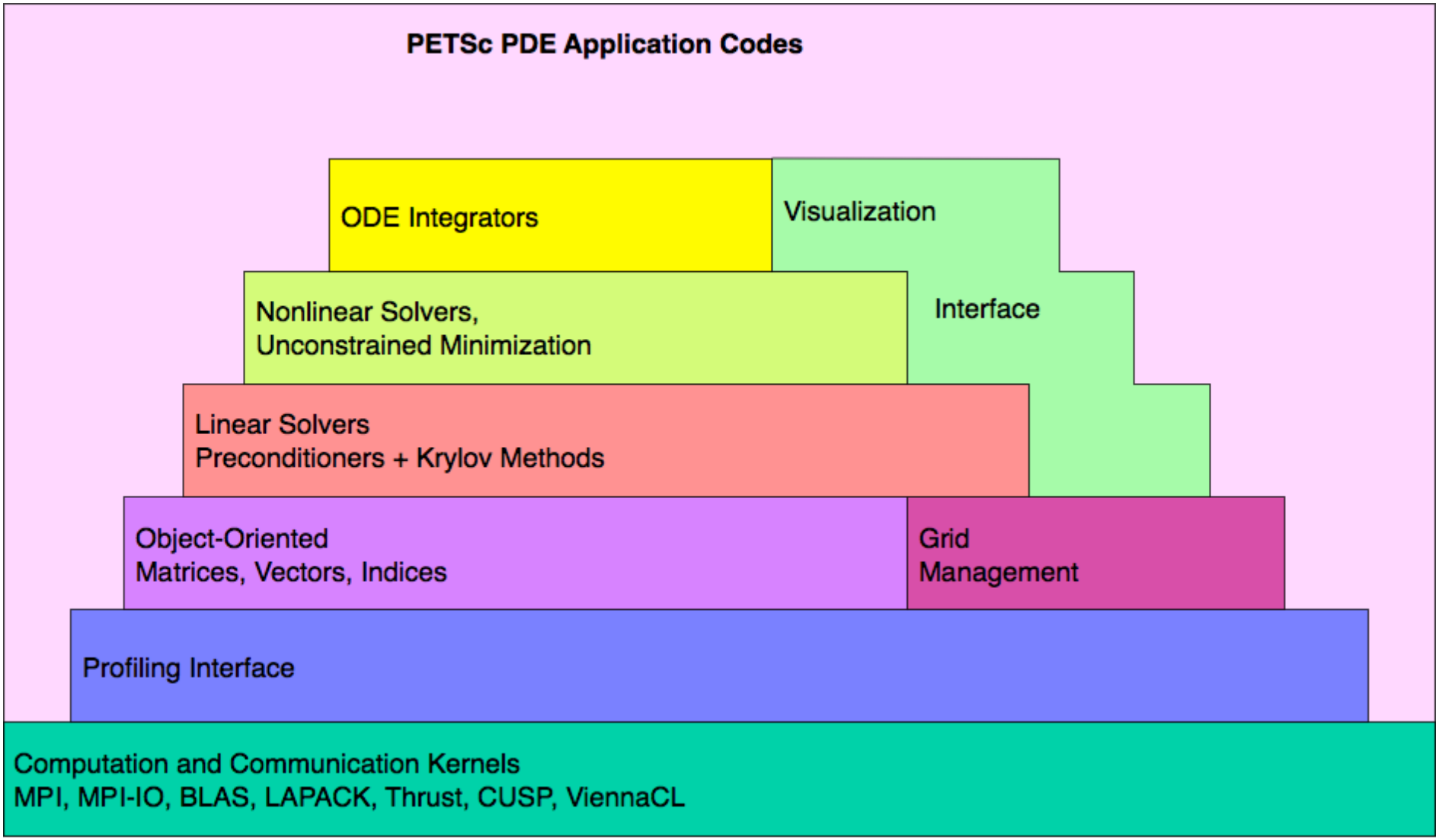
- Write robust, scalable MPI codes to solve PDE, without writing much MPI code yourself
- Use a combinatorial explosion of solvers, configurable at runtime
- Run your code essentially anywhere, from your laptop to Piz Daint
- Configure with a huge number of external packages (including external linear solvers)
- Excellent support and community
- Open Source (2-clause BSD) - you can contribute!

What's in a Name?

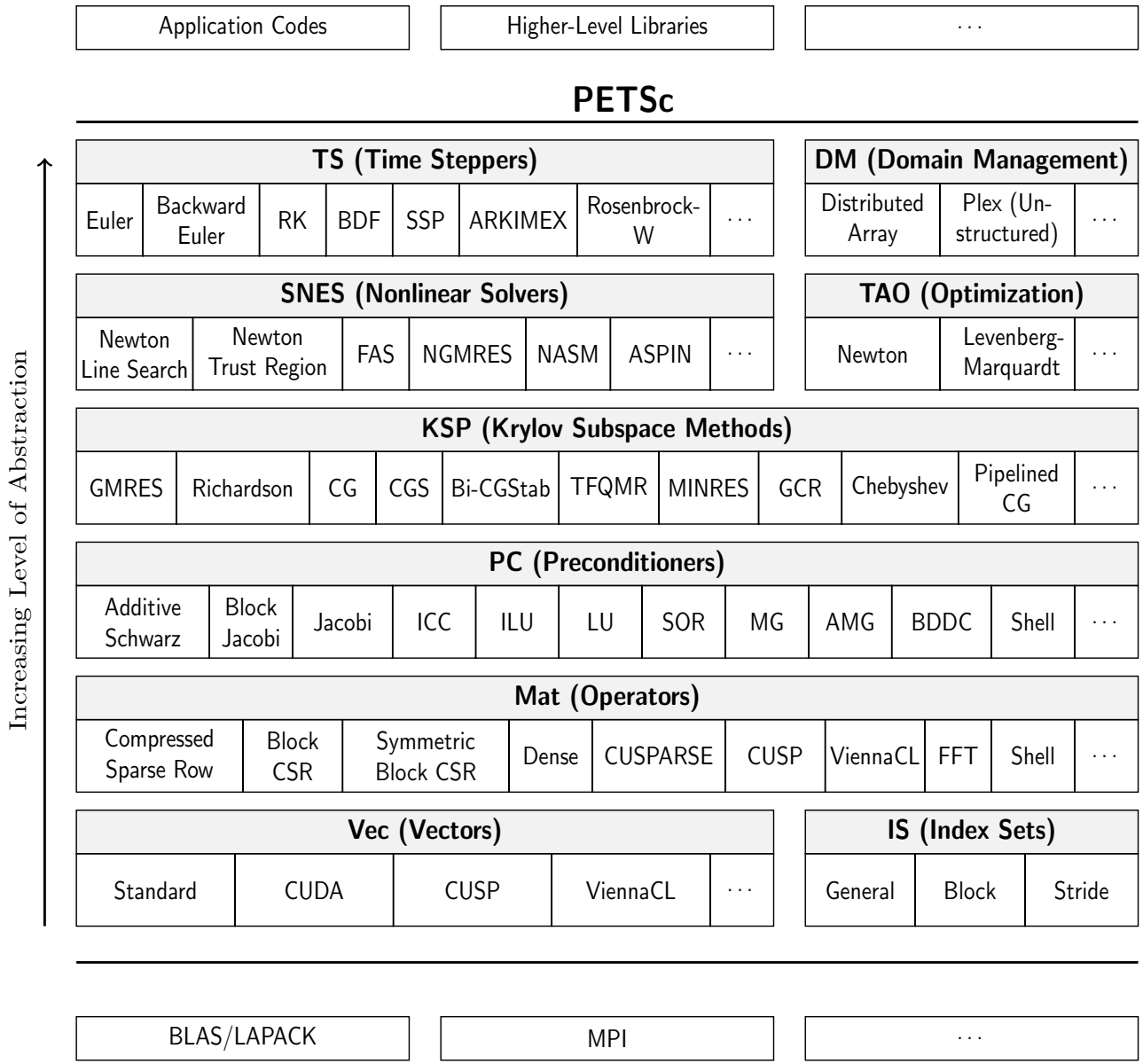
- **P**ortable
- **E**xtensible
- **T**oolkit for
- **S**cientific **c**omputation

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

PETSc Components



PETSc Numerical Libraries



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);
  /* Continued ... */
```

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)

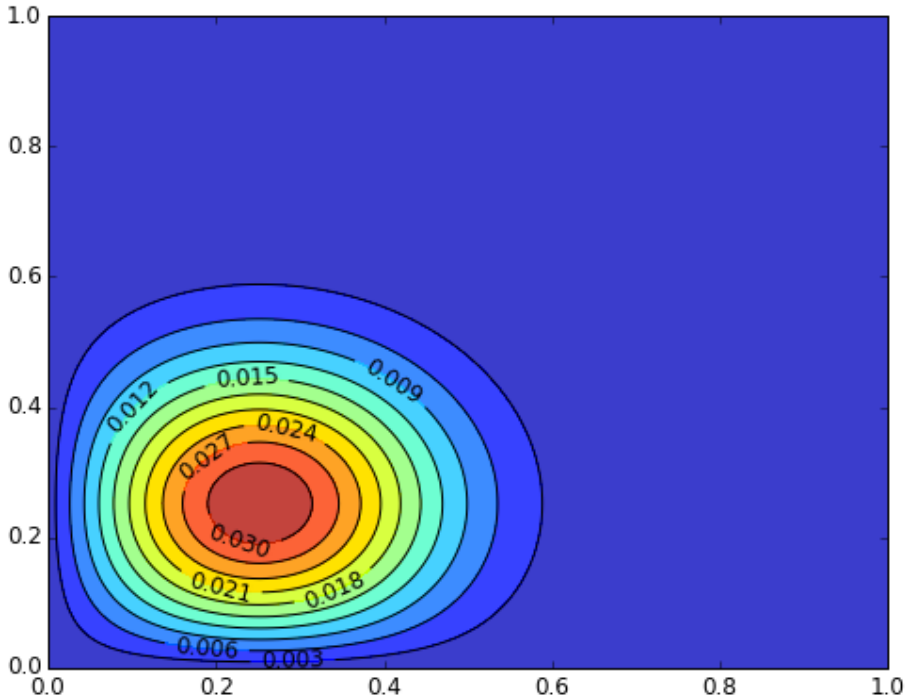
```
  /* Handle the interior points */
  for (j=jmin; j<jmax; ++j) {
    for (i=imin; i<imax; ++i) {
      val=0;
      val+=inarr[j-1][i  ] *       (-oneoverhy2);
      val+=inarr[j  ][i-1] *       (-oneoverhx2);
      val+=inarr[j  ][i+1] *       (-oneoverhx2);
      val+=inarr[j+1][i  ] *       (-oneoverhy2);
      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, you can configure and build PETSc yourself (see the bonus exercise later in these slides). Also see the included `Makefile.local`

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]

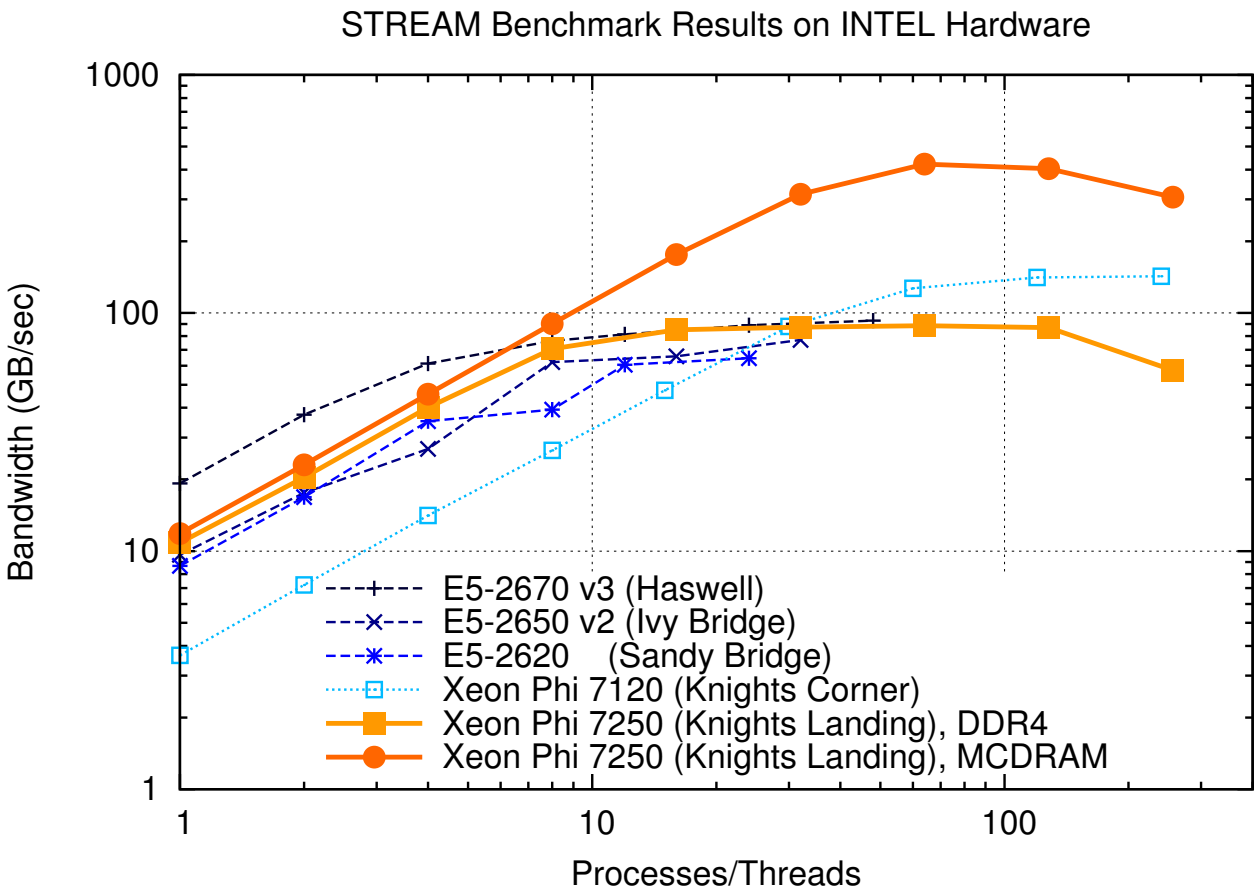
[4] This is algebraic multigrid

Performance Profiling

- `-log_view` 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)

STREAMS Benchmark

- Performance FAQ: "Why doesn't using N processors give an N-fold speedup?". One answer is that memory bandwidth is saturating.



Dual socket except for KNL. From the upcoming PETSc v3.8 manual, courtesy Karl Rupp.

Exercise 5: Algorithmic Experimentation

- Using only the command line options and `-log_view`, 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 1): Comparing AMG packages

Configure your own build of PETSc, based on the GNU compilers, and experiment with three different AMG preconditioners: GAMG, ML, and Hypre's BoomerAMG. (Allow 10-15 minutes to configure)

```
cd $SCRATCH
module unload PrgEnv-cray && module load daint-gpu PrgEnv-gnu
git clone https://bitbucket.org/petsc/petsc -b maint petsc-maint --depth=1
cd petsc-maint
./configure PETSC_ARCH=arch-daint-gnu-amg \
  --with-cc=cc --with-cxx=CC --with-fc=ftn COPTFLAGS= CXXOPTFLAGS= FOPTFLAGS= \
  --with-shared-libraries=0 --with-debugging=0 --with-valgrind=0 --with-x=0 \
  --with-sowing=0 --known-mpi-shared-libraries=1 \
  --download-ml --download-hypre --download-suitesparse
export PETSC_DIR=$PWD
export PETSC_ARCH=arch-daint-gnu-amg
make
cd /path/to/SummerSchool2017/miniapp/petsc
make -f Makefile.customPetsc clean && make -f Makefile.customPetsc
salloc -Cgpu
srun ./main -nx 128 -ny 128 -nt 1 -t 0.1  -options_left -ts_view -assemble \
  -ksp_converged_reason -snes_monitor -ksp_monitor \
  -pc_type ml -mg_coarse_pc_factor_mat_solver_package umfpack
srun ./main -nx 128 -ny 128 -nt 1 -t 0.1  -options_left -ts_view -assemble \
  -ksp_converged_reason -snes_monitor -ksp_monitor \
  -pc_type hypre
srun ./main -nx 128 -ny 128 -nt 1 -t 0.1  -options_left -ts_view -assemble \
  -ksp_converged_reason -snes_monitor -ksp_monitor \
  -pc_type gamg -mg_coarse_pc_type lu -mg_coarse_pc_factor_mat_solver_package umfpack
```

Exercise 7 (Bonus 2): 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