



PRACE Autumn School 2016

PETSc tutorial

Part I: Introduction

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Outline of the tutorial



- Part I: Introduction
- Part II: Hello World
- Part III: Vectors
- Part IV: Matrices
- Part V: KSP
- Part VI: advanced topics
(SNES, TAO, SLEPc)



First thing...



Try your connection to Anselm!

```
ssh anselm.it4i.cz
```

these slides: <http://tinyurl.com/pas16-petsc>



Frameworks for numerical computing



- „a **software framework** is a software providing **generic functionality** that can be selectively changed by user code, thus providing **application specific software**“ (wikipedia.org)
- There are only few such ones for **numerical computing**, e.g. **Trilinos** and **PETSc**
- don't reinvent the wheel!
- many **numerical algorithms** (LU, CG, SPMV, ...) **implemented** and **tested**
- focus on **novel** algorithms with an **added value**
- **PETSc** will be covered **in this talk**



What is PETSc



- **building blocks** (data structures and routines) for the scalable **parallel** solution of **scientific applications**, mainly **PDE-based**
- allows thinking in terms of **high-level objects** (matrices) instead of low-level objects (raw arrays)
- coded primarily in **C language** but good **FORTRAN** support, can also be called from **C++, Python** and **Java** codes
- highly **portable**
- source code and mailing lists **open to everybody**
- homepage: www.mcs.anl.gov/petsc



Role of PETSc

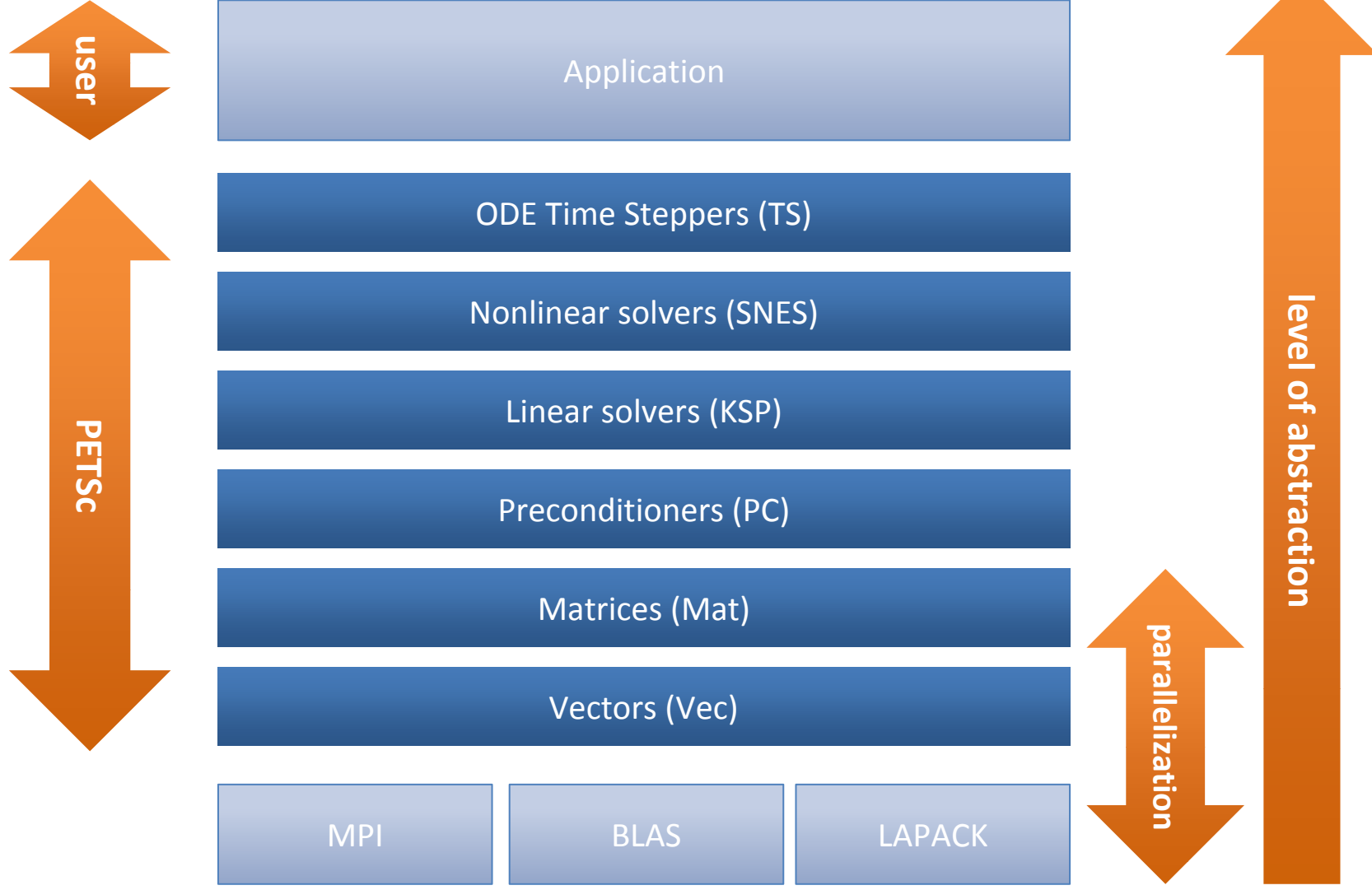


„Developing **parallel, nontrivial PDE solvers** that deliver **high performance** is still **difficult** and requires months (or even years) of concentrated effort. **PETSc** is a toolkit that can **ease these difficulties** and **reduce the development time**, but it is **not a black-box PDE solver, nor a silver bullet.**“

Barry Smith
(PETSc founder)



Hierarchy of components





Parallelism in PETSc



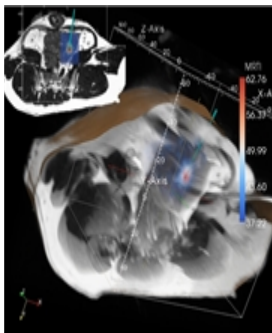
- PETSc is parallelized mostly using **MPI**
- **MPI** provides **low-level routines** to **exchange data primitives** between processes
- **PETSc** provides **mid-level routines** such as
 - insert matrix element to arbitrary location
 - parallel matrix-vector product
- you can **call MPI** directly if needed
- **same code** for **sequential** and **parallel** runs
- support for hybrid **MPI + {shared memory, accelerator} parallelism**
 - **thread-safe** but not **threaded**
 - **GPU-accelerated matrix types** `MATAIJCUSP`, `MATAIJCUSPARSE`, `MATAIJVIENNACL`
 - efficient use of MICs limited but is a hot topic now

Applications

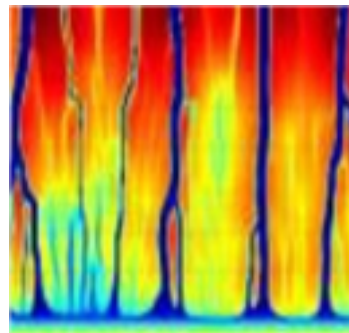
PETSc has been used for modeling in all of these areas:

Acoustics, Aerodynamics, Air Pollution, Arterial Flow, Bone Fractures, Brain Surgery, Cancer Treatment, Carbon Sequestration, Cardiology, Cells, CFD, Combustion, Concrete, Corrosion, Data Mining, Dentistry, Earth Quakes, Economics, Fission, Fusion, Glaciers, Linguistics, Mantle convection ...

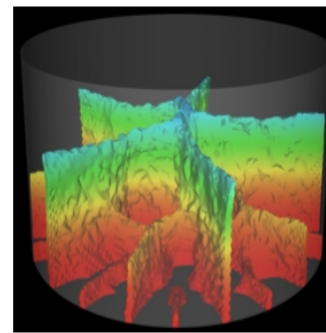
Real-time
surgery



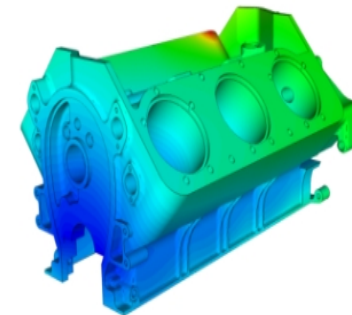
Magma
dynamics



Fracture
mechanics



Structure
Mechanics





PETSc interfaces...



- **Dense lin. algebra:** BLAS, LAPACK, Elemental
- **Sparse direct lin. sys. solvers:** MUMPS, SuperLU, SuperLU_Dist, PaStiX, UMFPACK, LUSOL
- **Iterative solvers / multigrid / preconditioners:** HYPRE, Trilinos ML, SPAI
- **Graph partitioning:** ParMetis, Scotch, Party, Chaco
- **FFT:** FFTW
- **ODE:** Sundials
- **Data exchange:** HDF5
- **Mathematics packages:** MATLAB, Mathematica
- ...



PETSc is interfaced by ...



- **TAO** - Toolkit for Advanced Optimization
- **SLEPc** - Scalable Library for Eigenvalue Problems
- **fluidity** - a finite element/volume fluids code
- **OpenFVM** - finite volume based CFD solver
- **OOFEM** - object oriented finite element library
- **libMesh** - adaptive finite element library
- **MOOSE** - Multiphysics Object-Oriented Simulation Environment
- **DEAL.II** - sophisticated C++ based finite element simulation package
- **PHMAL** - The Parallel Hierarchical Adaptive MultiLevel Project
- **Chaste** - Cancer, Heart and Soft Tissue Environment
- **PetIGA** - A framework for high performance Isogeometric Analysis



Getting PETSc



- homepage: <http://www.mcs.anl.gov/petsc/>
- download tarball: <http://www.mcs.anl.gov/petsc/download/index.html>
- `git clone -b maint https://bitbucket.org/petsc/petsc petsc`
- documentation hub: <http://www.mcs.anl.gov/petsc/documentation/index.html>
 - PDF Users Manual – recommended for beginners
 - Alphabetical index of functions (“Index of all manual pages”)
 - examples

these slides: <http://tinyurl.com/pas16-petsc>



Thanks for your attention.