Firedrake/PyOP2: an overview

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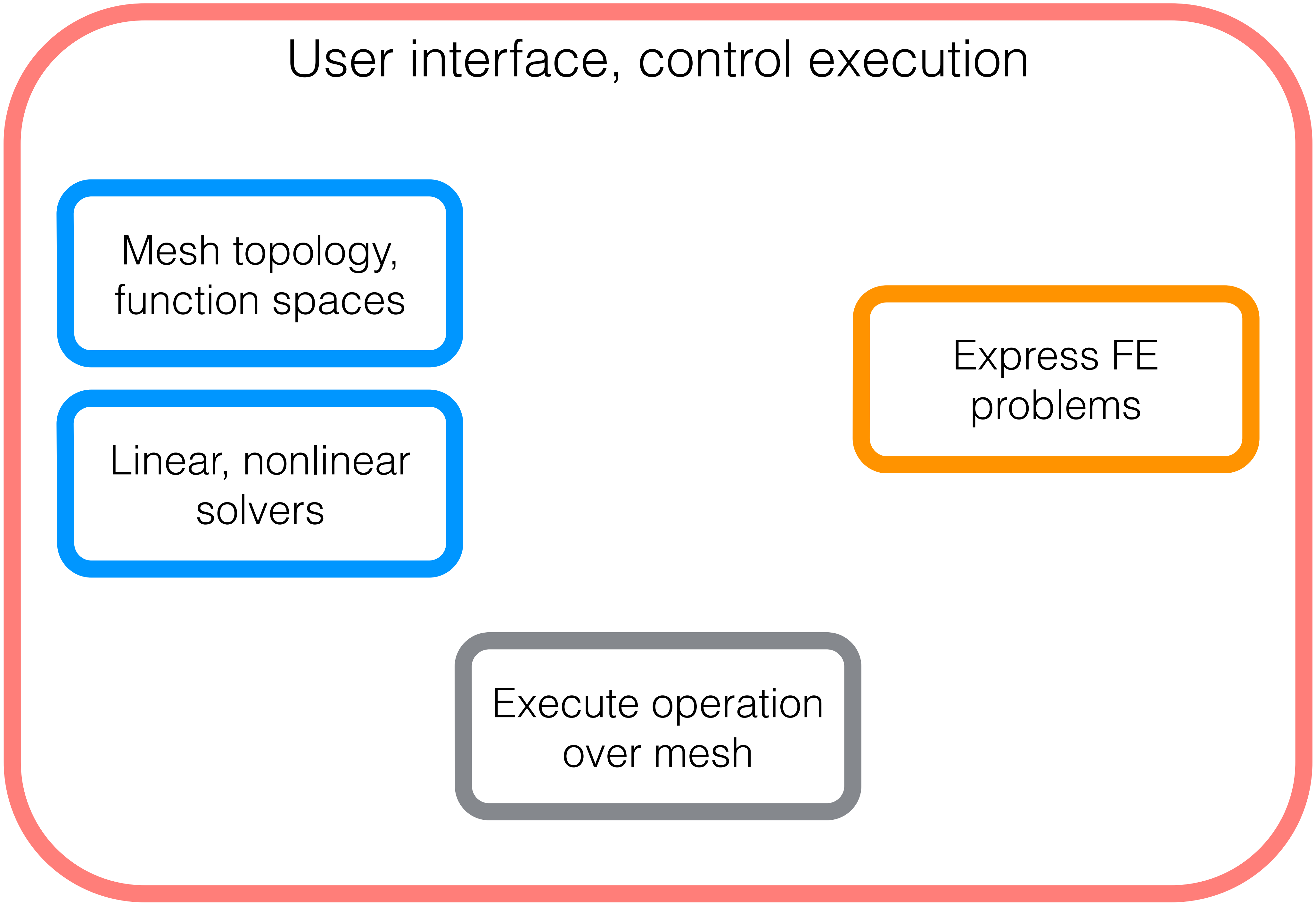
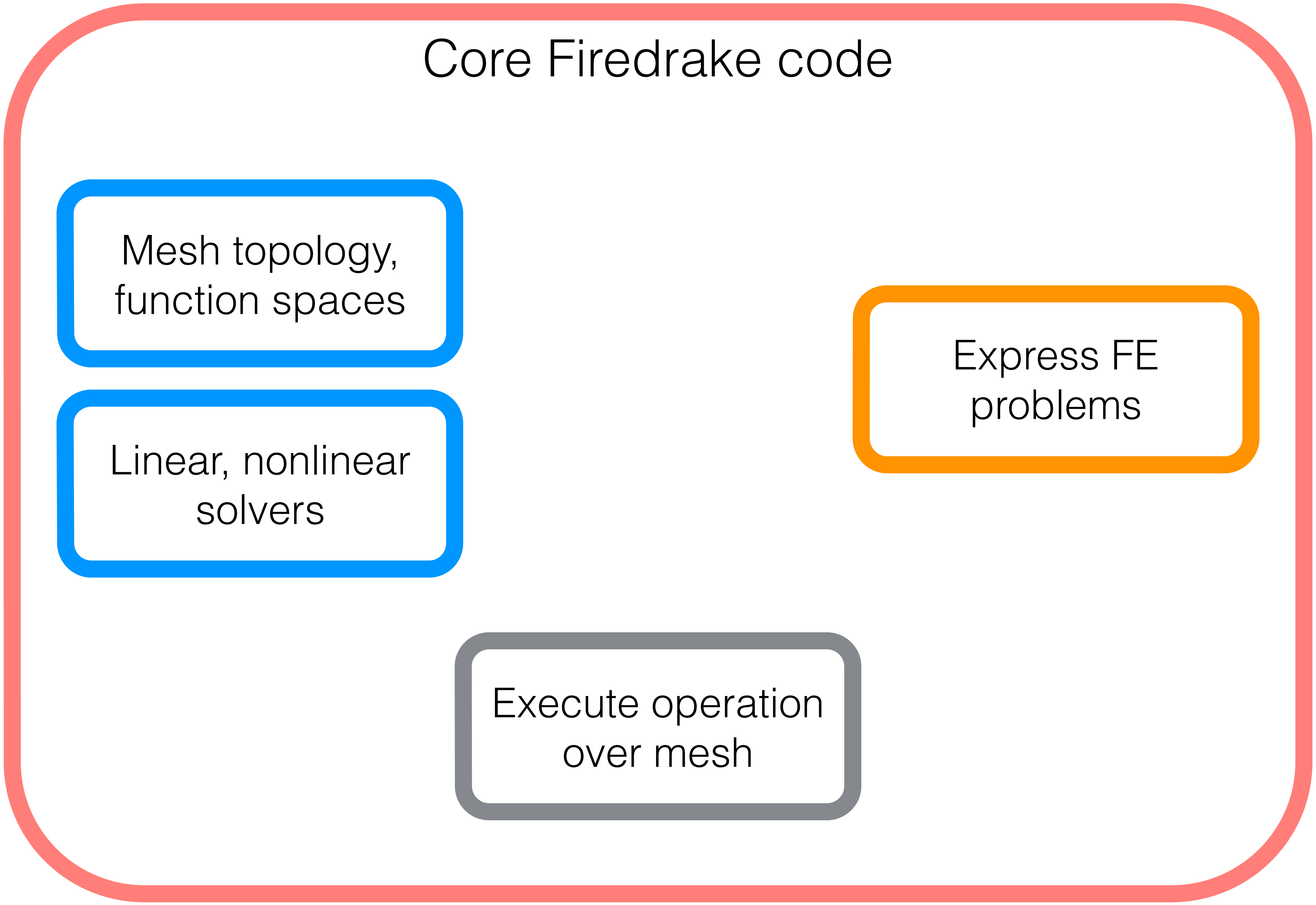
- www.firedrakeproject.org
- github.com/OP2/PyOP2
- github.com/firedrakeproject/firedrake
- firedrake@imperial.ac.uk (subscribe first)
- #firedrake on irc.freenode.net
- WPL upstairs (modulo summer building works)

...and a cast of thousands

- Computing
  - Doru Bercea, Fabio Luporini, Florian Rathgeber, Lawrence Mitchell, David Ham, Paul Kelly
- Maths
  - Andrew McRae, Colin Cotter, David Ham, Jemma Shipton, Hiroe Yamazaki
- ESE
  - Michael Lange, Christian Jacobs
- Bath
  - Eike Müller
- Simula
  - Simon Funke
- Former members
  - Graham Markall, Nicolas Loriant
- UROP/project students
  - Kaho Sato, George Boutsioukis


User interface, control execution
Mesh topology, function spaces
Linear, nonlinear solvers
Express FE problems
Execute operation over mesh


Core Firedrake code
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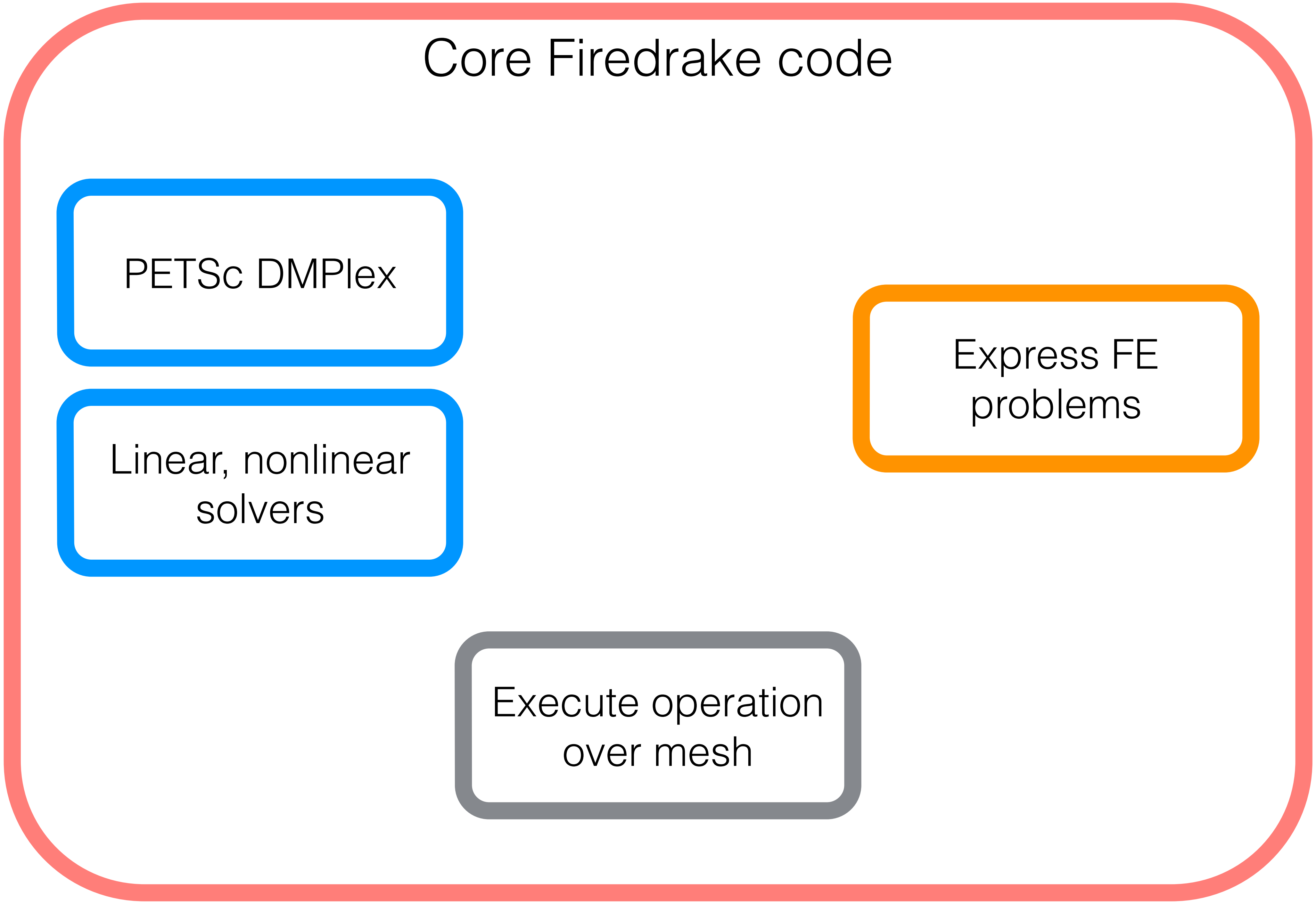
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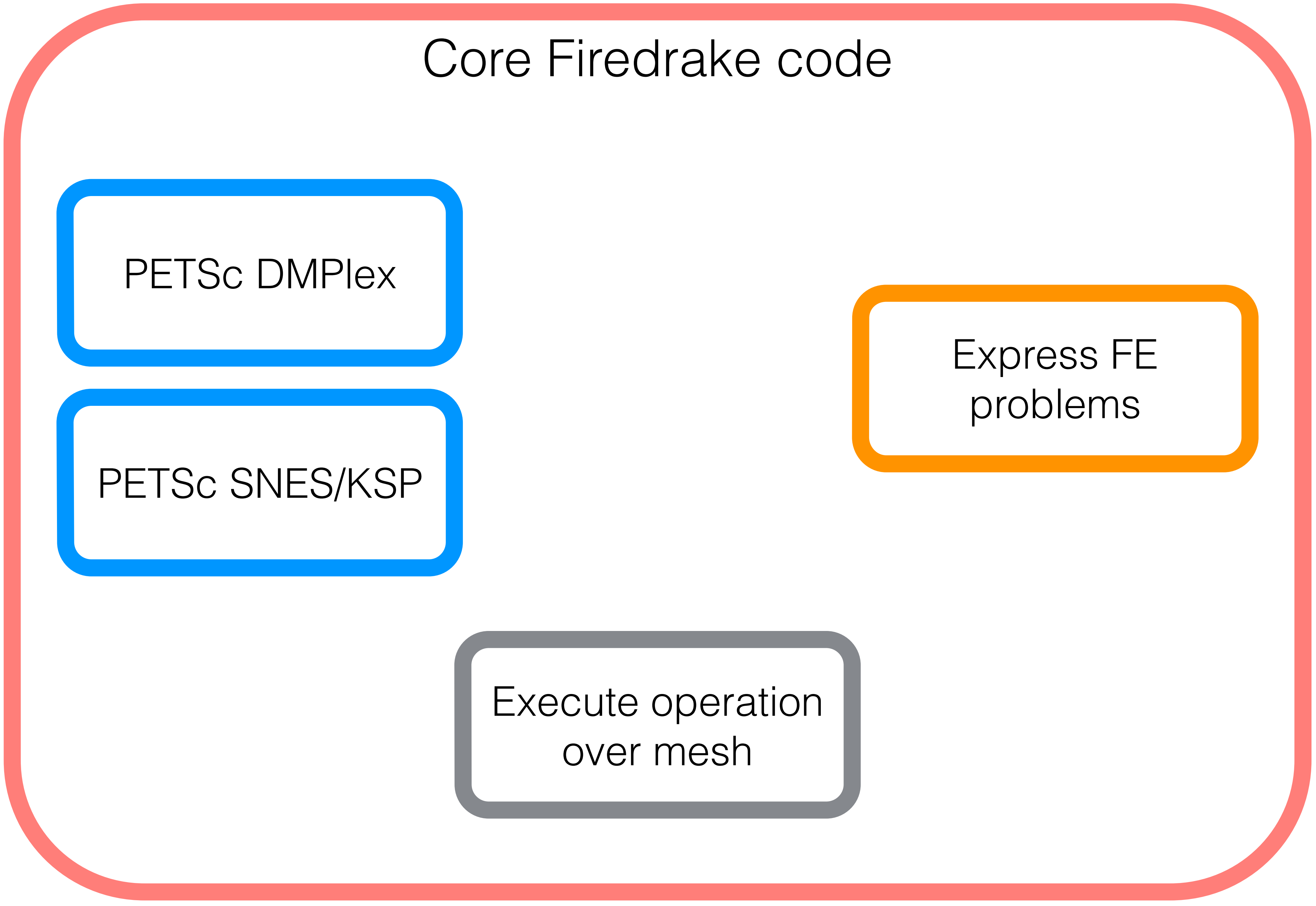
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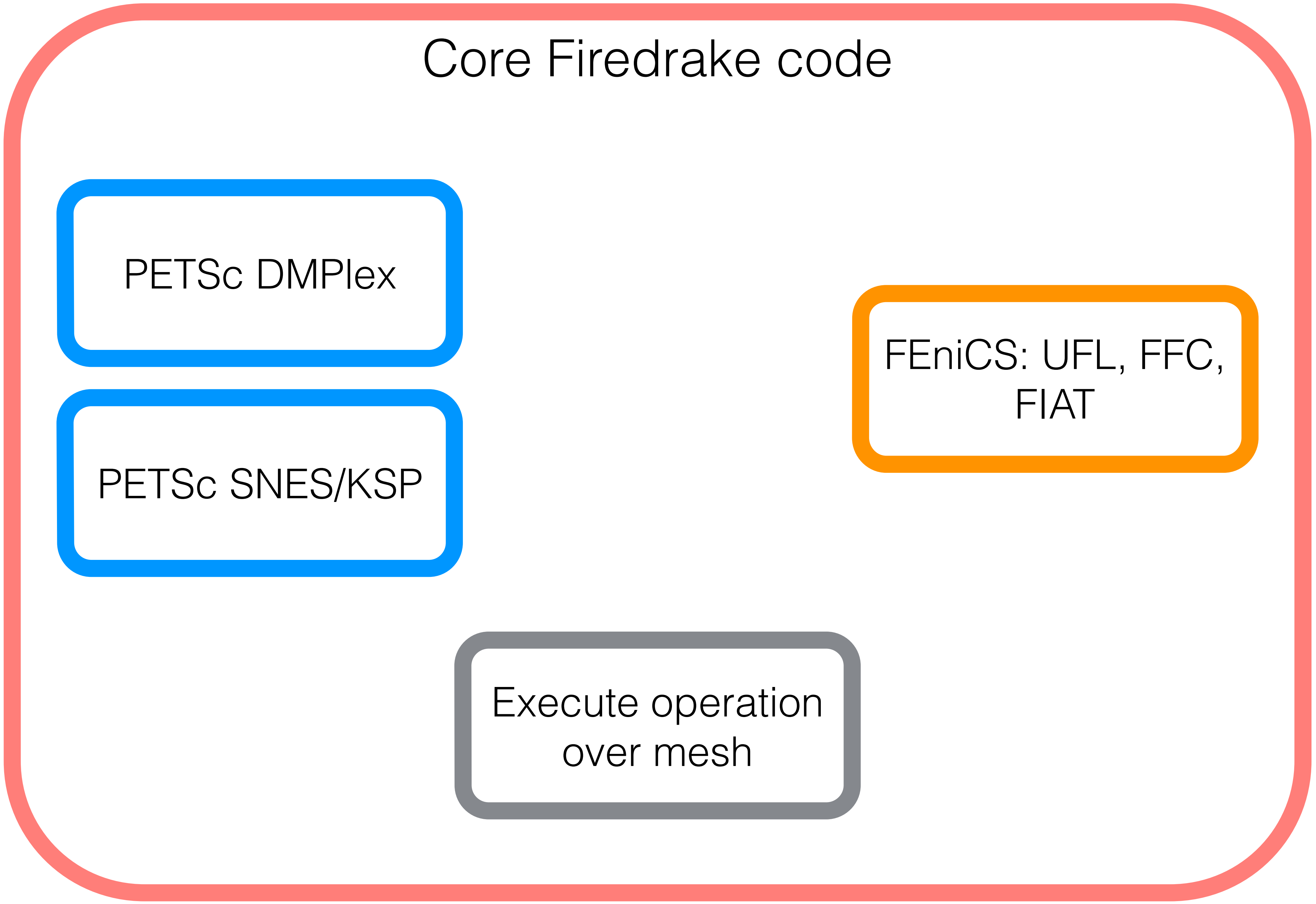
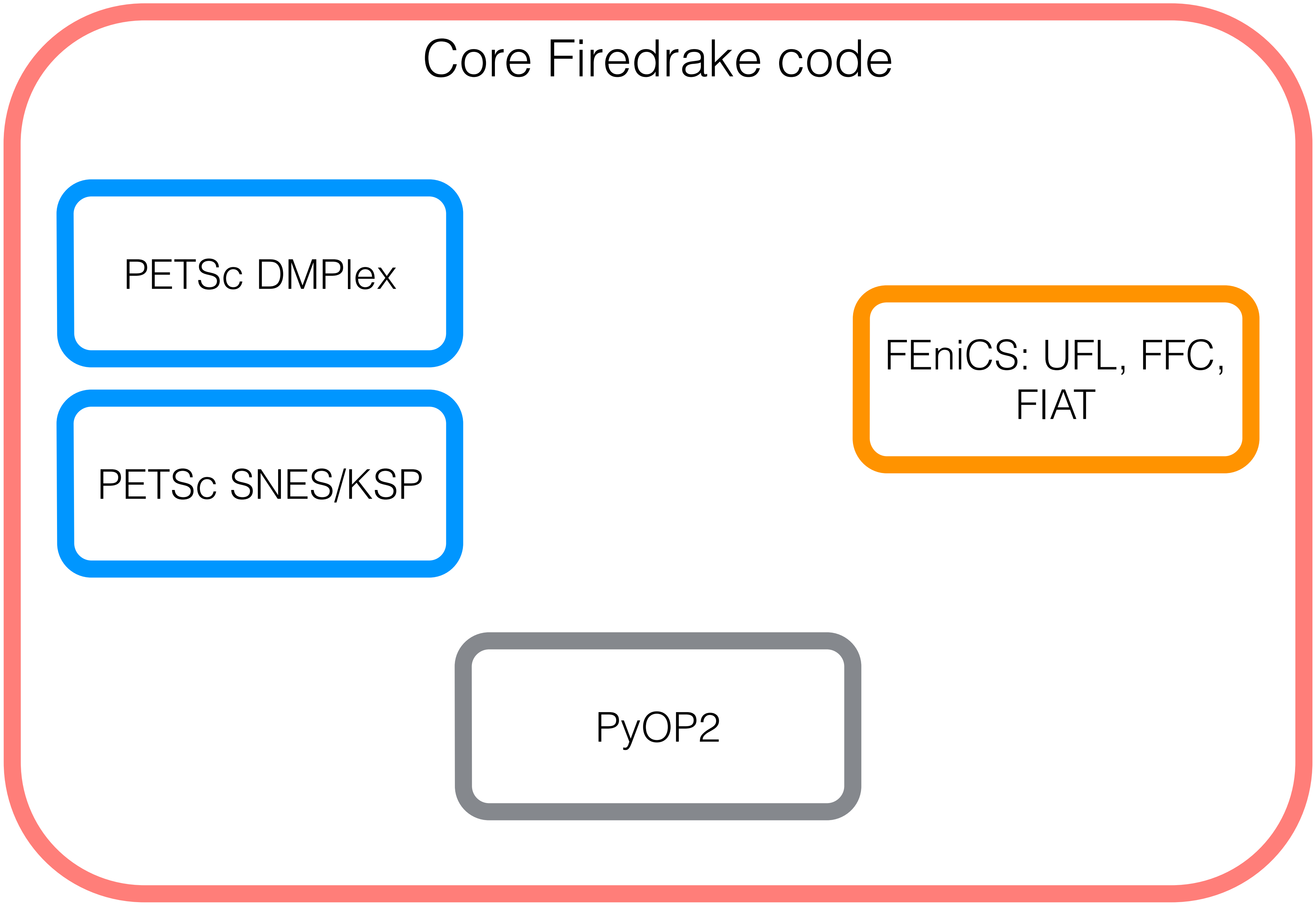


Core Firedrake code
PETSc DMPlex
PETSc SNES/KSP
FEniCS: UFL, FFC, FIAT
Execute operation over mesh


Core Firedrake code
PETSc DMPlex
PETSc SNES/KSP
FEniCS: UFL, FFC, FIAT
PyOP2

```python
from firedrake import *

m = Mesh('...')

mesh = ExtrudedMesh(m, layers=20, extrusion_type='uniform')

element1 = ...
element2 = ...

V = FunctionSpace(mesh, element1)
Q = FunctionSpace(mesh, element2)

W = V*Q

u, p = TrialFunctions(W)
v, q = TestFunctions(W)

a = fn(u, p, v, q)
L = fn(v, q)

solve(a == L, ...)
```

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Michael's talk (DMPlex)

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u, p = TrialFunctions(W)
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```

Extrusion

```python
from firedrake import *

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solve(a == L, ...)
```

UFL

```python
from firedrake import *

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Q = FunctionSpace(mesh, element2)

W = V*Q

u, p = TrialFunctions(W)
v, q = TestFunctions(W)

a = fn(u, p, v, q)
L = fn(v, q)

solve(a == L, ...)
```

← Firedrake

```python
from firedrake import *

m = Mesh('...')

mesh = ExtrudedMesh(m, layers=20, extrusion_type='uniform')

element1 = ...
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u, p = TrialFunctions(W)
v, q = TestFunctions(W)

a = fn(u, p, v, q)
L = fn(v, q)
solve(a == L, ...)
```
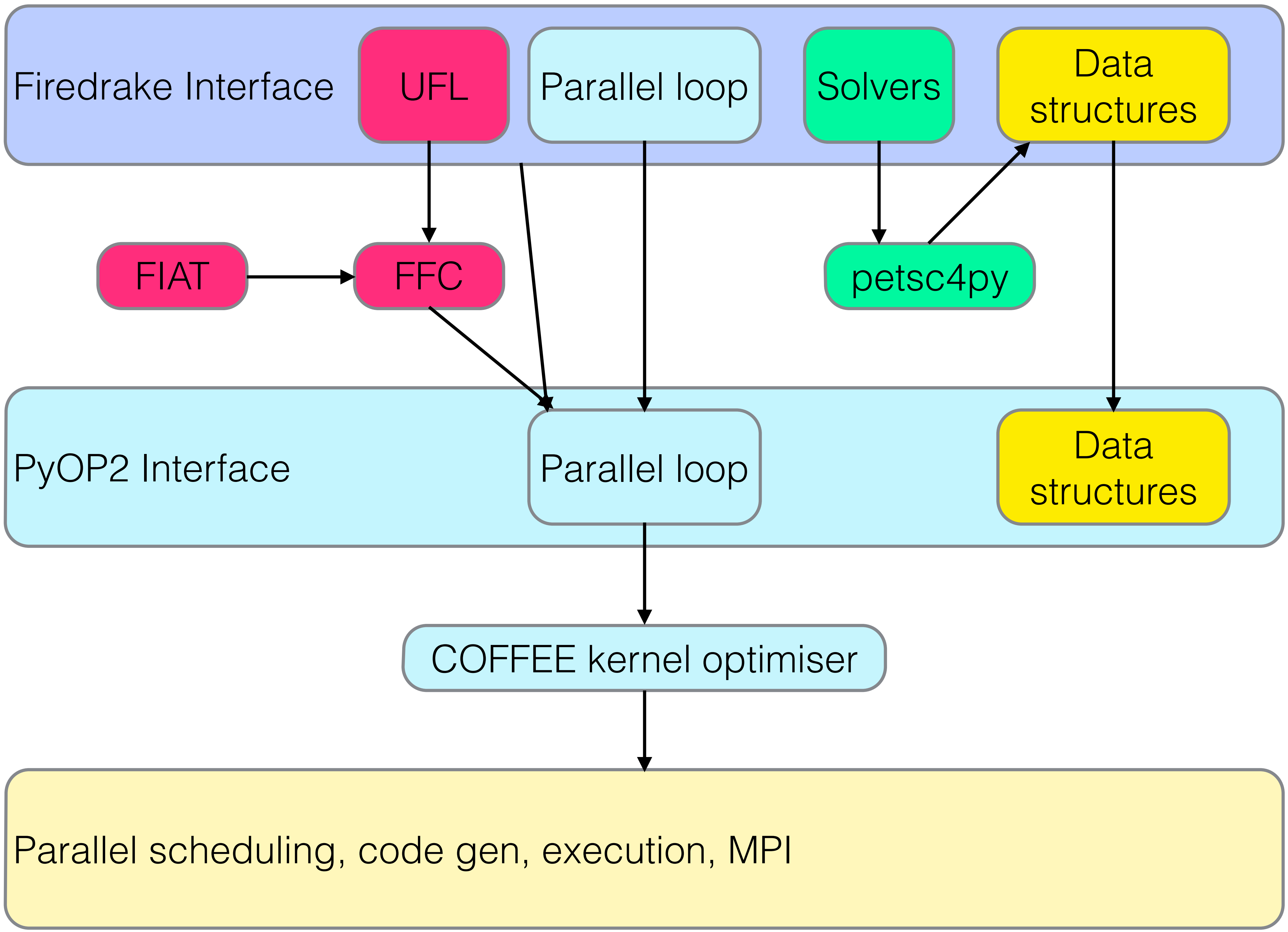

Firedrake, PyOP2, FFC, FIAT, UFL, PETSc


Firedrake Interface
UFL
Parallel loop
Solvers
Data structures
FIAT
FFC
petsc4py
PyOP2 Interface
Parallel loop
Data structures
COFFEE kernel optimiser
Parallel scheduling, code gen, execution, MPI

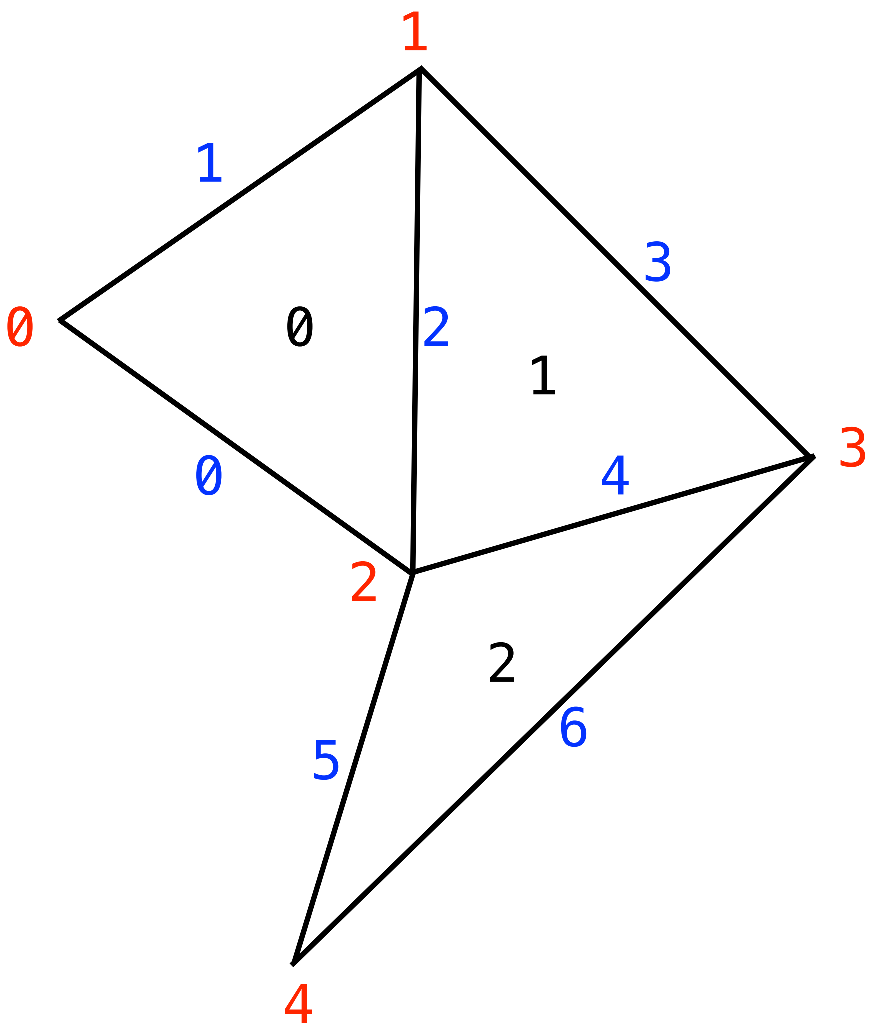
PyOP2

- Computation on a fixed-degree graph (unstructured mesh)
- Local computation *kernel* executed everywhere
    - Data parallel
- *Reductions* aggregate contributions into result
- No finite element assumption (almost)

Mesh topology

- Effectively a graph
- Sets represent nodes in the graph
- Maps define edges between nodes
- Maps are constant *arity*
    - Cannot have map from vertices to cells (say)

```python
from pyop2 import op2
op2.init()

cells = op2.Set(3)
edges = op2.Set(7)
vertices = op2.Set(5)

c2e = op2.Map(cells, edges, 3,
              [[0, 1, 2],
               [2, 3, 4],
               [4, 5, 6]])
c2v = op2.Map(cells, vertices, 3,
              [[0, 1, 2],
               [1, 2, 3],
               [2, 3, 4]])
e2v = op2.Map(edges, vertices, 2,
              [[0, 2],
               [0, 1],
               [1, 2],
               [1, 3],
               [2, 3],
               [2, 4],
               [3, 4]])
```



Data

- Data defined on DataSets (Set + number of entries per set entity), any C type

```
from pyop2 import op2
op2.init()
cells = op2.Set(3)
dofs = op2.Set(18)
```

```
field = op2.Dat(dofs**1, dtype=np.float64)
```

1 dof per set entity

```
vector_field = op2.Dat(dofs**2, dtype=np.float32)
```

2 dofs per set entity

Kernel

- Acts on *local* data, cannot read outside it

```
from pyop2 import op2
op2.init()

edges = op2.Set(...)
vertices = op2.Set(...)

midpoint = op2.Dat(edges**2)
coords = op2.Dat(vertices**2)

e2v = op2.Map(edges, vertices, 2, ...)

midpoint_kernel = op2.Kernel("""
     void midpoint(double *mid, double **vtx_coords) {
         mid[0] = (vtx_coords[0][0] + vtx_coords[1][0]) / 2;
         mid[1] = (vtx_coords[0][1] + vtx_coords[1][1]) / 2;
     }""", "midpoint")
```

Parallel loop

- Execute *kernel* over set, reading/writing data
  - Describe: iteration space (set/subset), data to be accessed, access type (READ, WRITE, RW, INC), indirection.
- MPI-collective
  - All processes must hit parallel loop (even if they are iterating over zero-sized domain)
    - Careful applying boundary conditions!
  - Kernel must be *identical* everywhere
    - Run with `export PYOP2_DEBUG=1` to find issues

```python
from pyop2 import op2
op2.init()

edges = op2.Set(...)
vertices = op2.Set(...)

midpoint = op2.Dat(edges**2)
coords = op2.Dat(vertices**2)

e2v = op2.Map(edges, vertices, 2, ...)

midpoint_kernel = ...

op2.par_loop(midpoint_kernel, edges,
             midpoint(op2.WRITE),
             coords(op2.READ, e2v))
```

Direct write to midpoint

Indirect read from coords through e2v

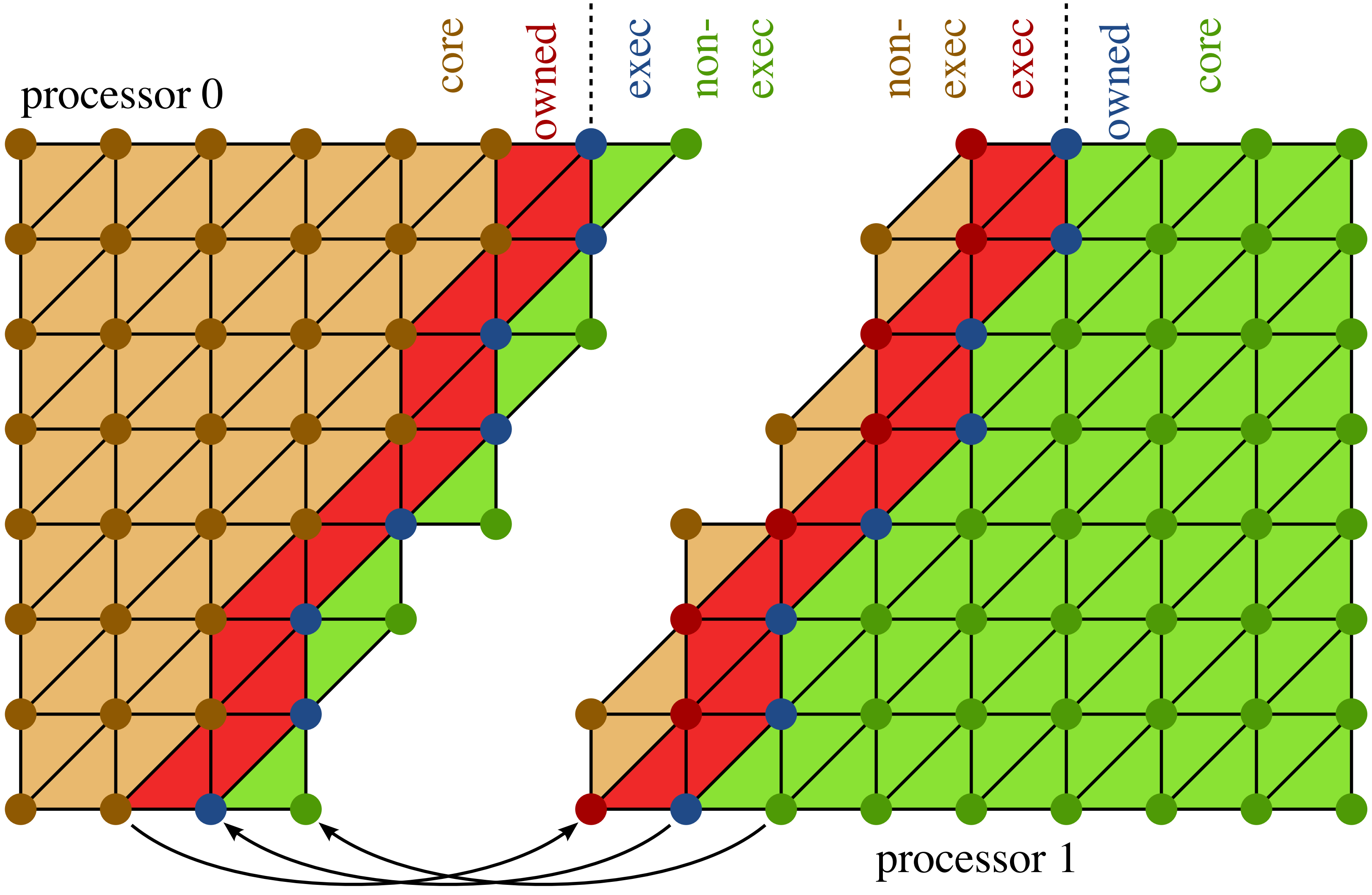
Code gen

- API carefully designed to make automated reasoning about execution *easy* "synthesis, not analysis"
- Access descriptors allow automatic reasoning about data dependencies
- e.g. no need to halo exchange on WRITE data
    - But mark as dirty so subsequent reads force exchange
- MPI-collective semantics mean we don't need to worry about other processes not posting halo sends/receives
- Shared memory: colour for non-conflicting execution
    - Assumption: we're allowed to reorder computations

```python
op2.par_loop(midpoint_kernel, edges,
             midpoint(op2.WRITE),
             coords(op2.READ, e2v))
```

```c
void midpoint(double *mid, double **vtx_coords) {
   mid[0] = (vtx_coords[0][0] + vtx_coords[1][0]) / 2;
   mid[1] = (vtx_coords[0][1] + vtx_coords[1][1]) / 2;
}

void wrap_midpoint(int start, int end,
                   double *midpoint, double *coords, int *e2v) {
   double *vtx_coords[2];
   for ( int i = start; i < end; i++ ) {
       vtx_coords[0] = coords + (e2v[i * 2 + 0])*2;
       vtx_coords[1] = coords + (e2v[i * 2 + 1])*2;
       midpoint(midpoint + i * 2, vtx_coords);
   }
}
```

- MPI parallelism handled in Python
- Entities must be *ordered*, extents can encode iteration order. Effectively, this puts constraint on numbering in Maps.

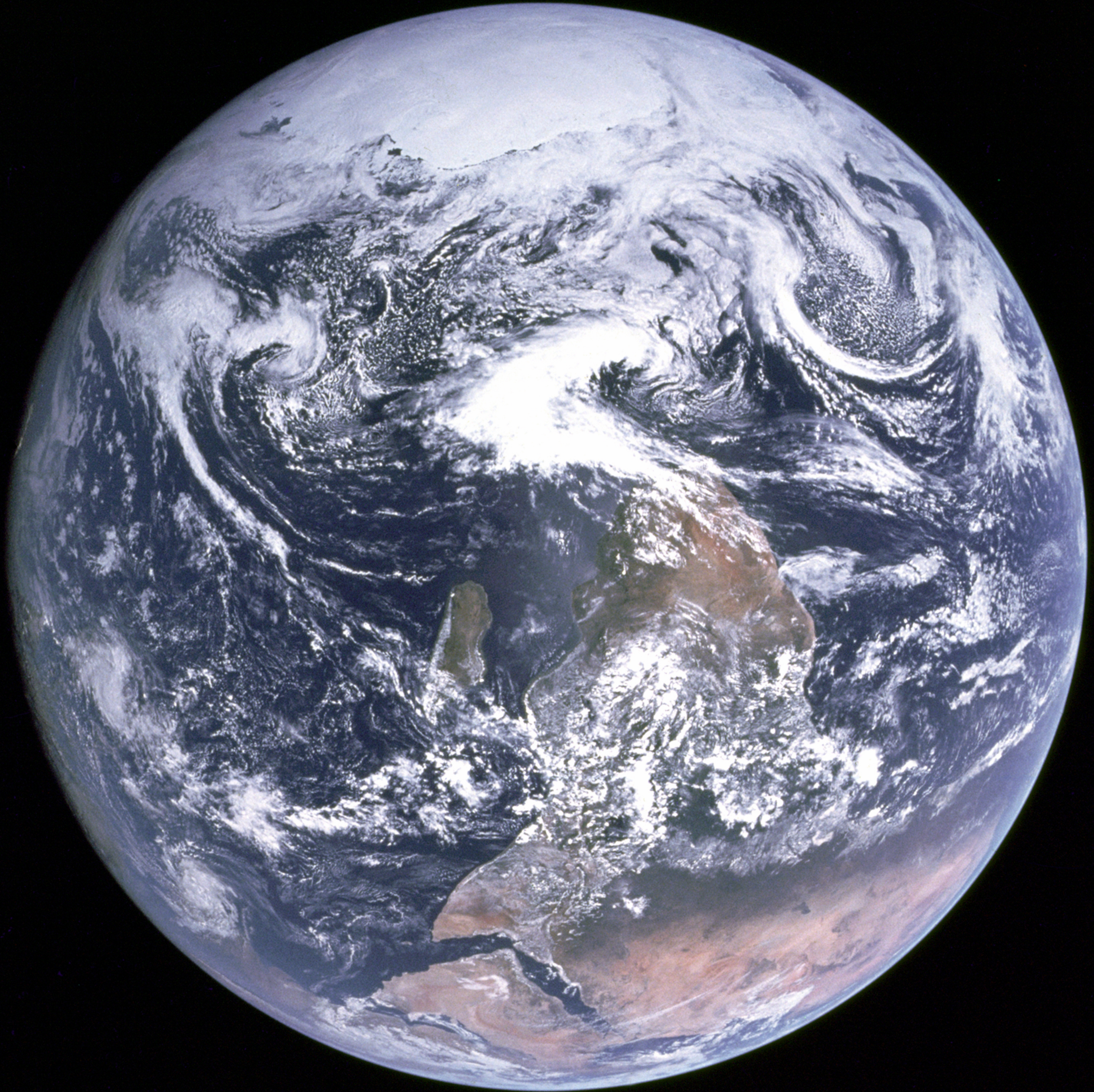


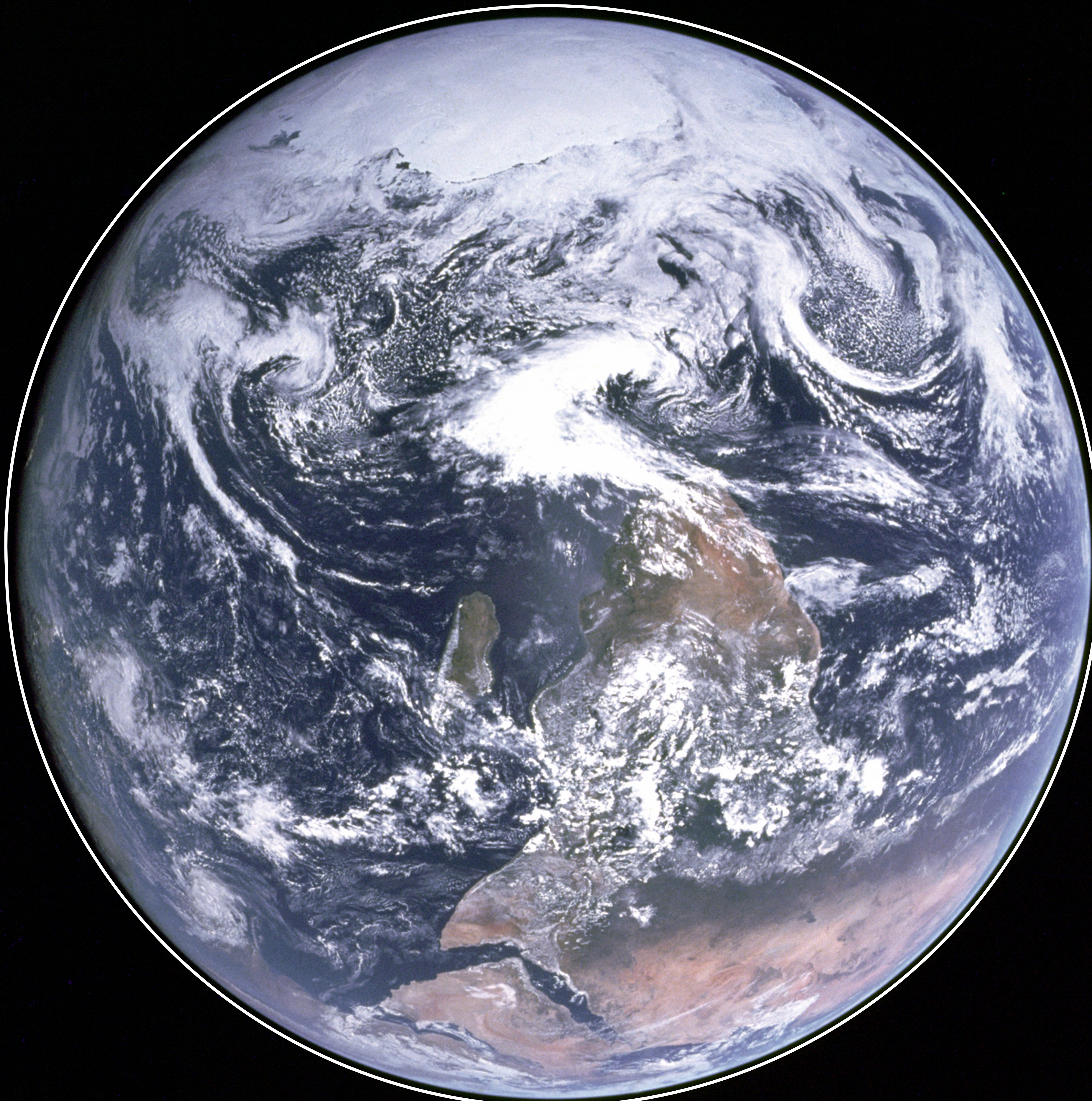
- *Core* entries: can compute without up to date halos
- *Owned* entries: local data, needs up to date halos
- *Exec halo* entries: remote data, but writes (through a map) to local data
- *Non-exec halo* entries: remote data, read (through a map) when computing on exec halo
- For FE, the stencil *on the topology* tells us how to mark topological entities, and hence degrees of freedom

```
cells = op2.Set([1, 3, 5, 6])
dofs = op2.Set([43, 52, 63, 68])

c2d = op2.Map(cells, dofs, 3,
             [
              # core entry (points to within first 43 dofs)
              [0, 32, 40],
              # owned entries (point to within first 52 dofs, but not
              # all within first 43)
              [0, 43, 44],
              [1, 45, 51],
              # exec halo entries (point to within first 63 dofs, but
              # not all within first 52)
              [2, 52, 57],
              [55, 56, 62],
              # non-exec halo entries (anything else)
              [63, 64, 65]
             ])
```

Extruded meshes

PyOP2 support



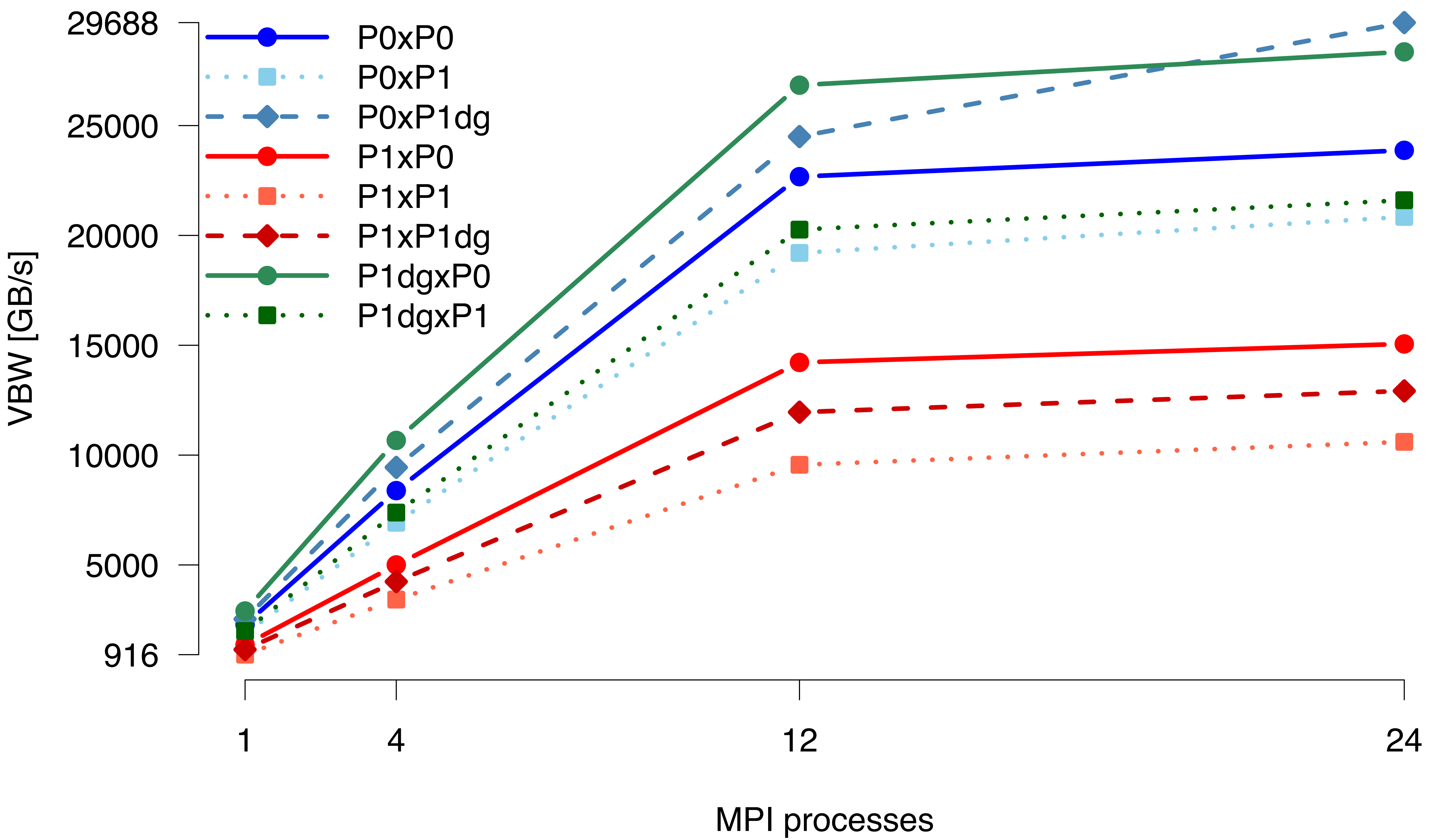


- Structured in *vertical* direction
- Map implicit (just provide *base* map plus offsets)
- Amortizes cost of indirect lookups
  - 70% peak memory bandwidth
- We measure *valuable bandwidth*: assume we could move data *perfectly* and therefore only ever touch it once. A *lower bound* on actual data movement.

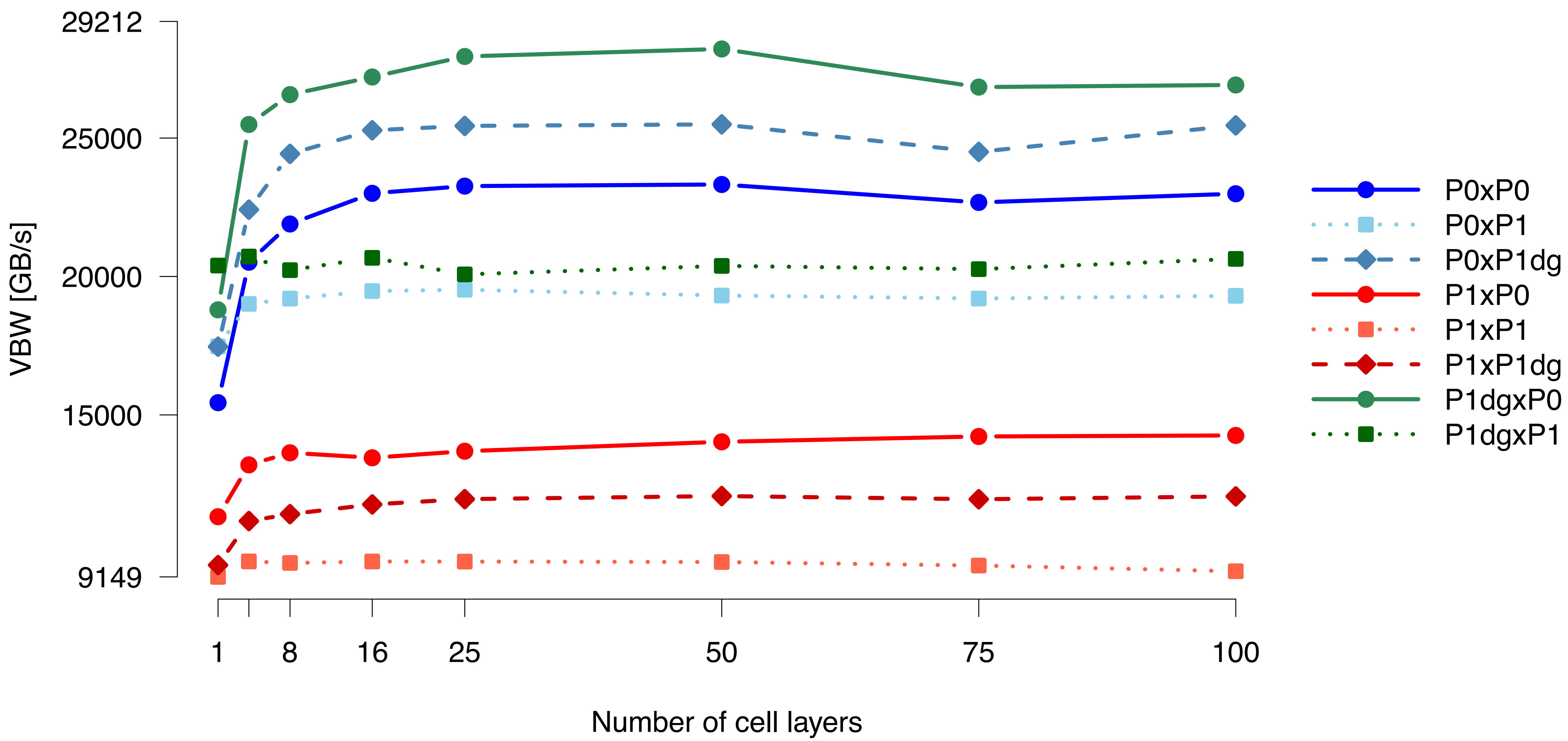
Does it work?

12 core SandyBridge; STREAM triad 42 GB/s

`assemble(v*dx)`



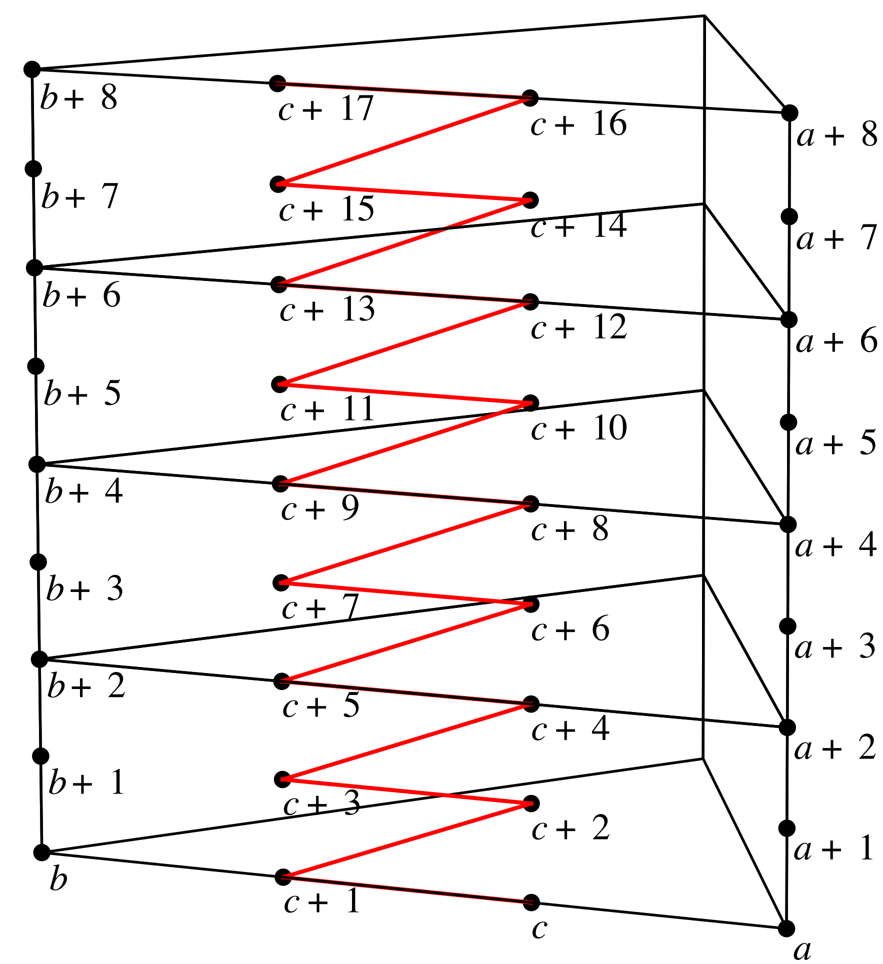
Indirection amortized after around 20 layers



How does it work?

- Indirect lookup for base cell dofs
- Direct increment walking up column
- Extra PyOP2 types
- Sets carry number of layers
- Maps carry offset for each indirected dof

```
base_cells = op2.Set(1)
ext_cells = op2.ExtrudedSet(base, layers=5)
base_dofs = op2.Set(total_dofs)
ext_dofs = op2.ExtrudedSet(base_dofs, layers=5)

cell2dof = op2.Map(ext_cells, ext_dofs,
                  12,
                  vals=[a, a+1, a+2, b, b+1, b+2,
                   c, c+1, c+2, c+3, c+4, c+5],
                  offset=[2, 2, 2, 2, 2, 2,
                          4, 4, 4, 4, 4, 4])
```



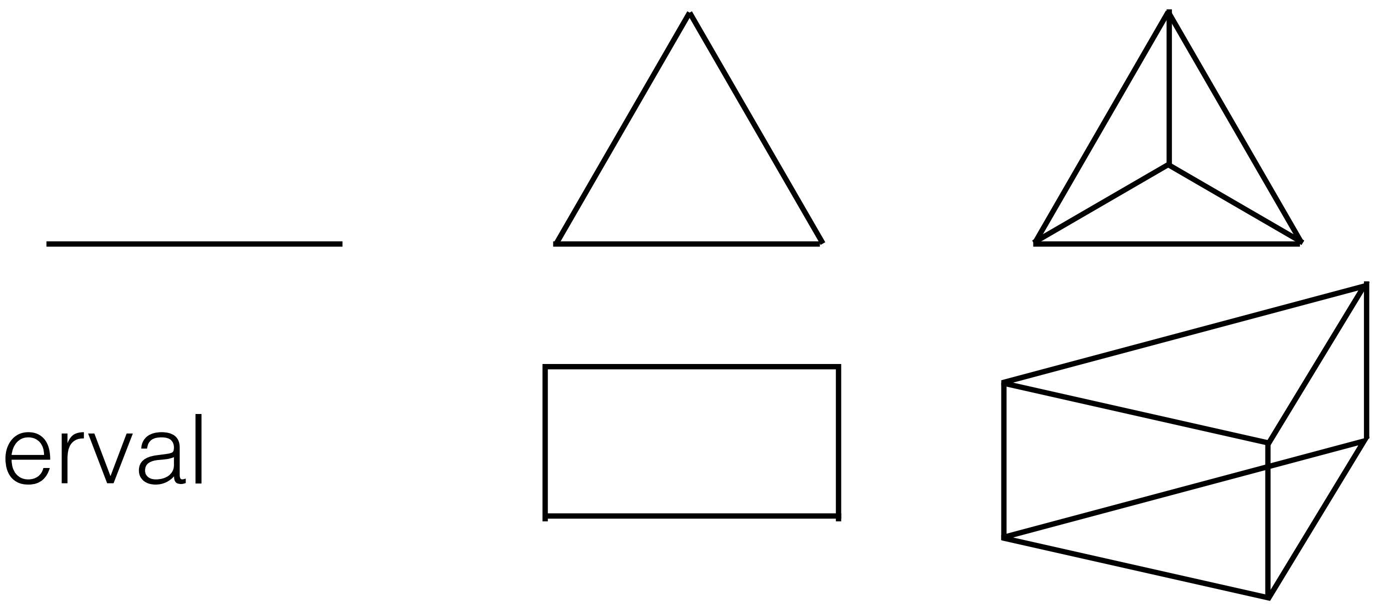
```c
void uniform_extrusion_kernel(double **base_coords, double **ext_coords,
                              int **layer, double *layer_height) {
   for ( int d = 0; d < 3; d++ ) {
       for ( int c = 0; c < 2; c++ ) {
           ext_coords[2*d][c] = base_coords[d][c];
           ext_coords[2*d+1][c] = base_coords[d][c];
       }
       ext_coords[2*d][2] = *layer_height * (layer[0][0]);
       ext_coords[2*d+1][2] = *layer_height * (layer[0][0] + 1);
   }
}
void wrap_uniform_extrusion_kernel(int start, int end, double *base_coords,
                                  int *base_coords_map, double *ext_coords,
                                  int *ext_coords_map, int *layer,
                                  int *layer_map, double *layer_height,
                                  int start_layer, int end_layer) {
   double *base_packed[3];
   double *ext_packed[6];
   int *layer_packed[1];
   for ( int i = start; i < end; i++ ) {
       base_packed[0] = base_coords + (base_coords_map[i * 3 + 0])* 2;
       base_packed[1] = base_coords + (base_coords_map[i * 3 + 1])* 2;
       base_packed[2] = base_coords + (base_coords_map[i * 3 + 2])* 2;
       ext_packed[0] = ext_coords + (ext_coords_map[i * 6 + 0])* 3;
       ext_packed[1] = ext_coords + (ext_coords_map[i * 6 + 1])* 3;
       ext_packed[2] = ext_coords + (ext_coords_map[i * 6 + 2])* 3;
       ext_packed[3] = ext_coords + (ext_coords_map[i * 6 + 3])* 3;
       ext_packed[4] = ext_coords + (ext_coords_map[i * 6 + 4])* 3;
       ext_packed[5] = ext_coords + (ext_coords_map[i * 6 + 5])* 3;
       layer_packed[0] = layer + (layer_map[i * 1 + 0])* 1;
       for (int j = start_layer; j < end_layer; ++j) {
           uniform_extrusion_kernel(base_packed, ext_packed, layer_packed, layer_height);
           ext_packed[0] += 3;
           ext_packed[1] += 3;
           ext_packed[2] += 3;
           ext_packed[3] += 3;
           ext_packed[4] += 3;
           ext_packed[5] += 3;
           layer_packed[0] += 1;
       }
   }
}
```

Platform portability

- Theory: PyOP2 code is portable across hardware platforms (CPU/GPU) since intent of iteration is separated from its implementation
- Some PyOP2 codes work on both CPU and GPU
- FEM kernels need different implementations on CPU/GPU (practice)
  - CPU: assemble multiple element tensors per thread
  - GPU: one element tensor *entry* per thread
- Reality: PyOP2 offers *potential* for platform portability, but is currently single (CPU (+ shared memory)) platform for practical purposes.

Firedrake

- Simplices
- Simplex x interval



- H^1, H(div), H(curl) and L^2 discretisations
- Mixed finite elements
- Parallel (MPI [+ OpenMP]) via PyOP2

No computation

- Firedrake carries out (almost) zero computation itself
  - Constructing dof maps for function spaces is our job (not really an abstraction available here)
- All solving is devolved to PETSc
  - Abstraction: non-linear solves require residual evaluation and matrix-vector products (of the linearisation of the residual)
- All FE assembly devolved to PyOP2
  - Abstraction: FE assembly is the evaluation of a *local* kernel repeatedly over a mesh of *global* data

(Almost) no code

```
$ cloc firedrake/
      30 text files.
      30 unique files.
       1 file ignored.

http://cloc.sourceforge.net v 1.60  T=0.17 s (168.6 files/s, 50255.0 lines/s)
-------------------------------------------------------------------------------
Language                     files          blank        comment           code
-------------------------------------------------------------------------------
Python                          27           1359           1865           4282
Cython                           1            107            138            620
C/C++ Header                     1             33             37            204
-------------------------------------------------------------------------------
SUM:                            29           1499           2040           5106
-------------------------------------------------------------------------------
```

Why?

- Use existing solutions wherever possible
- Militant about sticking to abstractions
    - The only way to do mesh-size operations is with PyOP2 loops
    - Mesh setup an exception, it is by far the most difficult bit of code

Behind the solve call

```
from firedrake import *

m = Mesh('...')

mesh = ExtrudedMesh(m, layers=20, extrusion_type='uniform')

element1 = ...
element2 = ...

V = FunctionSpace(mesh, element1)
Q = FunctionSpace(mesh, element2)

W = V*Q

u, p = TrialFunctions(W)
v, q = TestFunctions(W)

a = fn(u, p, v, q)
L = fn(v, q)

solve(a == L, ...)
```

```
solve(a == L, u, ...)
```

- Always solve using nonlinear solver
  - Jacobian is `a`
  - Residual is `action(a, u) - L =: F`
  - Solver is a PETSc SNES
    - provide residual evaluation `assemble(F)`
    - and Jacobian `assemble(a)`

Inside assemble

- Call ffc to turn form into PyOP2 kernels (COFFEE AST)
- inspect form to determine coefficients and any (maybe) trial and test functions
- Construct arguments to PyOP2 par_loop
- Call par_loop

```python
for integral_type, coords, coefficients, kernel in kernels:
   m = coords.function_space().mesh()
   if integral_type == 'cell':
       if is_mat:
           tensor_arg = mat_tensor(op2.INC,
                                   (s.cell_node_map()[op2.i[0]],
                                    s.cell_node_map()[op2.i[1]]))
       elif is_vec:
           tensor_arg = vec_tensor(op2.INC,
                                   s.cell_node_map()[op2.i[0]])
       else:
           tensor_arg = tensor(op2.INC)

       itspace = m.cell_set
       itspace._extruded_bcs = extruded_bcs
       args = [kernel, itspace, tensor_arg,
               coords.dat(op2.READ, coords.cell_node_map(),
                          flatten=True)]

       for c in coefficients:
           args.append(c.dat(op2.READ, c.cell_node_map(),
                             flatten=True))

       op2.par_loop(*args)
```

Inside par_loop

- Kernel optimised by COFFEE
    - LICM, padding and alignment, vectorisation
    - `arxiv:1407.0904 [cs.MS]`
    - For low-order extruded elements obtain 70% FP peak on prisms for matrix assembly.
- Wrapper code generated, compiled, loaded into process
- Call generated function with appropriate code

Boundary conditions

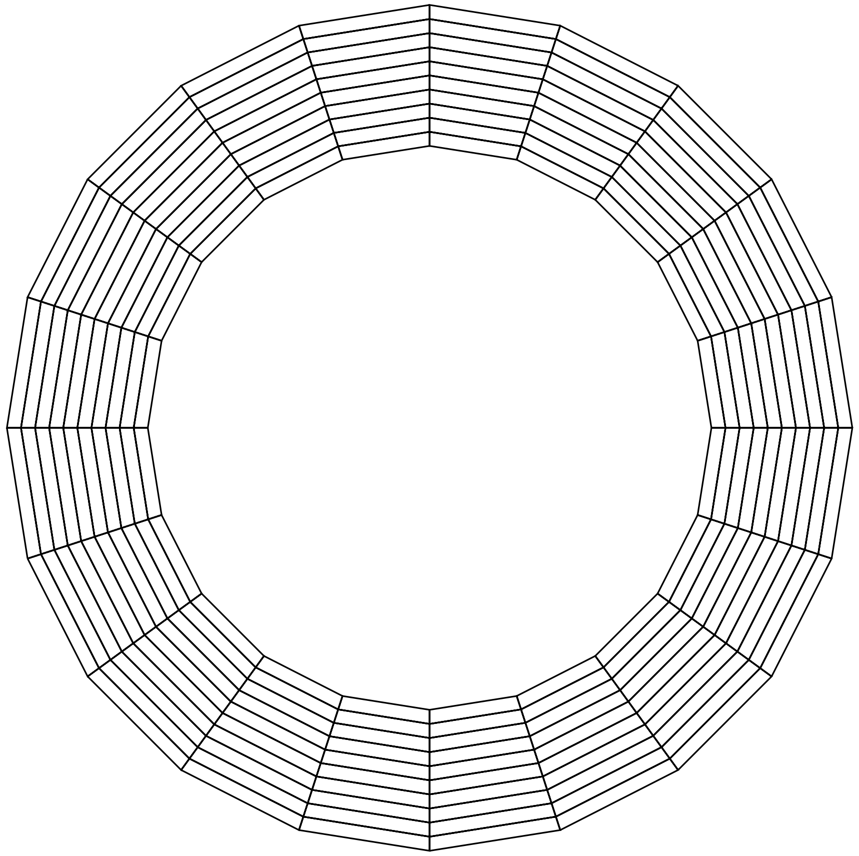
- http://firedrakeproject.org/boundary_conditions.html
- Effectively just throw away entries in Jacobian corresponding to bc dofs, put a 1 on the diagonal
  - PETSc makes this easy: pass negative row/column index to MatSetValues
- Set residual on boundary dofs to zero
- This approach maintains:
  - symmetry (or skew-symmetry)
  - positive (semi-)definiteness
  - diagonal dominance

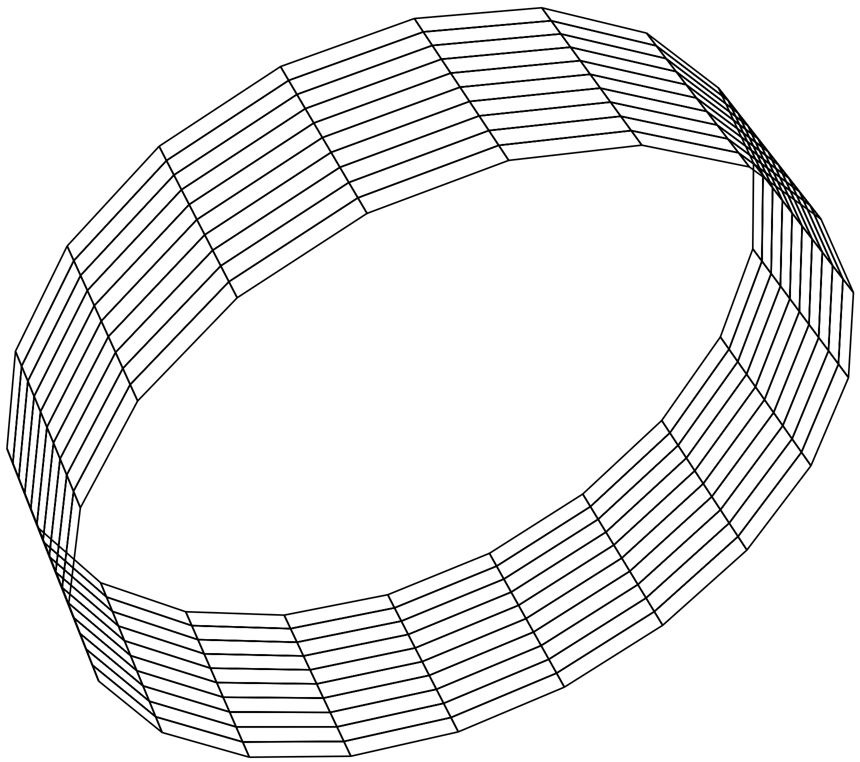
Extruded Firedrake

- *Extensions* to existing UFL syntax
- *Extensions* to PyOP2 types (seen these)
    - Not all extruded composes with non-extruded
    - can't do *direct* loops over extruded and non-extruded dats, can loop over extruded set and read non-extruded dat *indirectly*

Meshes

```python
from firedrake import *

m = CircleManifoldMesh(20, radius=10)
annulus = ExtrudedMesh(m, layers=10, layer_height=0.5,
                       extrusion_type='radial')
cylinder = ExtrudedMesh(m, layers=10, layer_height=0.5,
                        extrusion_type='uniform')

File('annulus.pvd') << annulus.coordinates
File('cylinder.pvd') << cylinder.coordinates
```

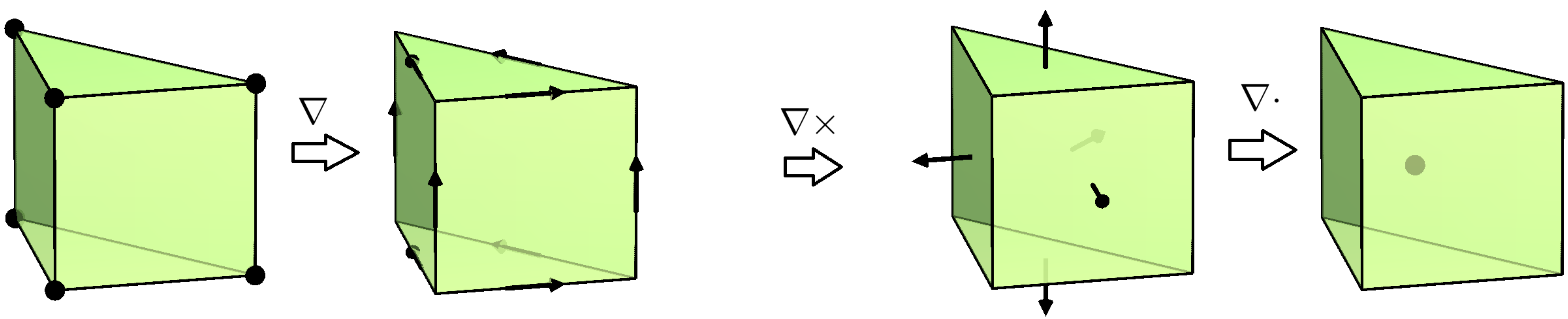




- *Uniform* extrusion increases topological and geometric dimension of cells
- *Radial* extrusion increases topological, but maintains geometric dimension
- Jacobians (currently) assume affine cells

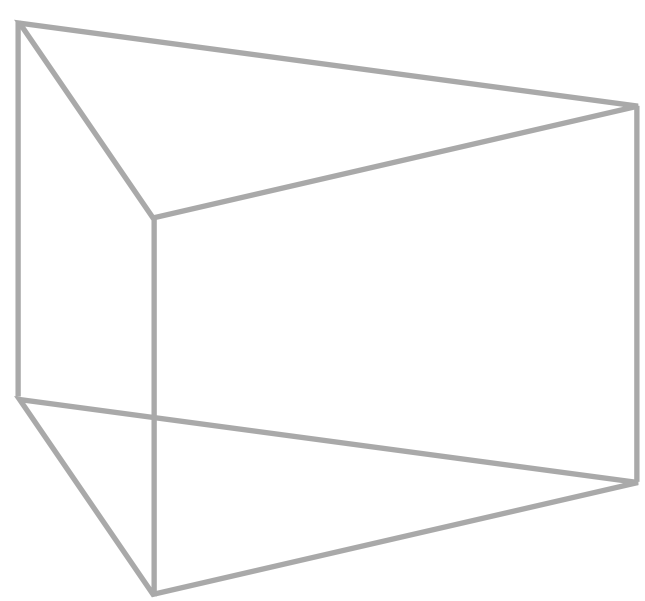
Elements

- Anything that can be expressed as tensor product of simplex (1 or 2d) with interval
  - e.g. Q2-P1dg for Stokes not supported
- You can have a full discrete de Rham product complex



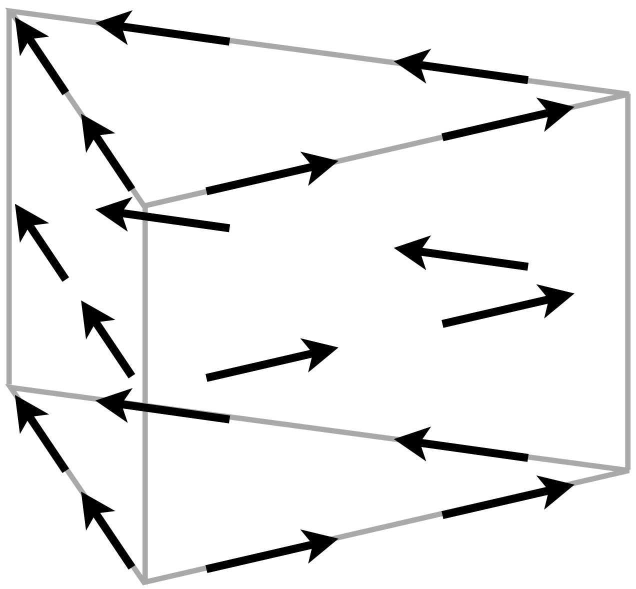
N2curl on prism

N2curl on prism



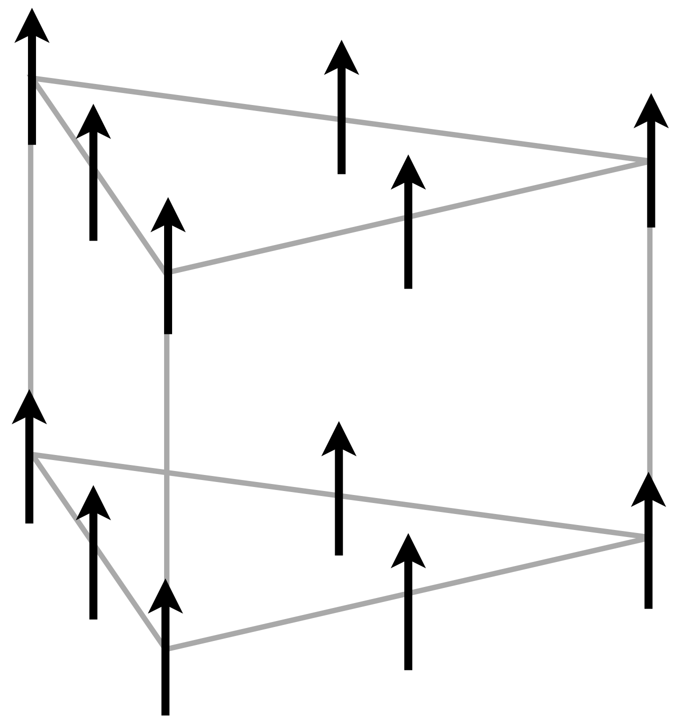
N2curl on prism

```
N2_1 = FiniteElement("N2curl", triangle, 1)
CG_2 = FiniteElement("CG", interval, 2)
Ned_horiz = HCurl(OuterProductElement(N2_1, CG_2))
```



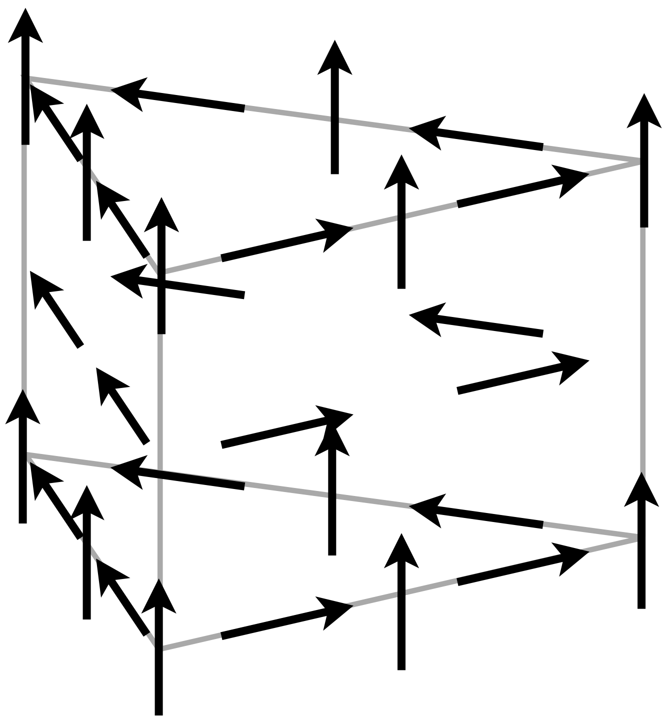
N2curl on prism

```
N2_1 = FiniteElement("N2curl", triangle, 1)
CG_2 = FiniteElement("CG", interval, 2)
Ned_horiz = HCurl(OuterProductElement(N2_1, CG_2))
P2tri = FiniteElement("CG", triangle, 2)
P1dg = FiniteElement("DG", interval, 1)
Ned_vert = HCurl(OuterProductElement(P2tri, P1dg))
```



N2curl on prism

```
N2_1 = FiniteElement("N2curl", triangle, 1)
CG_2 = FiniteElement("CG", interval, 2)
Ned_horiz = HCurl(OuterProductElement(N2_1, CG_2))
P2tri = FiniteElement("CG", triangle, 2)
P1dg = FiniteElement("DG", interval, 1)
Ned_vert = HCurl(OuterProductElement(P2tri, P1dg))
Ned_wedge = Ned_horiz + Ned_vert
```



Escaping abstractions

- What if I want to code a slope limiter?
  - UFL no good
- Firedrake allows you to code PyOP2 par_loops directly
  - Also some syntax to ease things
- PyOP2 doesn't have an "escape hatch"

- P1 field on vertices taking maximum value of P0 field on cells adjacent to those vertices

```
m = UnitSquareMesh(20,20)
cg = FunctionSpace(m, "CG", 1)
dg = FunctionSpace(m, "DG", 0)
c = Function(cg)
d = Function(dg)
par_loop("""for (int i=0; i<c.dofs; i++)
              c[i][0] = fmax(c[i][0], d[0][0]);""",
        # walk over cells
        dx,
        # associate 'c' variable with c field, 'd' with d
        {'c': (c, RW), 'd': (d, READ)})
```

Block solvers

- PETSc provides nice interface to block preconditioning
  - Schur complements (2x2 blocks)
  - Block Jacobi/Gauss-Seidel (nxn blocks)
- We (basically) inherit this
- Can either precondition with approximation of inverse of operator, or with approximation of inverse of some spectrally equivalent operator

Mixed Poisson

Find $\sigma \in \Sigma \subset \mathrm{H(div)}$, $v \in V \subset L^2$ satisfying

$$\begin{aligned} \langle \sigma, \tau \rangle - \langle u, \nabla \cdot \tau \rangle &= 0, \quad \forall\, \tau \in \Sigma, \\ \langle \nabla \cdot \sigma, v \rangle &= \langle f, v \rangle, \quad \forall\, v \in V \end{aligned}$$

A good preconditioner for this problem is the inverse of the H(div) inner product for the H(div) piece, and the inverse of the L^2 mass matrix for the L^2 piece
[Arnold, Falk, Winther, Multigrid in H(div) and H(curl)]

```python
from firedrake import *
m = UnitSquareMesh(40, 40)
Sigma = FunctionSpace(m, 'BDM', 2, name="sigma")
V = FunctionSpace(m, 'DG', 1, name="v")
W = Sigma * V
sigma, u = TrialFunctions(W)
tau, v = TestFunctions(W)
n = FacetNormal(m)
a = (inner(sigma, tau) - div(tau)*u + div(sigma)*v)*dx
L = - 4*dot(tau, n)*ds(4) - 2*dot(tau, n)*ds(3)
aP = (inner(sigma, tau) + div(sigma)*div(tau) + u*v)*dx
bcs = [DirichletBC(W[0], (0, 0), (1, 2))]
w = Function(W)
solve(a == L, w, Jp=aP, bcs=bcs,
      solver_parameters={'ksp_type': 'gmres',
                         'pc_type': 'fieldsplit',
                         'ksp_converged_reason': True,
                         'pc_fieldsplit_type': 'additive',
                         'fieldsplit_sigma_ksp_type': 'preonly',
                         'fieldsplit_sigma_pc_type': 'lu',
                         'fieldsplit_v_ksp_type': 'richardson',
                         'fieldsplit_v_pc_type': 'jacobi',
                         'fieldsplit_v_ksp_max_it': 5})

uexact = Function(V)
uexact.interpolate(Expression("2 + 2*x[1]"))
sigma, u = w.split()
assert errornorm(u, uexact) < 1e-6
```

Could have used full Schur complement PC on original system, converges in fewer iterations but takes about 5x as long.

```
solve(a == L, w, bcs=bcs,
     solver_parameters={'ksp_type': 'gmres',
                        'pc_type': 'fieldsplit',
                        'ksp_converged_reason': True,
                        'ksp_monitor_true_residual': True,
                        'pc_fieldsplit_type': 'schur',
                        'pc_fieldsplit_schur_fact_type': 'full',
                        'fieldsplit_sigma_ksp_type': 'preonly',
                        'fieldsplit_sigma_pc_type': 'lu'})
```

Obviously for large problems we can't invert with LU, working on good PCs for problems in H(div) and H(curl)

More questions?