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Practical PETSc Tutorial

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Why use PETSc?

- Write robust, scalable PDE codes without the pain of writing MPI.

- Use a combinatorial explosion of solvers, configurable at runtime.

- Run your code anywhere, from your laptop to Piz Daint

- Configure with a huge number of external packages (including external linear solvers)

- Excellent support and community (but documentation that could still use some polishing)

- **P**ortable : compile-anywhere C (and Fortran) with a robust configuration process
- **E**xtensible : plug-in oriented design, so you can write your own implementations of any object, from a vector to an ODE solve
- **T**oolkit for **S**cientific **c**omputation : originally developed on top of MPI to allow for domain-decomposition approaches to solving numerical PDE based on sparse matrix operations, now provides that and more!

See the PETSc web site for tutorials, the manual, etc.
mcs.anl.gov/petsc

Here we will quickly move to some example code!

PETSc Mini-app

- We will use the same simple nonlinear PDE (Fischer's equation) that you have become familiar with during the week.

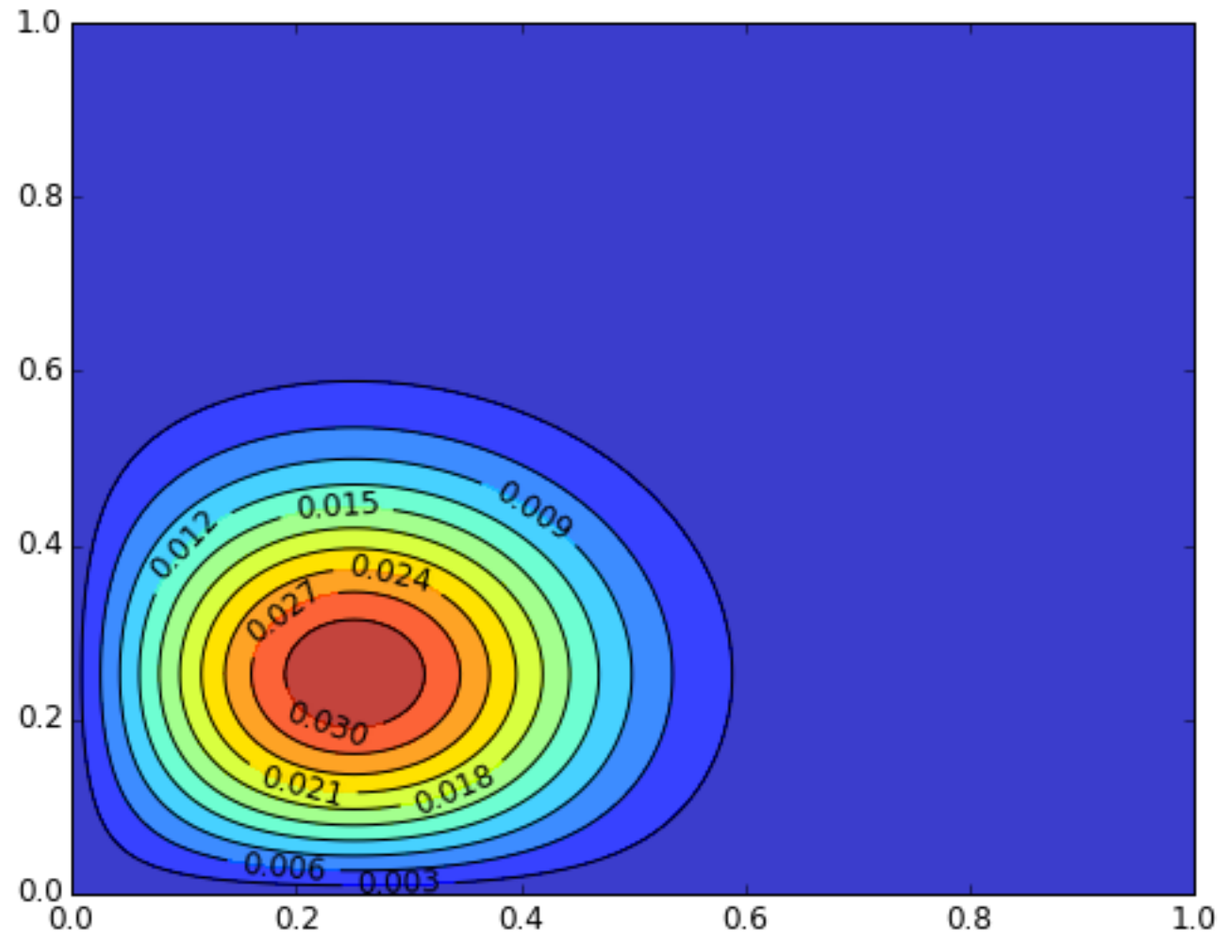
$$\frac{\partial s}{\partial t} = D\overbrace{\left(\frac{\partial^2 s}{\partial x^2} + \frac{\partial^2 s}{\partial y^2}\right)}^{\text{diffusion}} + \overbrace{Rs(1-s)}^{\text{reaction/growth}}$$

- A key design point of PETSc is that it is run-time configurable.
- This means that we can completely change our solvers **from the command line**.
- We can easily change the linear solver, add preconditioners, change the nonlinear solver, or change the timestepping scheme.
- Further, we write a straightforward code that can **scale to huge numbers of MPI processes** with a uniform interface which hides the details of the halo exchanges and other communication details.

Exercise 1

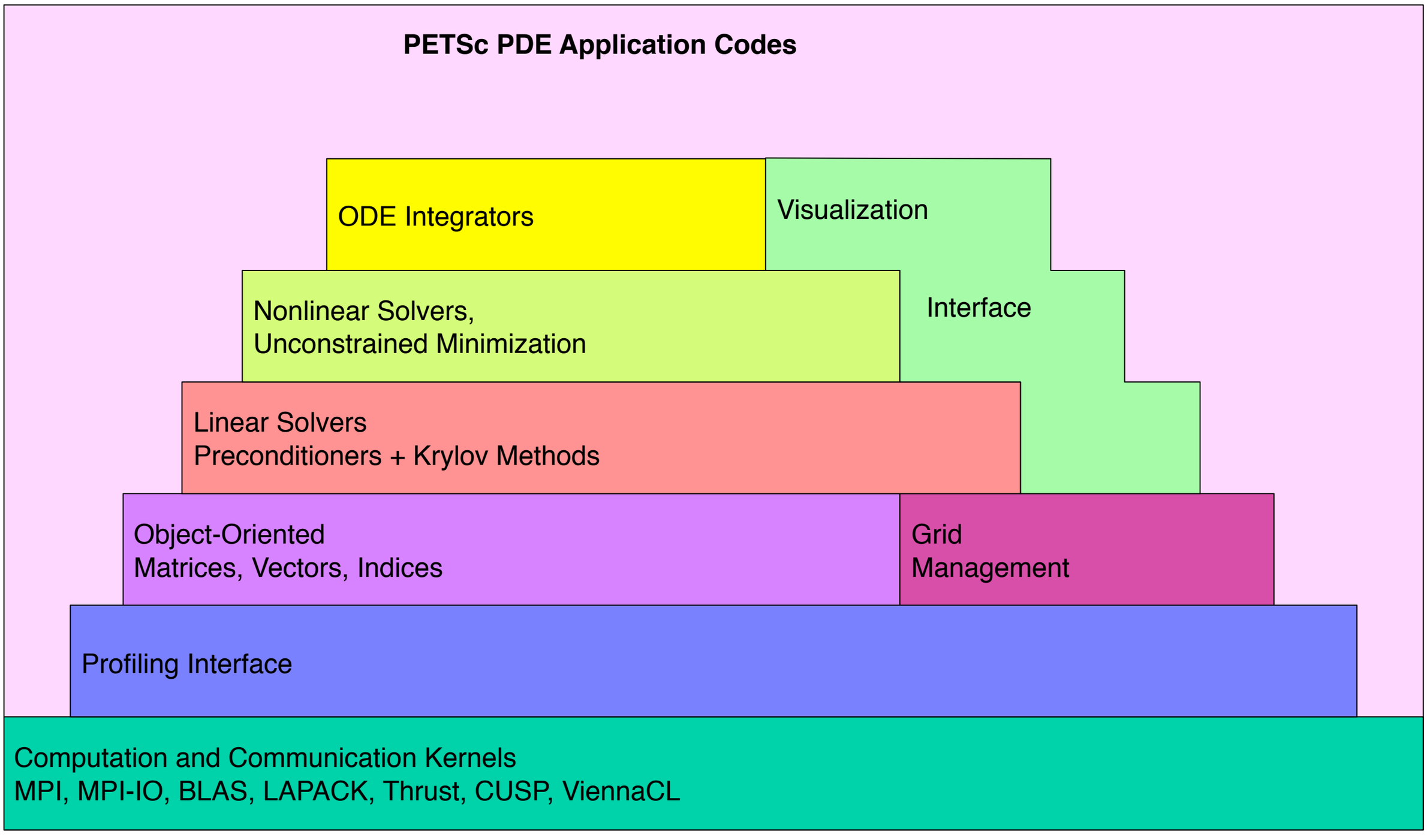
Get the code running!

- Obtain the source
- Follow the instructions in `libraries/petsc-miniapp/README.md`



(Note that it is very convenient to use the **`cray-petsc`** module, as we will do here, but that you can, with relative ease, build a more recent version of the library on essentially any machine, and use/modify the included makefile.local)

We will touch (briefly) on all the major components pictured here



Code Walkthrough: ODE Solvers

see `main.c`

(Note that PETSc's TS also includes DAE solvers, though we only consider ODE here)

Exercise 2

Change the ODE integrator

- Experiment running the program with different numbers of grid points, time steps, and MPI processes
- Experiment with the command line options
  `-ts_view`, **`-ts_monitor`**
- Experiment with **`-ts_type`** (Not all will work - later on as a bonus exercise we can change this)

Table 10: Time integration schemes.

TS Name	Reference	Class	Type	Order
euler	forward Euler	one-step	explicit	1
ssp	multistage SSP [20]	Runge-Kutta	explicit	≤ 4
rk*	multistage	Runge-Kutta	explicit	≥ 1
beuler	backward Euler	one-step	implicit	1
cn	Crank-Nicolson	one-step	implicit	2
theta*	theta-method	one-step	implicit	≤ 2
alpha	alpha-method [18]	one-step	implicit	2
gl	general linear [5]	multistep-multistage	implicit	≤ 3
eimex	extrapolated IMEX [7]	one-step	≥ 1, adaptive	
arkimex	see Tab. 12	IMEX Runge-Kutta	IMEX	$1-5$
rosw	see Tab. 13	Rosenbrock-W	linearly implicit	$1-4$

http://www.mcs.anl.gov/petsc/petsc-current/docs/manual.pdf

Code Walkthrough: Distributed Vectors, Arrays, and Linear Operators

see **`system.c`**

(We see how to assemble an operator, but PETSc also supports matrix-free operators, as in the miniapp, with the **`MatShell`** object)

Code Walkthrough: Simple Viewing

see **dump.c**

Exercise 3

Parallel Preconditioners

- Use the **`-assemble 1`** option
- 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)
  - Hint: perform one time step and use **`-ksp_view`**, and look at the preconditioner being used
- Experiment with an additive Schwarz preconditioner with options like
  `-help –pc_type asm`

and learn how to set the subsolver type (note that **`-help`** should now give you options specific to the ASM preconditioner)

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
  - Try `-pc_type gamg`

(Challenging) **Bonus exercise for the bored or bold**
PETSc includes many very sophisticated “Implicit Explicit” integrators. Take a look in the PETSc manual and see if you can adapt the example to use TSARKIMEX.

Performance Profiling

-log_summary provides a wealth of information.

- Time and flops used by various functions
- Call counts
- load balances
- Memory usage
- Much more!

Exercise 5

Algorithmic experimentation

- See how much you can speed up the execution of the program just by selecting different options at the command line
- For a reasonable set of options, vary the number of MPI processes and use **`-log_summary`** to examine the strong-scaling efficiency (does doubling the number of process halve the time?)

Ask questions!

Also, note the manual and man pages at http://www.mcs.anl.gov/petsc/documentation/index.html

Continuing with PETSc

- Read the manual
- join the petsc-users mailing list (and petsc-dev if interested)
  - http://www.mcs.anl.gov/petsc/miscellaneous/mailing-lists.html
  - Note the archives
- Look at the many examples in the **`src/`** tree
- Ask for help on the petsc-users list, or at petsc-maint@mcs.anl.gov (if you must)
- To get the best help
  - Read the error message
  - In emails, include full error messages, **`configure.log`** and **`make.log`**, and the output of **`-log_summary`** if asking about performance.
- Have fun, and let me know how it goes, as I am working on a longer PETSc tutorial ! (sananp@usi.ch)