THE UNIVERSITY of York

Overview of the BOUT++ code structure

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BOUT++

- A toolbox for solving PDEs on parallel computers, together with pre- and post-processing codes. Aims to reduce duplication of effort, and allow quick development and testing of new physics models and simulations
- A collection of examples and test cases
- Focused on flute-reduced plasma models in field-aligned coordinate systems, but more general capabilities

Is not:

- A single plasma model or simulation
- A general library of numerical methods for parallel computing. Other tools like PETSc are available for that.
- Magic. Appropriate numerical schemes depend on the problem, and must be chosen intelligently by the user

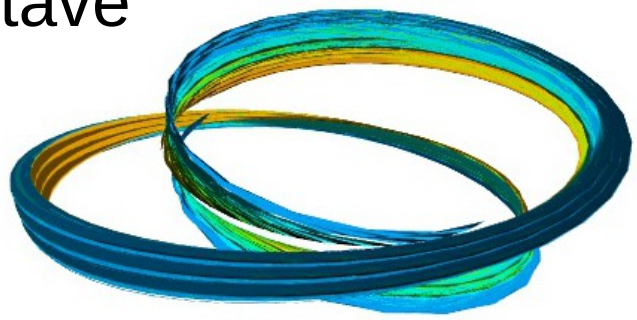
Key features

- Finite difference initial value code in 3D
- Implicit (e.g. BDF, C-N) or explicit (e.g. RK4, Karniadakis) time integration
- Coordinate system set in metric tensor components
- Handles complicated topology of X-point tokamak geometry
- Written in C++, quite modular design

- A growing community working to develop and exploit simulations using fluid and gyro-fluid models

Improvements since version 1.0

- Interfaces to PETSc (timestepping + linear solves) and MUMPS (linear solves).
  → Many sophisticated methods, more general problems
- Linear solvers for new classes of problems
  → Fast parabolic solves along (equilibrium) field lines
- Preconditioning schemes → faster simulations
- New differencing methods, flux conservative and limiter schemes, boundary conditions, ...
- Pre- and post-processing in more languages
  →IDL, Python, Matlab, Mathematica, Octave
- 3D visualisation using VisIt and Mayavi
- Many updates, fixes, restructuring configure scripts, manual, ...



Getting BOUT++

- Workshop release version 2.0

```
https://github.com/boutproject/BOUT-2.0
```

- Version control using **git**, a distributed system designed for large collaborative projects (e.g. Linux kernel)

→ See `http://git-scm.com`

- To download, run in terminal:

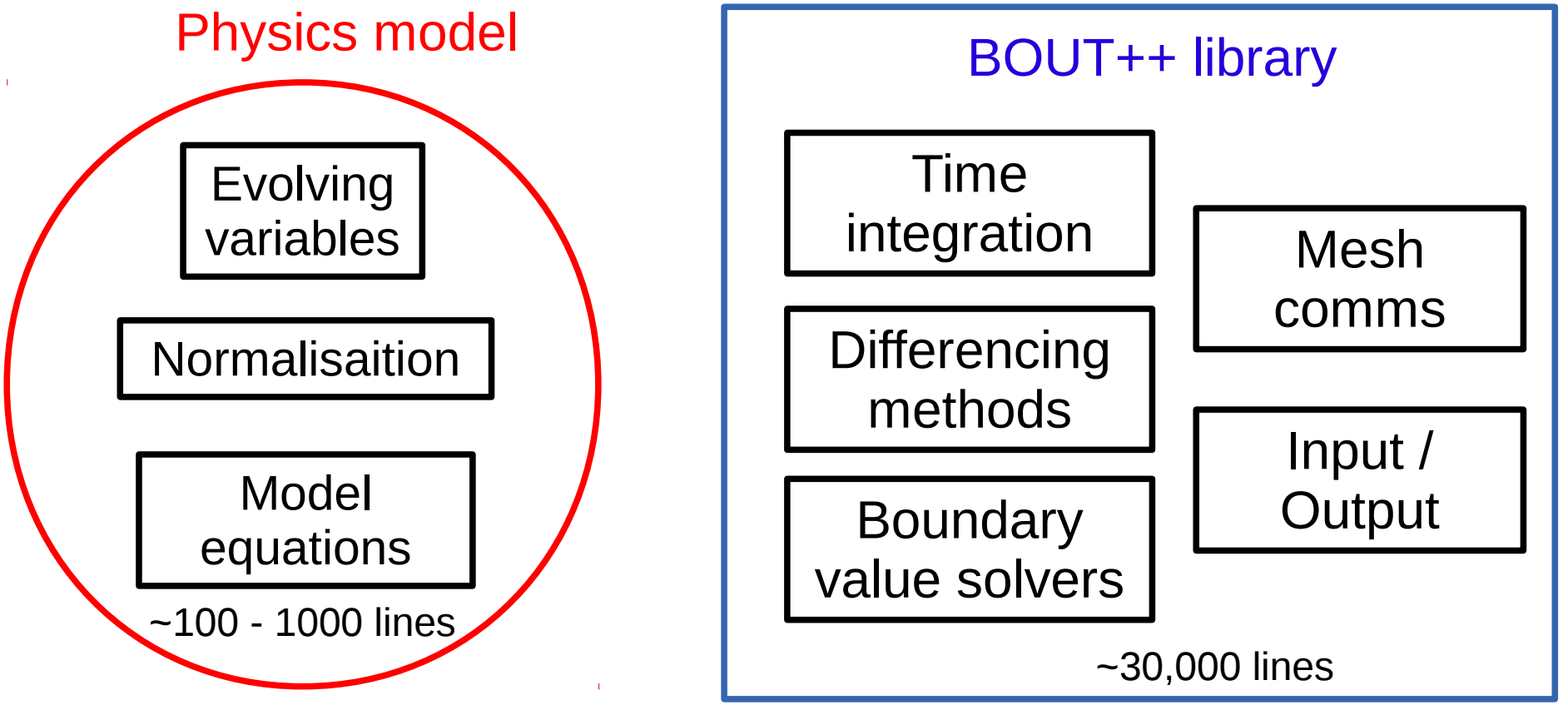
```
$ git clone
      https://github.com/boutproject/BOUT-2.0.git
```

- To later update to latest version, change to BOUT-2.0 directory and run

```
$ git pull
```

BOUT++ structure

- Separates generic methods from model-specific code
- Most of the code doesn't know or care about what a variable represents, its normalisation etc. Only needs to know the geometry and which operation to perform



Finding your way around

After downloading BOUT++ (or browsing online), you'll see

`manual`

`src`

`examples`

`tools`

- configure and make scripts
  (see user manual, and Maxim's talk)
- README and COPYING

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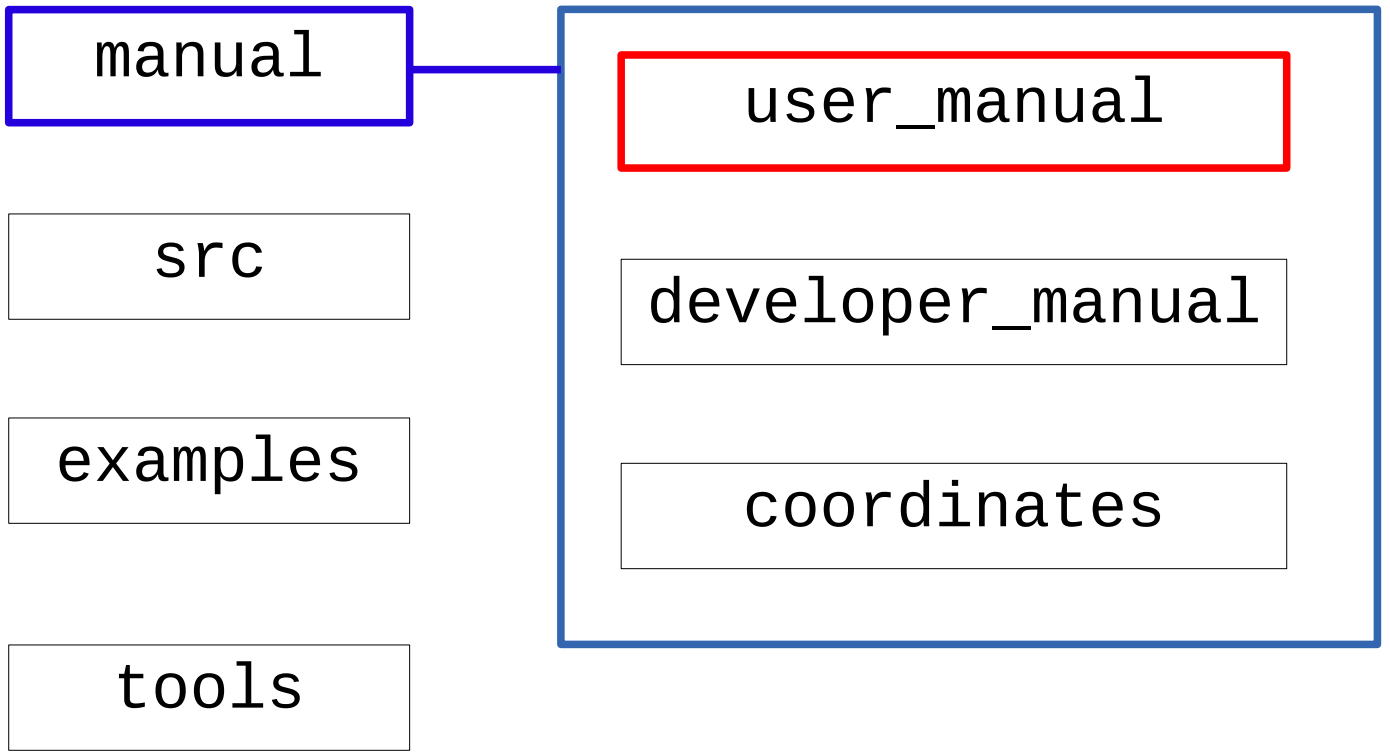

User manual describes how to get started with BOUT++.

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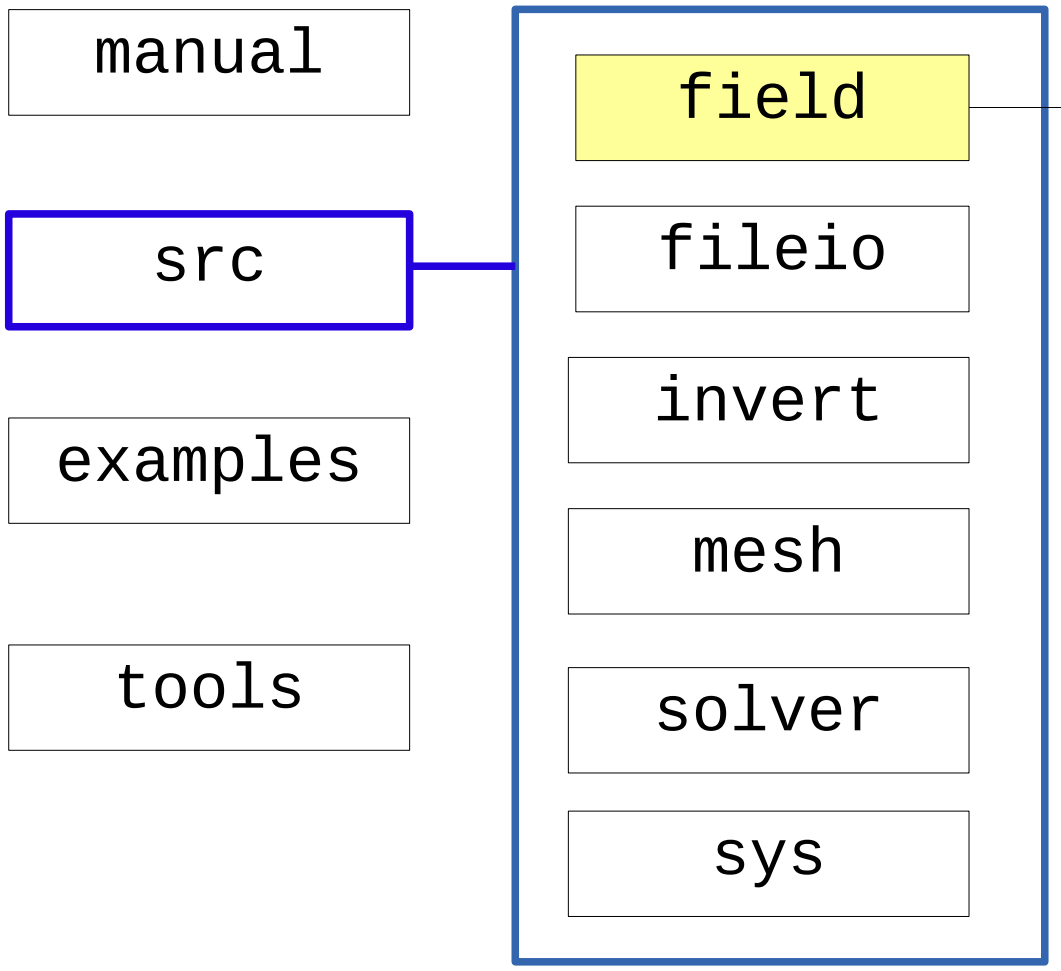

Data handling routines

- Memory allocation and handling
- Scalar and vector fields, and operations on them
- Initial and boundary conditions

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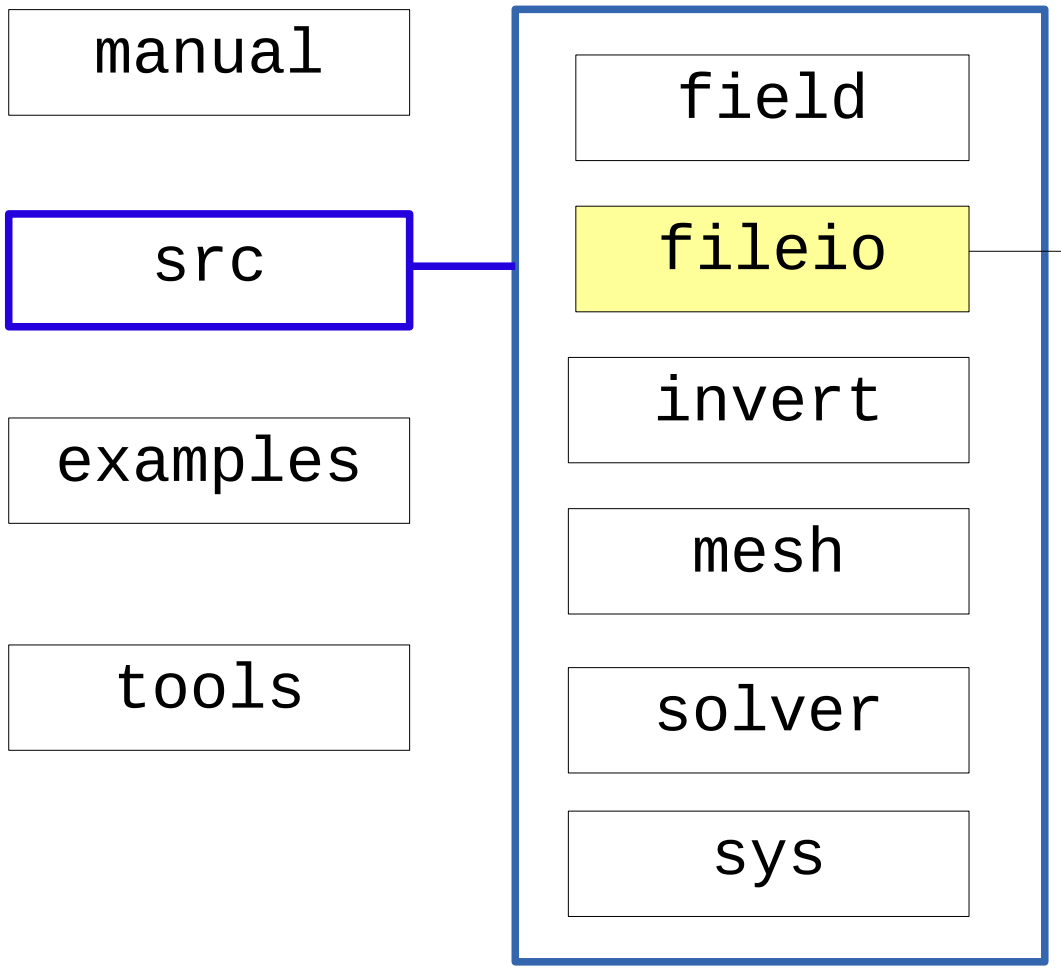

Data input and output

- Reading and writing binary file formats (pdb, netcdf, ...)
- Interface for writing scalar and vector fields

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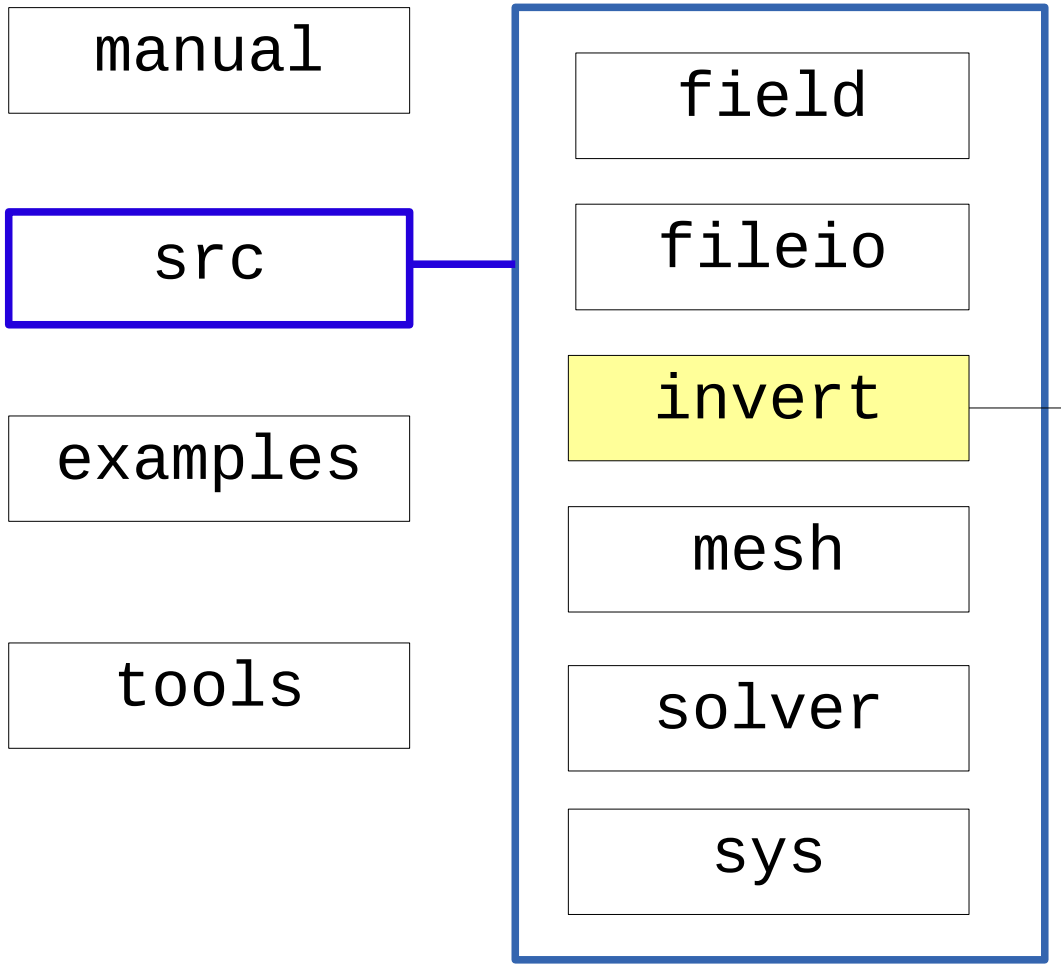

PDE solvers for boundary-value problems

- Common routines for inverting Laplacian type equations
- Interfaces to PETSc, MUMPS, … for some problems

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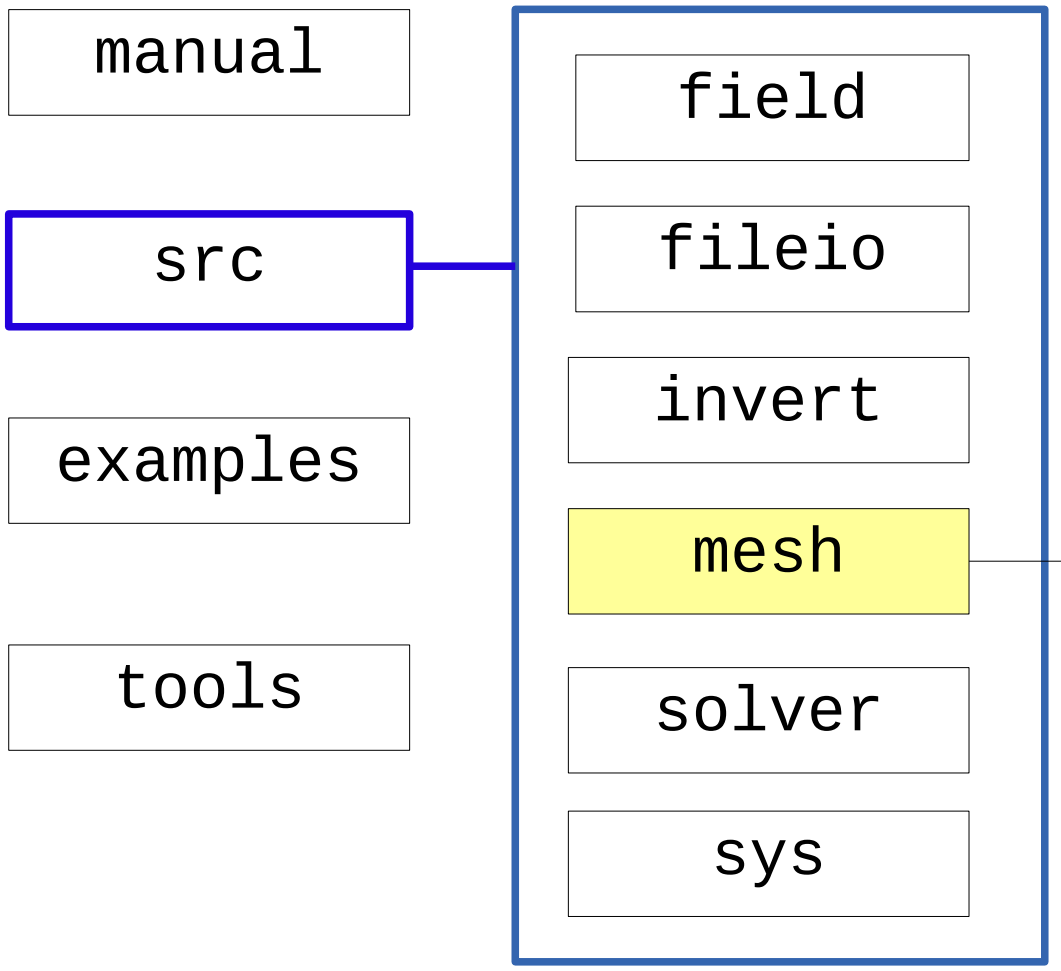

Mesh

- Distribution of grid points across processors
- Local ↔ Global
- Communications
- Metric tensor

Finding your way around

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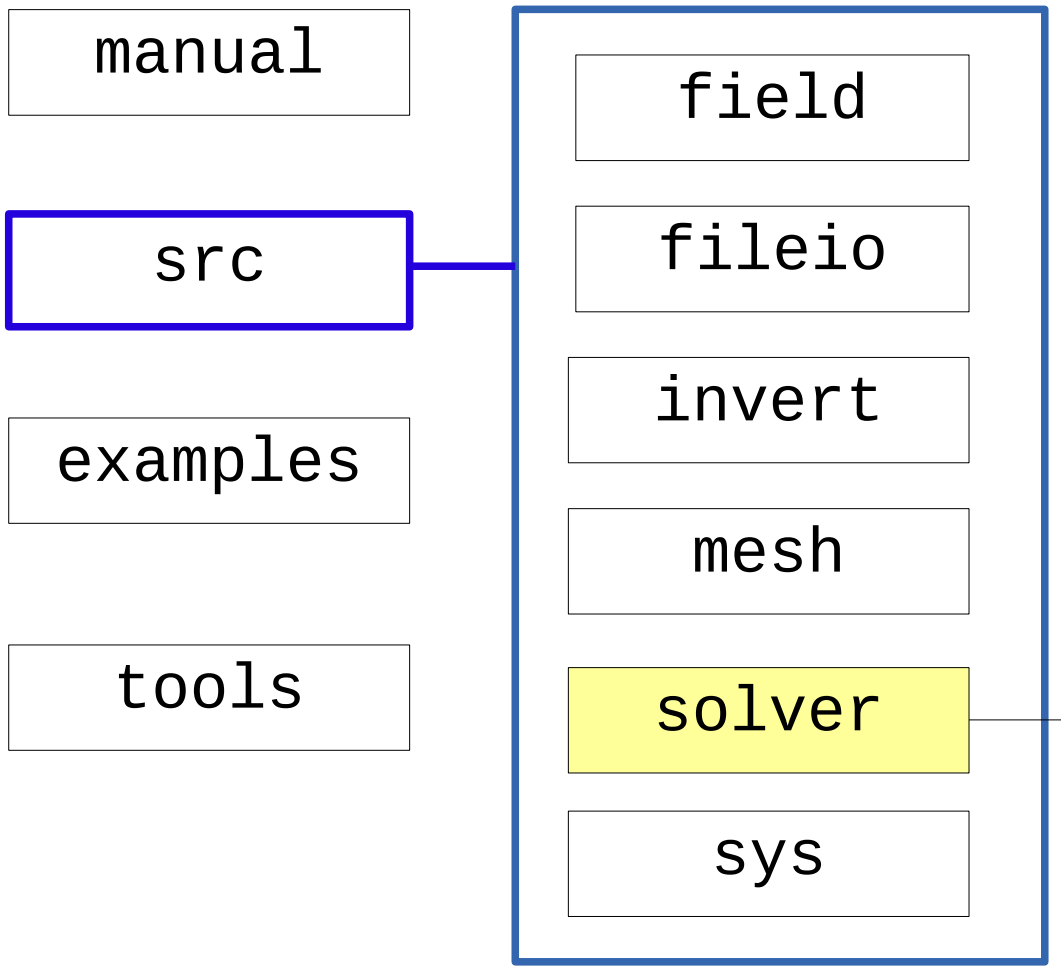

Time integration

- Explicit and implicit methods
- Interface to external solvers in SUNDIALS and PETSc

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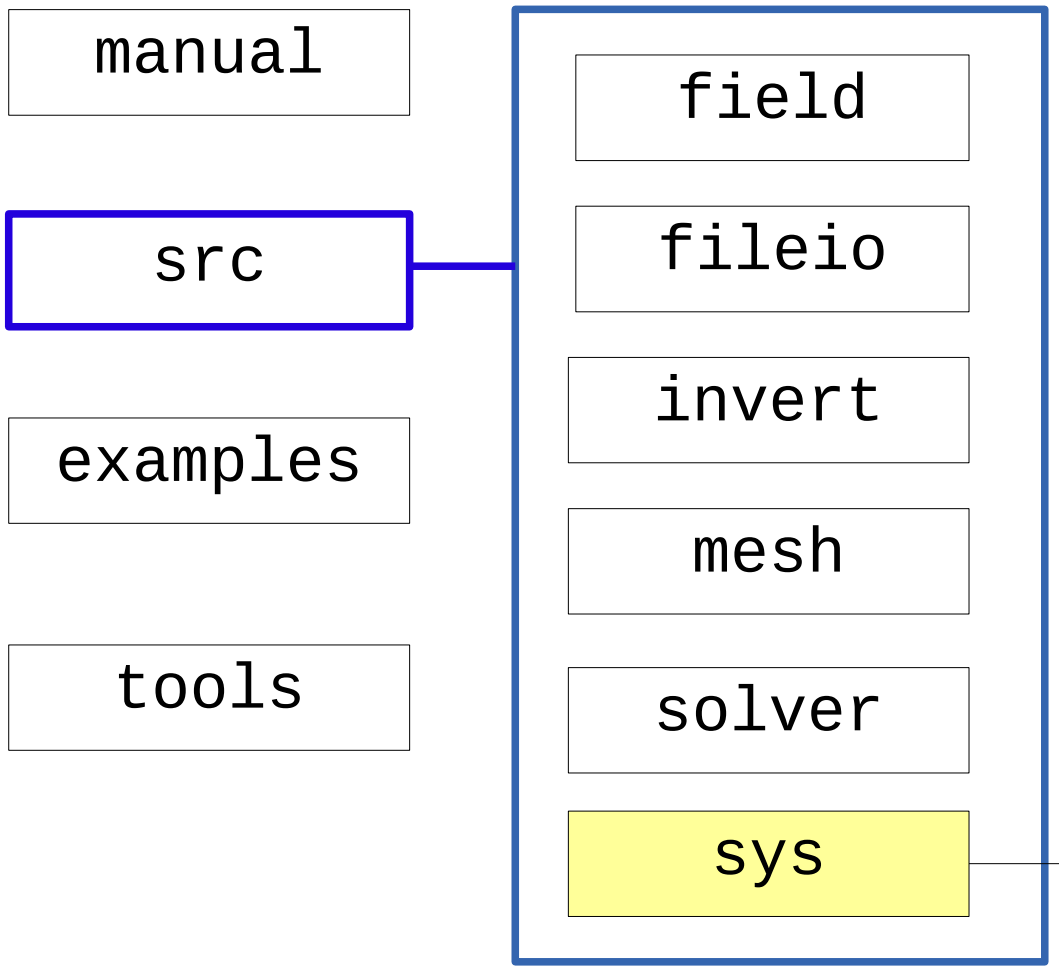

Miscellaneous utilities

- Options get/set to control behaviour
- Exception handling, timing and debugging aids
- MPI and PETSc start / stop
- Differencing methods

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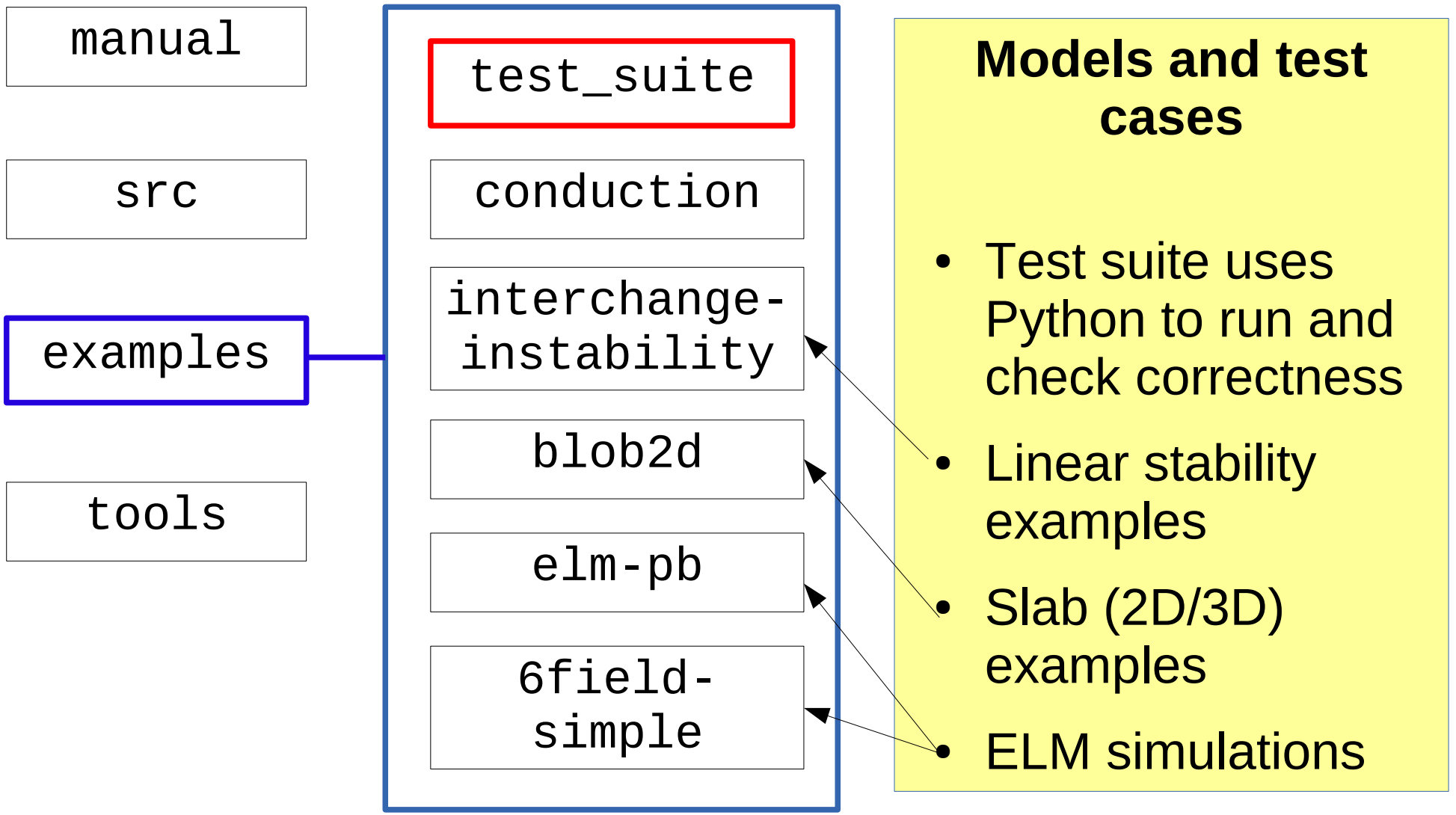

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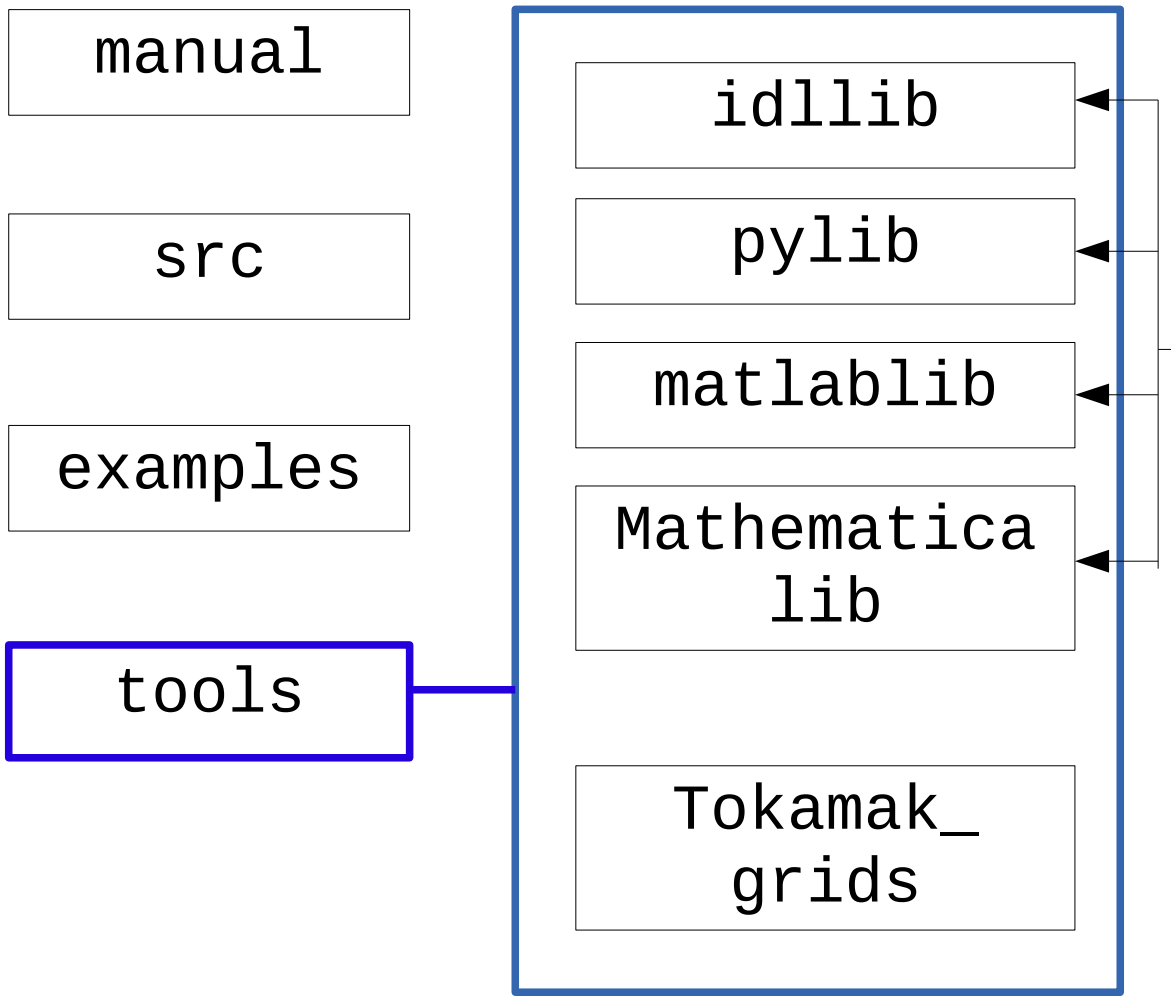

Pre- and post-processing

- “Collect” routines to read output data for various languages
- Processing and visualisation
- Mesh generation

Example: Hasegawa-Wakatani

```
Field3D n, vort, phi;
```

Objects represent scalar and vector fields over the mesh

```
Options *options = Options::getRoot()->getSection("hw");
OPTION(options, alpha, 1.0);
OPTION(options, kappa, 0.1);


SOLVE_FOR2(n, vort);

phiSolver = Laplacian::create();
```

RHS function evaluation (called by solver)

```
phi = phiSolver->solve(vort, phi);
mesh->communicate(n, vort, phi);

ddt(n) = -bracket(phi, n, bm) + alpha*(phi - n) – kappa*DDZ(phi)
         – Dn*Delp4(n);
ddt(vort) = -bracket(phi, vort, bm) + alpha*(phi – n)
         - Dvort*Delp4(vort);
```

Example: Hasegawa-Wakatani

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```

Tree of options controlling behaviour. Set in input file:

```
[hw]
alpha = 0.4
```

RHS function evaluation (called by solver)

```
phi = phiSolver->solve(vort, phi);
mesh->communicate(n, vort, phi);

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```

Macros for common tasks:

```
options->get(alpha, “alpha”, 1.0);
options->get(kappa, “kappa”, 0.1);

solver->add(n, “n”);
solver->add(vort, “vort”)
```

RHS function evaluation (called by solver)

```
phi = phiSolver->solve(vort, phi);
mesh->communicate(n, vort, phi);

ddt(n) = -bracket(phi, n, bm) + alpha*(phi - n) – kappa*DDZ(phi)
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phiSolver = Laplacian::create();
```

Factory options set in input file:

```
[solver]
type = cvode

[laplace]
type = petsc
```

(Can be passed an options object)

RHS function evaluation (called by solver)

```
phi = phiSolver->solve(vort, phi);
mesh->communicate(n, vort, phi);

ddt(n) = -bracket(phi, n, bm) + alpha*(phi - n) – kappa*DDZ(phi)
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```

Guard cell communication explicit to allow optimisation (send...calculate ...wait)

Equations appear in easily readable form

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Overloaded operators, not template expressions currently

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ddt(vort) = -bracket(phi, vort, bm) + alpha*(phi – n)
         - Dvort*Delp4(vort);
```

Derivative methods set in options e.g.

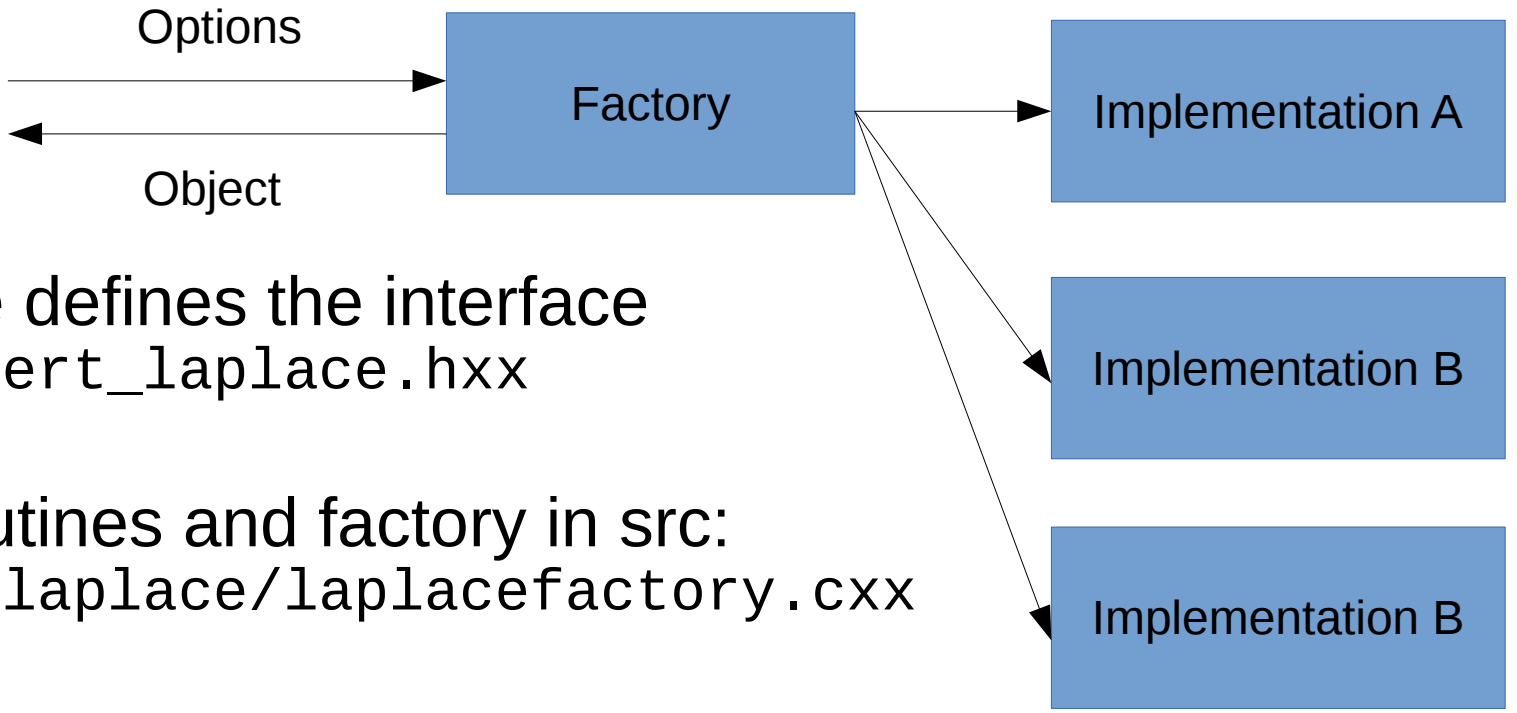
```
[ddz]
first =  C4   # 4th-order Central difference
```

Boundary conditions in input file e.g

```
[n]
bndry_all = dirichlet
```

BOUT++ component patterns

Most components now follow the same “**factory**” pattern



A header file defines the interface
`include/invert_laplace.hxx`

Common routines and factory in src:
`src/invert/laplace/laplacefactory.cxx`

Individual implementations in subdirectory
`src/invert/laplace/impls/...`

The factory is the only place where individual headers are included, so forces rest of the code to be independent.

See developer manual for more details

Using BOUT++ (conclusions)

- BOUT++ is open source, under the LGPL license.
- Allows linking to proprietary code, but modifications to core of BOUT++ come under LGPL.

- You are free to take and modify BOUT++ for any purpose
- Please contribute improvements and fixes back to the community
- Use of BOUT++ and contributed components should be acknowledged through co-authorship and/or citations

- One aim of this workshop is to establish a solid community basis for collaboration