pyop3: A new domain-specific language for automating high-performance mesh-based simulation codes

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January 2023

What came before: PyOP2

- Domain-specific language embedded in Python for doing mesh computations
- Uses code generation to produce fast code
- Handles the data structures used by Firedrake
- Used all over Firedrake for things like assembly and interpolation

Introducing pyop3

Key differences with PyOP2:

- Complete rewrite of the code generation part
- New more expressive and composable interface inspired by PETSc DMPlex
- **Has a new data layout model for describing mesh data**
- Work-in-progress!

pyop3 wishlist

We want an abstraction that lets us easily express and automate the following.

Features:

- ☐ Handle orientations (e.g. unstructured hexes)
- ☐ p-adaptivity
- ☐ Mixed meshes

Performance:

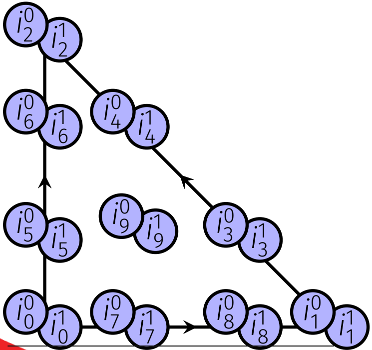
- ☐ Exploit mesh partial structure (e.g. extruded)
- ☐ Prescribe DoF ordering (e.g. in extruded mesh columns)

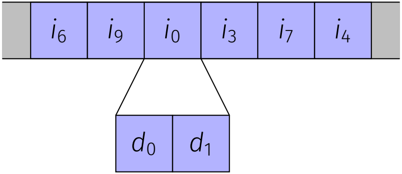
(And more...)

Claim: `pyop3`'s new mesh data layout abstraction facilitates all of these.

How does PyOP2 store mesh data?

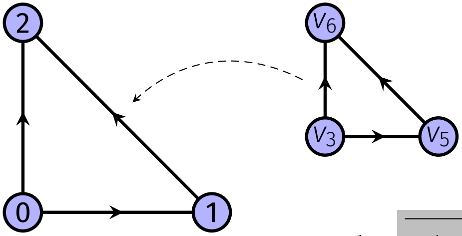
- Mesh data is stored by `Dats`[1]
- `Mixed Dats` and `Dats` for extruded meshes are also possible
- These associate a fixed inner shape (d_m) with a set of possibly unordered nodes (i_n)
- **This abstraction loses topological information**



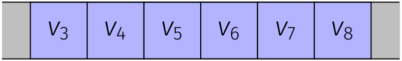


[1] Sparse matrices not discussed

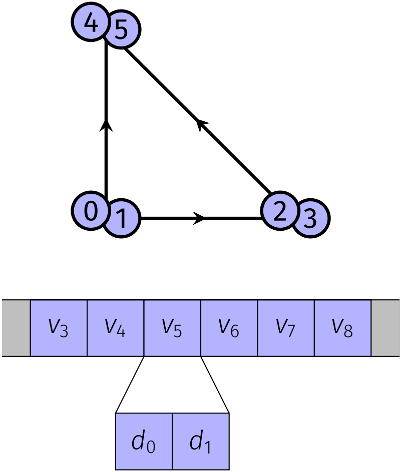
Starting simple: P1




```
root = (
  MultiAxis()
  .add_part(AxisPart(nverts))
)
```

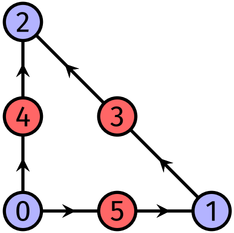


Adding shape: vector P1




```
root = (
  MultiAxis()
   .add_part(AxisPart(nverts))
   .add_subaxis(AxisPart(2))
)
```

Multiple entities: P2



e_0	...	e_m	v_0	...	v_n

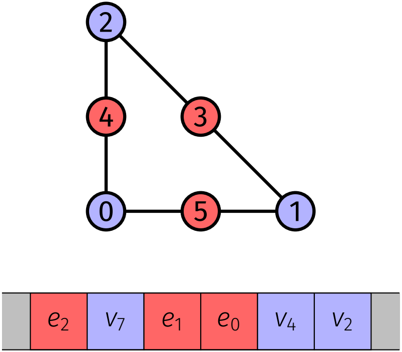
☑ p-adaptivity[2]
☑ Mixed meshes[2]

```
root = (
  MultiAxis()
  .add_part(AxisPart(nedges))
  .add_part(AxisPart(nverts))
)
```

[2] Since topological entities are now distinguishable

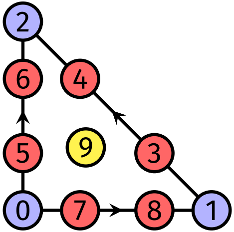
Now with renumbering

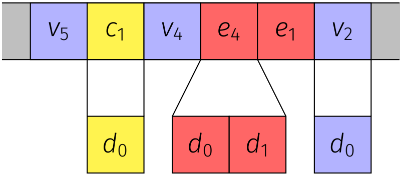
☑ Prescribe DoF ordering




```
root = (
  MultiAxis()
  .add_part(AxisPart(
    nedges,
    numbering=[4,2,5,...],
  ))
  .add_part(AxisPart(
    nverts,
    numbering=[3,0,1,...],
  ))
)
```

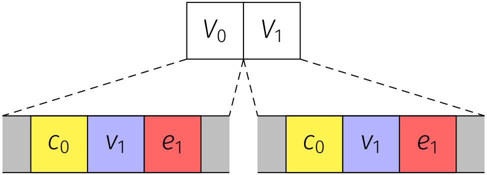
More complicated inner shape: P3






```
root = (
  MultiAxis()
  .add_part(AxisPart(ncells, "cells"))
  .add_part(AxisPart(nedges, "edges"))
  .add_part(AxisPart(nverts, "verts"))
  .add_subaxis("edges", AxisPart(2))
)
```

Mixed




```
root = (
  MultiAxis()
  .add_part(AxisPart(1, "V0"))
  .add_part(AxisPart(1, "V1"))
  .add_subaxis("V0", ...)
  .add_subaxis("V1", ...)
)
```

Features:

- ☐ Handle orientations
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Performance:

- ☐ Exploit mesh partial structure
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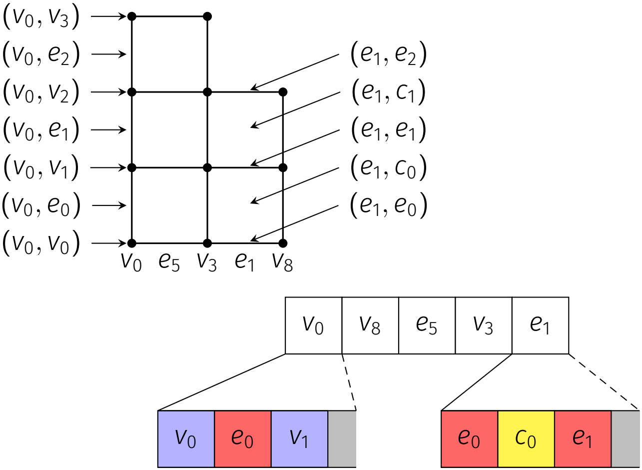
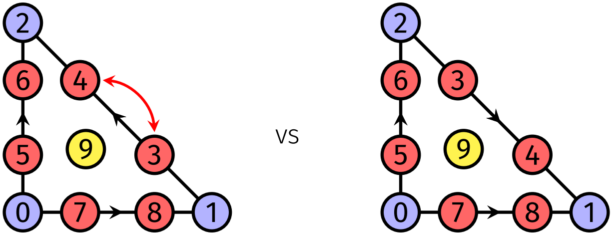
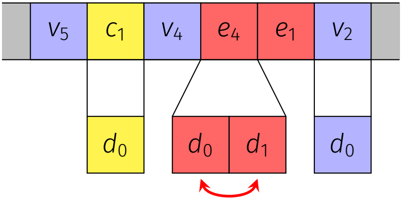
Partially-structured meshes: extruded



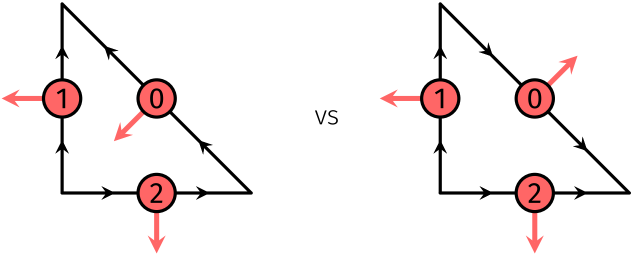
This might be overkill... but it works!

Orientation: P3





Orientation: Raviart-Thomas



e_5	e_9	e_0	e_4	e_1	e_2

$(\times -1)$

Imperial College London

pyop3 wishlist

Features:

☑ Handle orientations
☑ p-adaptivity
☑ Mixed meshes

Performance:

☑ Exploit mesh partial structure
☑ Prescribe DoF ordering

- `pyop3` has a unifying abstraction for all* of the data structures currently used in PyOP2
- This abstraction should let us do a lot of cool things, automatically!

*I claim

Things I missed

- The cool new interface (inc. map and loop composition)
- Tight integration with PETSc (esp. DMPlex)
- Support for sparse matrices
- Support for ragged data structures (e.g. variable layer extrusion, PIC, mixed-arity maps)
- MPI parallelism
- Could streamline PCPATCH and multigrid code (via loop/map composition)
- Should retain PyOP2's work on GPUs and inter-element vectorisation
- Additional data layout transformations/optimisations
- Could potentially do a similar mesh structure trick for refined meshes

Appendix

```
do_loop(
  c := mesh.cells.index,
  kernel(dat0[closure(c)], dat1[closure(c)])
)

do_loop(
  f := mesh.interior_facets.index,
  kernel(
    dat0[closure(support(f))],
    dat1[closure(support(f))]
  )
)
```

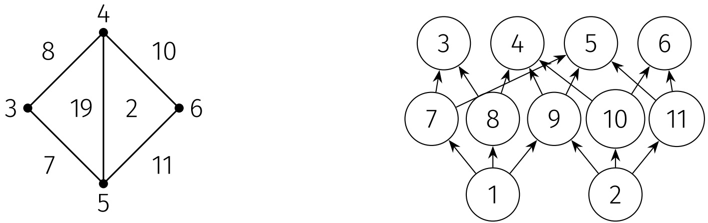
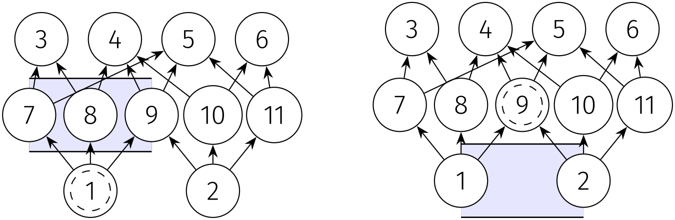
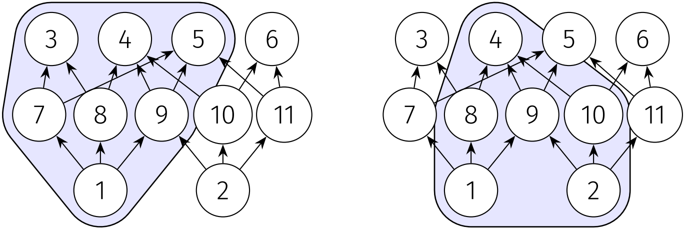


Figure 1: An example mesh and its Hasse diagram representation. Note that the topological entities are numbered according to the DMPlex convention of first cells, then vertices, then faces.



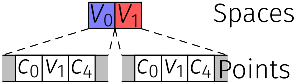
(a) $\operatorname{cone}(1) = \{7, 8, 9\}$ (b) $\operatorname{supp}(9) = \{1, 2\}$



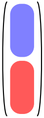
(c) $\operatorname{cl}(1) = \{1, 3, 4, 5, 7, 8, 9\}$ (d) $\operatorname{st}(4) = \{4, 8, 9, 10, 1, 2\}$

Figure 2: The possible DMPlex covering queries (applied to the Hasse

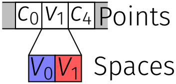
Mixed reordering



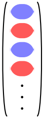
(a) A typical data layout for a ‘mixed’ system with the spaces V_0 and V_1 forming the ‘outer’ axis.



(b) The resulting block-structured vector.

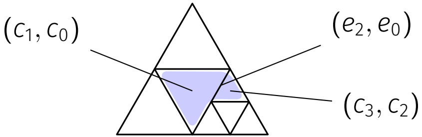


(c) A transformed data layout where the “Spaces” and “Points” axes have been swapped.

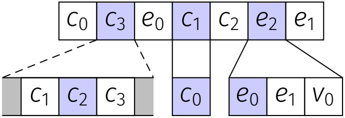


(d) The resulting interleaved vector.

Figure 3: A possible data layout transformation for a ‘mixed’ system permitted by **pyop3**. The entries V_0 and V_1 represent the spaces of the mixed system and the “Points” axis is representative of the mesh



(a) An example of a stencil - $\mathfrak{st}((e_2, e_0))$ - over a refined mesh. Note that the unrefined cell (c_1, c_0) is still indexed with two indices. We say that it has been refined using the identity transformation.



(b) Example data layout for the refined mesh shown above. Note that the base mesh in unstructured which is why the top axis is unordered.

Figure 4: Example data layout and stencil for a refined mesh.

PCPATCH

```
loop(v := mesh.vertices.index, [
  loop(p := star(v).index, [
    assemble_jacobian(dat1[closure(p)], dat2[closure(p)], "mat"),
    assemble_residual(dat3[closure(p)], "vec"),
  ]),
  solve_and_update("mat", "vec", dat4[v]),
])
```