PETSc

Portable, Extensible Toolkit for Scientific Computation

Mathematics and Computer Science Division
Argonne National Laboratory

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Argonne NATIONAL LABORATORY

U.S. DEPARTMENT OF ENERGY

PETSc Overview

PETSc Origins

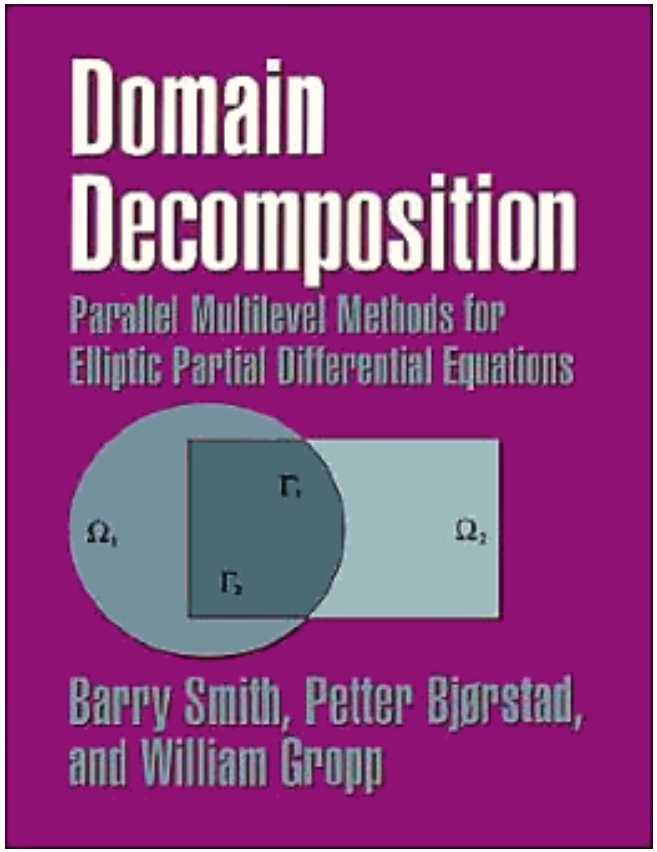
PETSc was developed as a Platform for

Experimentation

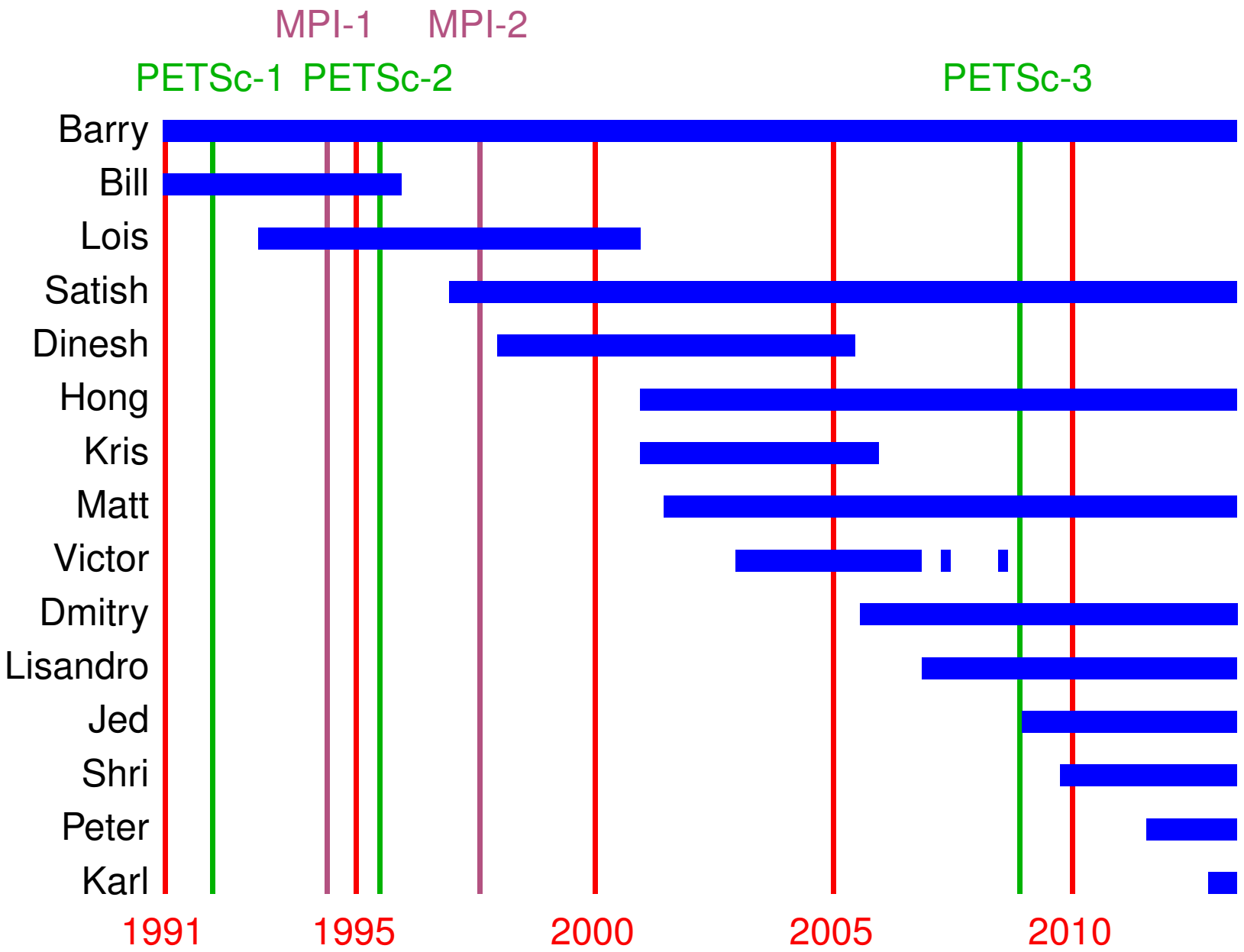
We want to experiment with different

- Models
- Discretizations
- Solvers
- Algorithms

These boundaries are often blurred...



Timeline


MPI-1
MPI-2
PETSc-1
PETSc-2
PETSc-3
Barry
Bill
Lois
Satish
Dinesh
Hong
Kris
Matt
Victor
Dmitry
Lisandro
Jed
Shri
Peter
Karl
1991
1995
2000
2005
2010

PETSc

Portable Extensible Toolkit for Scientific Computing

Architecture

- tightly coupled (e.g. XT5, BG/P, Earth Simulator)
- loosely coupled such as network of workstations
- GPU clusters (many vector and sparse matrix kernels)

Software Environment

- Operating systems (Linux, Mac, Windows, BSD, proprietary Unix)
- Any compiler
- Usable from C, C++, Fortran 77/90, Python, and MATLAB
- Real/complex, single/double/quad precision, 32/64-bit int

System Size

- 500B unknowns, 75% weak scalability on Jaguar (225k cores) and Jugene (295k cores)
- Same code runs performantly on a laptop

Free to everyone (BSD-style license), open development

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

Example

Vendor supplies matrix format and associated preconditioner, distributes compiled shared library.

Application user loads plugin at runtime, no source code in sight.

PETSc

Portable Extensible **Toolkit** for Scientific Computing

Toolset

algorithms

(parallel) debugging aids

low-overhead profiling

Composability

try new algorithms by choosing from product space

composing existing algorithms (multilevel, domain decomposition, splitting)

Experimentation

Impossible to pick the solver *a priori*

PETSc's response: expose an algebra of composition

keep solvers decoupled from physics and discretization

PETSc

Portable Extensible Toolkit for **Scientific Computing**

Computational Scientists

PyLith (CIG), Underworld (Monash), Magma Dynamics (LDEO, Columbia), PFLOTRAN (DOE), SHARP/UNIC (DOE)

Algorithm Developers (iterative methods and preconditioning)

Package Developers

SLEPc, TAO, Deal.II, Libmesh, FEniCS, PETSc-FEM, MagPar, OOFEM, FreeCFD, OpenFVM

Funding

Department of Energy

SciDAC, ASCR ISICLES, MICS Program, INL Reactor Program

National Science Foundation

CIG, CISE, Multidisciplinary Challenge Program

Documentation and Support

Hundreds of tutorial-style examples

Hyperlinked manual, examples, and manual pages for all routines

Support from `petsc-maint@mcs.anl.gov`

The 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

The Role of PETSc

You want to think about how you decompose your data structures, how you think about them globally. [...]

If you were building a house, you'd start with a set of blueprints that give you a picture of what the whole house looks like. You wouldn't start with a bunch of tiles and say. "Well I'll put this tile down on the ground, and then I'll find a tile to go next to it."

But all too many people try to build their parallel programs by creating the smallest possible tiles and then trying to have the structure of their code emerge from the chaos of all these little pieces. You have to have an organizing principle if you're going to survive making your code parallel.

— Bill Gropp
— http://www.rce-cast.com/Podcast/rce-28-mpich2.html

Obtaining PETSc

Linux Package Managers

Web: http://mcs.anl.gov/petsc, download tarball

Git: https://bitbucket.org/petsc/petsc

Mercurial: https://bitbucket.org/petsc/petsc-hg

Installing PETSc

```
$> cd /path/to/petsc/workdir
$> git clone \
     https://bitbucket.org/petsc/petsc.git \
     --branch master --depth 1
$> cd petsc
```

```
$> export PETSC_DIR=$PWD PETSC_ARCH=mpich-gcc-dbg
$> ./configure --with-cc=gcc --with-fc=gfortran
                 --download-f-blas-lapack
                 --download-{mpich,ml,hypre}
```

PETSc External Packages

Most packages can be automatically

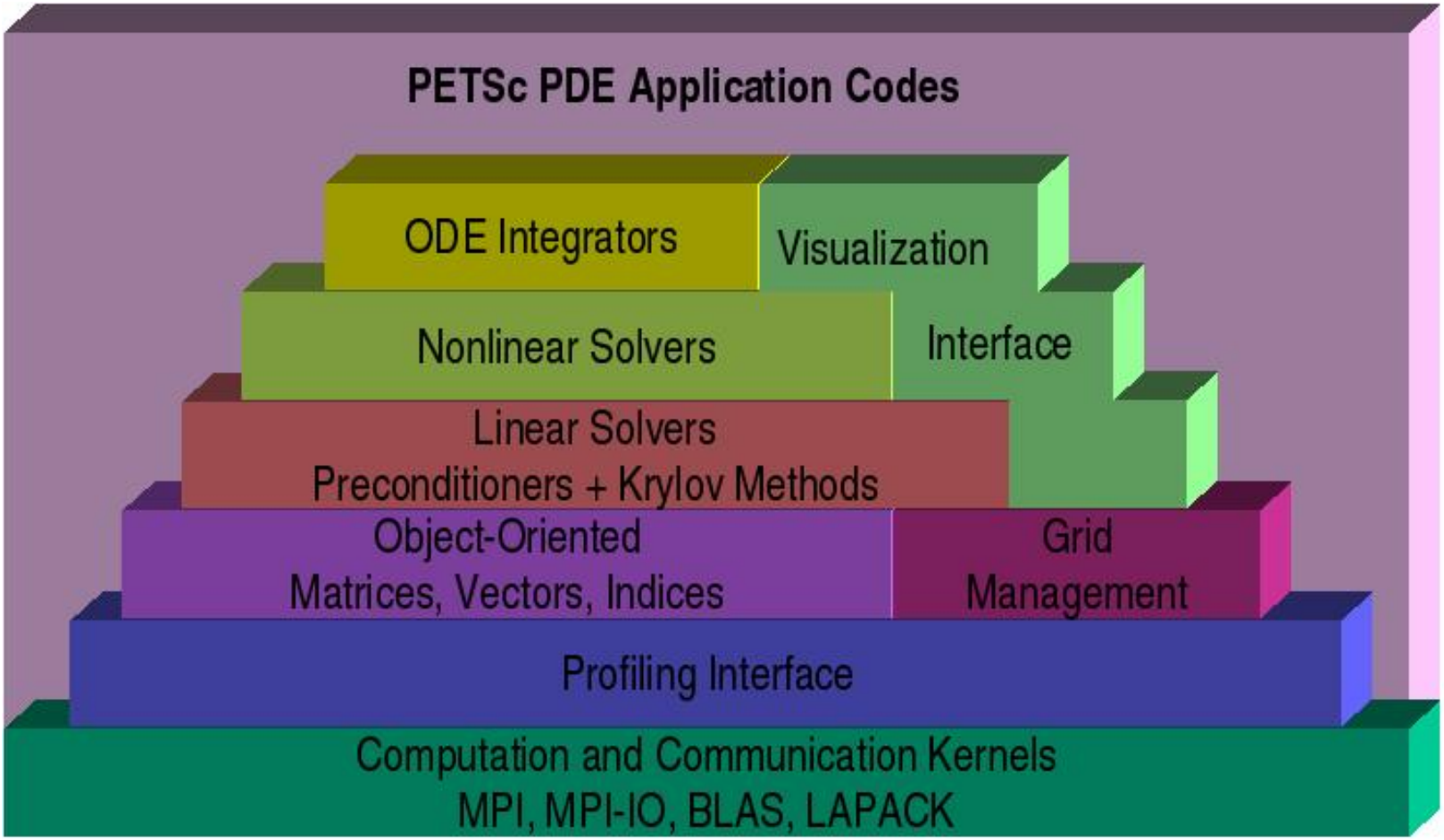
- Downloaded
- Configured and Built (in `$PETSC_DIR/externalpackages`)
- Installed with PETSc

Currently works for

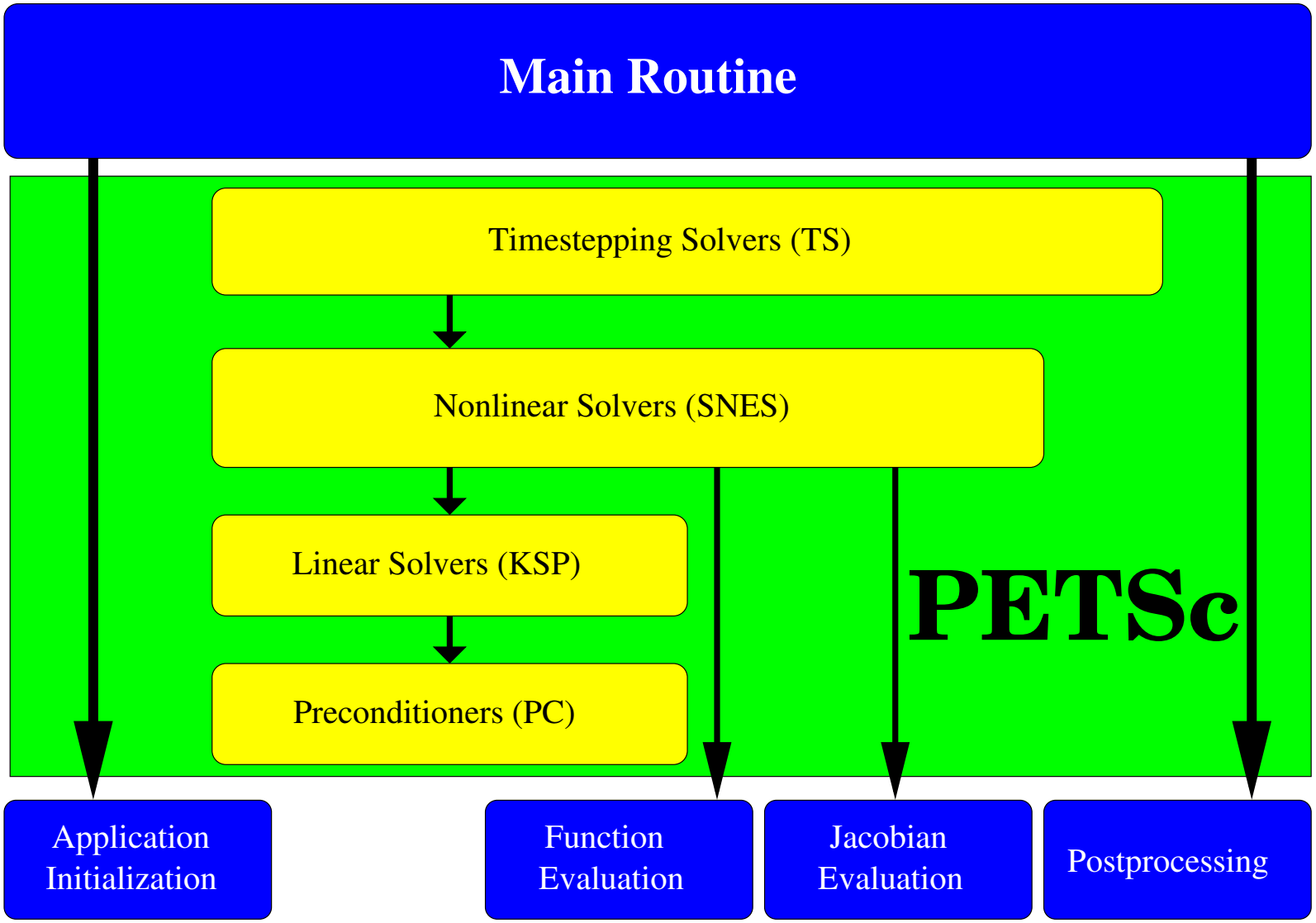
- petsc4py
- PETSc documentation utilities (Sowing, lgrind, c2html)
- BLAS, LAPACK, BLACS, ScaLAPACK, PLAPACK
- MPICH, MPE, OpenMPI
- ParMetis, Chaco, Jostle, Party, Scotch, Zoltan
- MUMPS, Spooles, SuperLU, SuperLU_Dist, UMFPack, pARMS
- PaStiX, BLOPEX, FFTW, SPRNG
- Prometheus, HYPRE, ML, SPAI
- Sundials
- Triangle, TetGen, FIAT, FFC, Generator
- HDF5, Boost

PETSc Pyramid

PETSc Structure



Flow Control for a PETSc Application



PETSc Objects

Sample Code

```
Mat A;
PetscInt m,n,M,N;
MatCreate(comm,&A);
MatSetSizes(A,m,n,M,N);        /* or PETSC_DECIDE */
MatSetOptionsPrefix(A,"foo_");
MatSetFromOptions(A);
/* Use A */
MatView(A,PETSC_VIEWER_DRAW_WORLD);
MatDestroy(A);
```

Remarks

- `Mat` is an opaque object (pointer to incomplete type)
  - Assignment, comparison, etc, are cheap
- What's up with this "Options" stuff?
  - We will discuss this later...

Basic PetscObject Usage

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.

PETSc 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]`

PETSc Options

Example of Command Line Control

```
$> ./ex5 -da_grid_x 10 -da_grid_y 10 -par 6.7
     -snes_monitor -{ksp,snes}_converged_reason
     -snes_view
$> ./ex5 -da_grid_x 10 -da_grid_y 10 -par 6.7
     -snes_monitor -{ksp,snes}_converged_reason
     -snes_view -mat_view_draw -draw_pause 0.5
$> ./ex5 -da_grid_x 10 -da_grid_y 10 -par 6.7
     -snes_monitor -{ksp,snes}_converged_reason
     -snes_view -mat_view_draw -draw_pause 0.5
     -pc_type lu -pc_factor_mat_ordering_type natural
```

Use `-help` to find other ordering types

Application Integration

Application Integration

Be willing to experiment with algorithms

No optimality without interplay between physics and algorithmics

Adopt flexible, extensible programming

Algorithms and data structures not hardwired

Be willing to play with the real code

Toy models have limited usefulness

But make test cases that run quickly

If possible, profile before integration

Automatic in PETSc

Incorporating PETSc into Existing Codes

PETSc does not seize `main()`, does not control output

Propogates errors from underlying packages, flexible

Nothing special about `MPI_COMM_WORLD`

Can wrap existing data structures/algorithms

- `MatShell`, `PCShell`, full implementations
- `VecCreateMPIWithArray()`
- `MatCreateSeqAIJWithArrays()`
- Use an existing semi-implicit solver as a preconditioner
- Usually worthwhile to use native PETSc data structures unless you have a good reason not to

Uniform interfaces across languages

- C, C++, Fortran 77/90, Python, MATLAB

Do not have to use high level interfaces (e.g. SNES, TS, DM)

- but PETSc can offer more if you do, like MFFD and SNES Test

Integration Stages

Version Control

It is impossible to overemphasize

Initialization

Linking to PETSc

Profiling

Profile before changing

Also incorporate command line processing

Linear Algebra

First PETSc data structures

Solvers

Very easy after linear algebra is integrated

PETSc and Accelerators

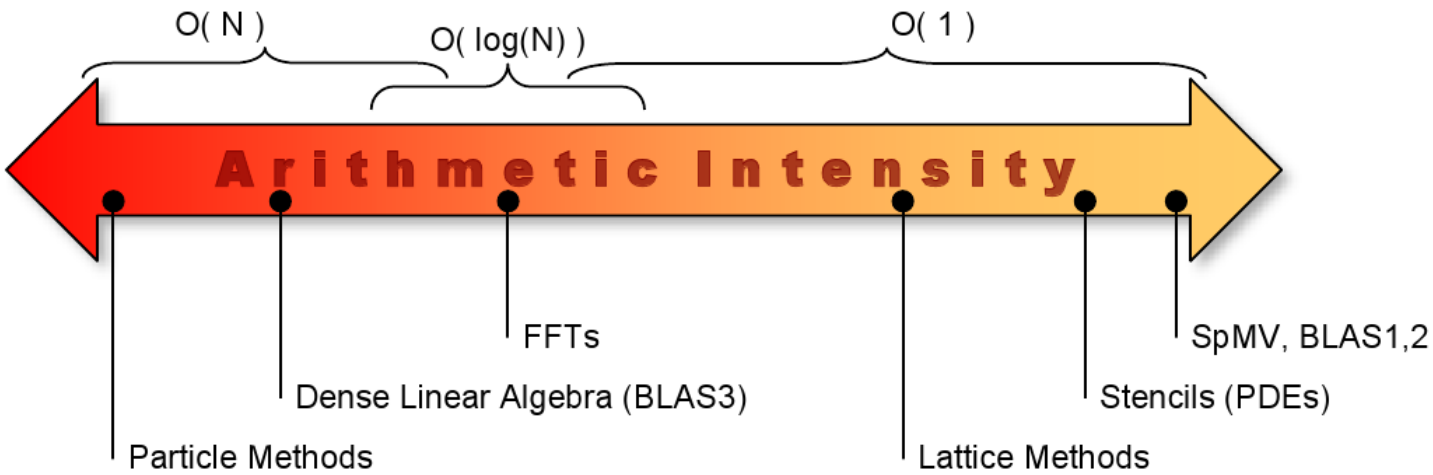
Typical PETSc Operations

“Sparse” Linear Algebra

Sparse Matrix-Vector Operations (on-node)

Vector Operations (on and across nodes)

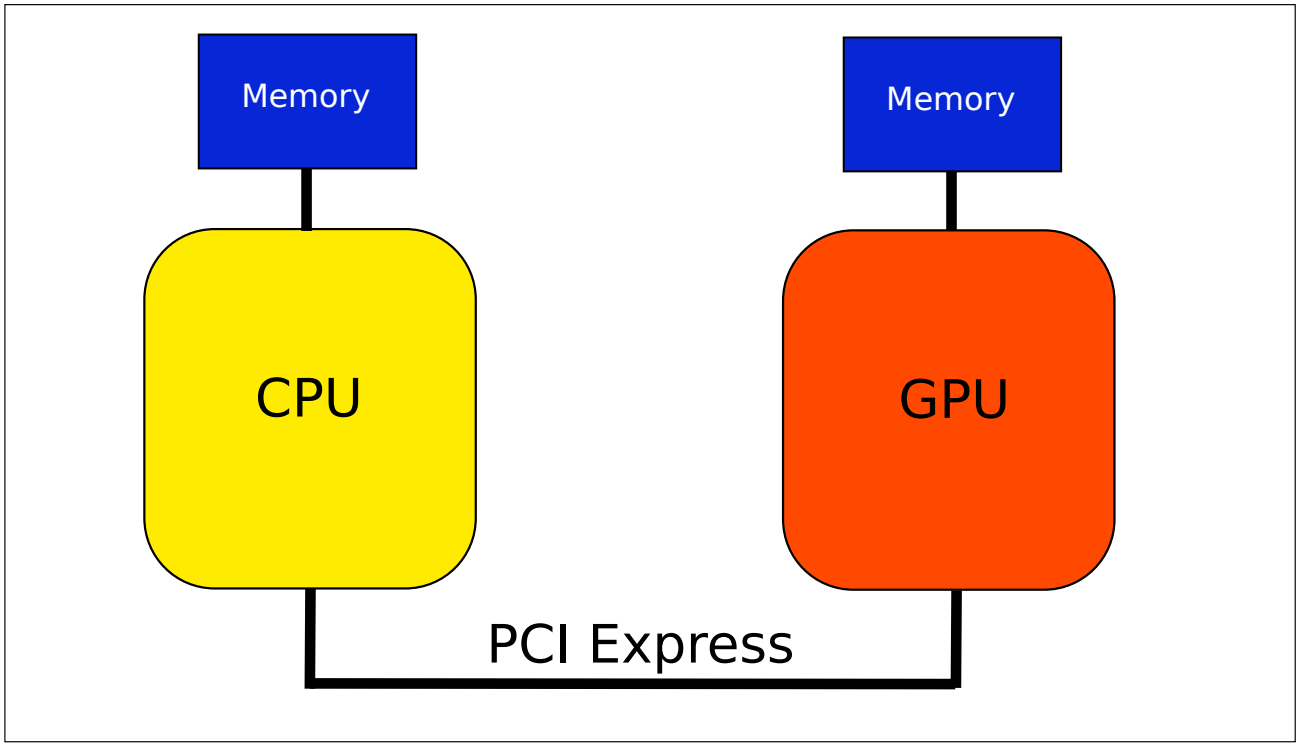
Only on small patches: Dense Operations (*small* matrices)



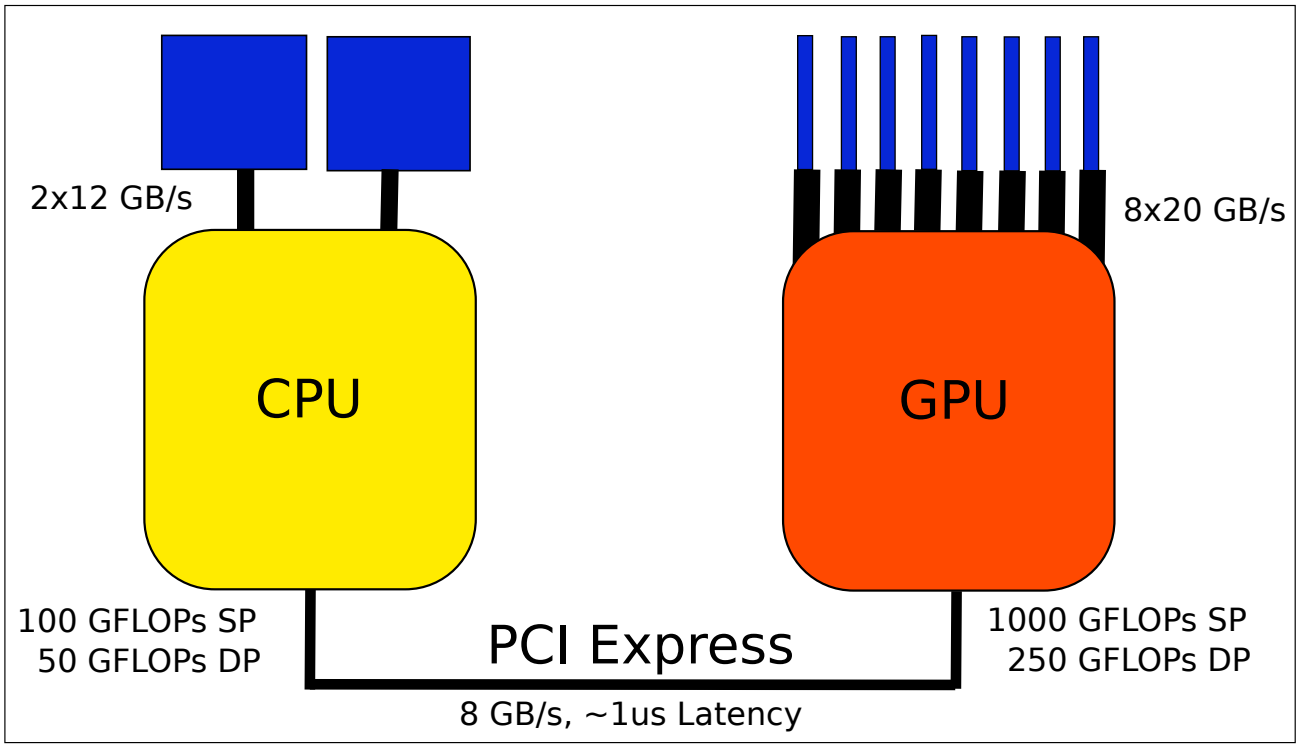
← Look at FLOPs

Look at Mem-BW →

Computing Architecture Schematic



Computing Architecture Schematic



Good for large FLOP-intensive tasks, high memory bandwidth

PCI-Express can be a bottleneck

$\gg$ 10-fold speedups (usually) not backed by hardware

GPU Programming Approaches

CUDA

- Almost no additional code required
- Vendor-lock
- Relies on `nvcc` being available

OpenCL

- Additional boilerplate code required (low-level API)
- Broad hardware support (separate SDKs)
- No more development effort from NVIDIA

Directives

- Annotate existing code with OpenMP-style Pragmas
- OpenACC and others

PETSc GPU Support

NVIDIA Cusp/Thrust/CUSPARSE

Compile PETSc with CUDA support

Use command line options to enable types, e.g.

```
-vec_type cusp -mat_type aijcusp
```

ViennaCL (OpenCL)

Compile PETSc with OpenCL support

Use command line options to enable types, e.g.

```
-vec_type viennacl -mat_type aijviennacl
```

Used for subsequent benchmarks

No change in application code required!

Which Accelerator is Right for Me?

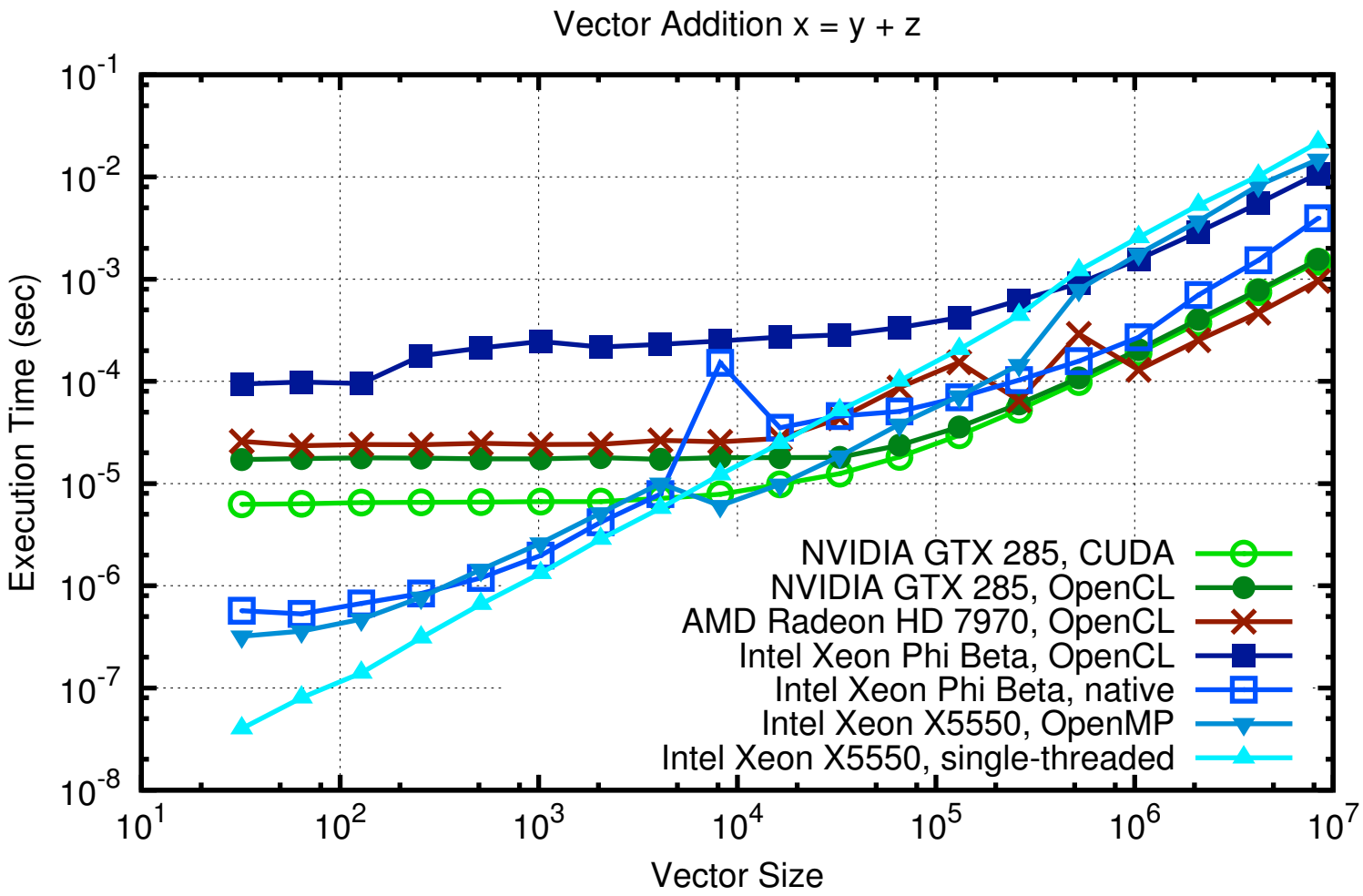
Available Accelerators (Rough Sketch)

Name	TFLOP/s	RAM (GB)	GB/s	TDP	Price
NVIDIA GTX 580	1.5/∼0.2	1.5-3.0	192	244	$500
NVIDIA GTX Titan	4.5/1.3	6.0	288	250	$∼1k
NVIDIA Tesla 2050	1.3/0.5	3.0-6.0	150	225	$∼2k
NVIDIA K20	3.5/1.2	5.0	200	220	$∼3k
AMD HD 7970	3.5/∼0.9	3.0-6.0	264	250	$550
AMD FirePro W9k	4.0/1.0	6.0	264	274	$∼3k
Intel Xeon Phi	∼2.0/∼1.0	8	320	225	$∼3k
Intel Xeon E5-264x	0.2/0.1	∼64	∼48	100	$∼1k

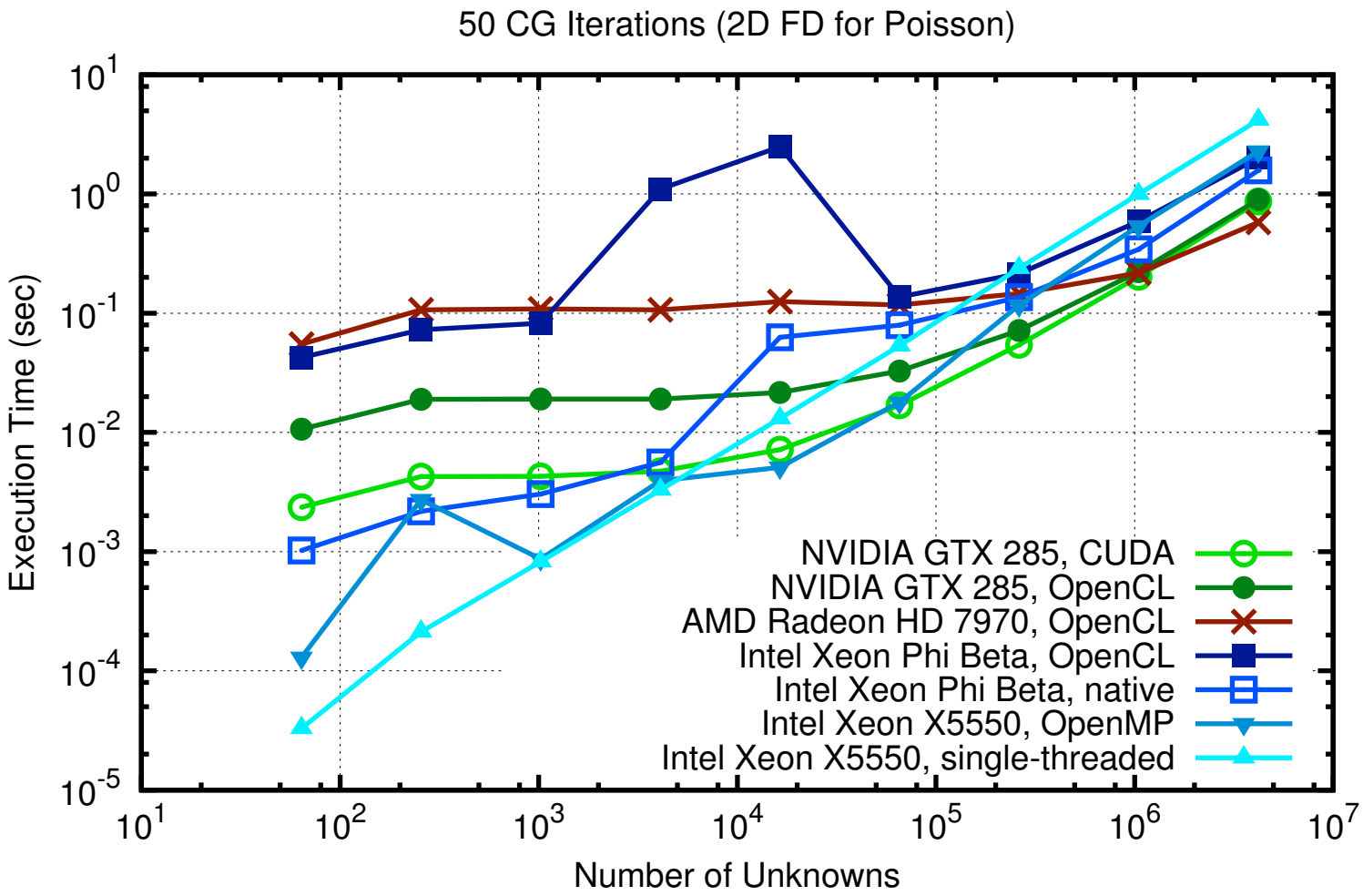
PETSc Considerations

- Single precision performance doesn't matter
- Essentially all kernels memory bandwidth limited
- Memory access patterns rather irregular

Benchmarks


Vector Addition x = y + z
Execution Time (sec)
Vector Size
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
10^{-8}
10^{1}
10^{2}
10^{3}
10^{4}
10^{5}
10^{6}
10^{7}
NVIDIA GTX 285, CUDA
NVIDIA GTX 285, OpenCL
AMD Radeon HD 7970, OpenCL
Intel Xeon Phi Beta, OpenCL
Intel Xeon Phi Beta, native
Intel Xeon X5550, OpenMP
Intel Xeon X5550, single-threaded

Benchmarks


50 CG Iterations (2D FD for Poisson)
Execution Time (sec)
Number of Unknowns
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{1}
10^{2}
10^{3}
10^{4}
10^{5}
10^{6}
10^{7}
NVIDIA GTX 285, CUDA
NVIDIA GTX 285, OpenCL
AMD Radeon HD 7970, OpenCL
Intel Xeon Phi Beta, OpenCL
Intel Xeon Phi Beta, native
Intel Xeon X5550, OpenMP
Intel Xeon X5550, single-threaded

PETSc can help You

solve algebraic and DAE problems in your application area

rapidly develop efficient parallel code, can start from examples

develop new solution methods and data structures

debug and analyze performance

advice on software design, solution algorithms, and performance

`petsc-{users,dev,maint}@mcs.anl.gov`

You can help PETSc

report bugs and inconsistencies, or if you think there is a better way

tell us if the documentation is inconsistent or unclear

consider developing new algebraic methods as plugins, contribute if your idea works