# University of Numerical Simulation Laboratory

## Time integration with PETSc

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- 1 Lecture 1: Introduction and Installation
- 2 Lecture 2: Data structures and classes overview
- 3 Lecture 3: Data structures and classes continued
- 4 Lecture 4: Solving ODE IVPs with TS
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# 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.

- 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<sup>12</sup> unknowns, full-machine scalability on Top-10 systems
- Same code runs performantly on a laptop

Philosophy: Everything has a plugin architecture

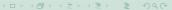
- Vectors, Matrices, Coloring/ordering/partitioning algorithms
- Preconditioners, Krylov accelerators
- Nonlinear solvers, Time integrators
- Spatial discretizations/topology

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.



- 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.

Lecture 1 Lecture 2 Lecture 3 Lecture 4 Lecture 5 Lecture 6

Lecture resource Overview Installation Using Exercises

# 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.

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