Latest developments in pyop3

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13 September 2023

Overview

What is **pyop3**?

A simple-ish example

What's the point?

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What is `pyop3`?

TL;DR

- A programming language for mathematicians
- Comes with a compiler
- The language lets you express how to read and write from complicated data structures

In more detail

- A **domain-specific** programming language for mathematicians **embedded in Python (like UFL)**
- Comes with a **just-in-time** compiler **that targets loopy and then C/CUDA/OpenCL**
- The language lets you express how to read and write from complicated data structures
- **Never need to create a `PetscSection` ever again!**

Why is this hard?

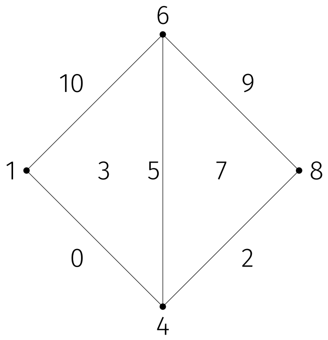
- FEM codes have diverse and complicated data structures
- These data structures also need to be accessed in non-trivial ways

A simple-ish example

Outline of a pyop3 program

1. Create data structures
2. Execute loop expressions acting on the data structures

Create a data layout for a 2 cell mesh




```
mesh_axis = Axis(
  [
    AxisComponent(2, "cells"),
    AxisComponent(5, "edges"),
    AxisComponent(4, "verts"),
  ],
  "mesh"
  permutation=[3, 7, 0, 10, 5, 9, 2, 1, 6, 4, 8],
)
```

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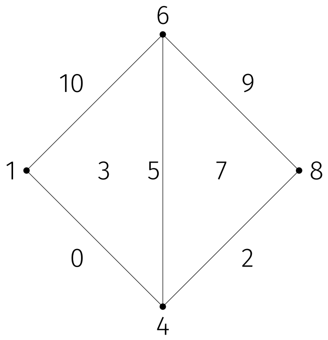


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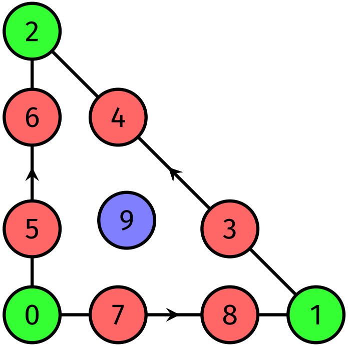
```

0	0	4	0	2	2	1	1	3	3	1

Now make it a P3 function space




```
axes = (
  AxisTree(mesh_axis)
    .add_subaxis(Axis(1), mesh_axis.id, "cells")
    .add_subaxis(Axis(2), mesh_axis.id, "edges")
    .add_subaxis(Axis(1), mesh_axis.id, "verts")
)
```

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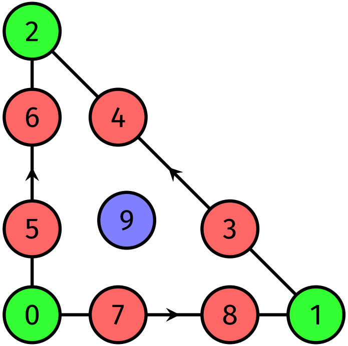


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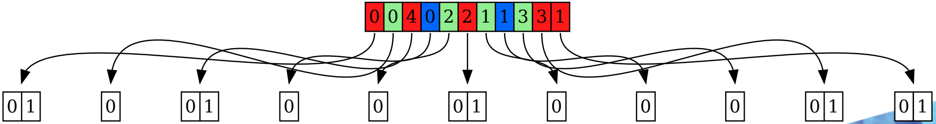

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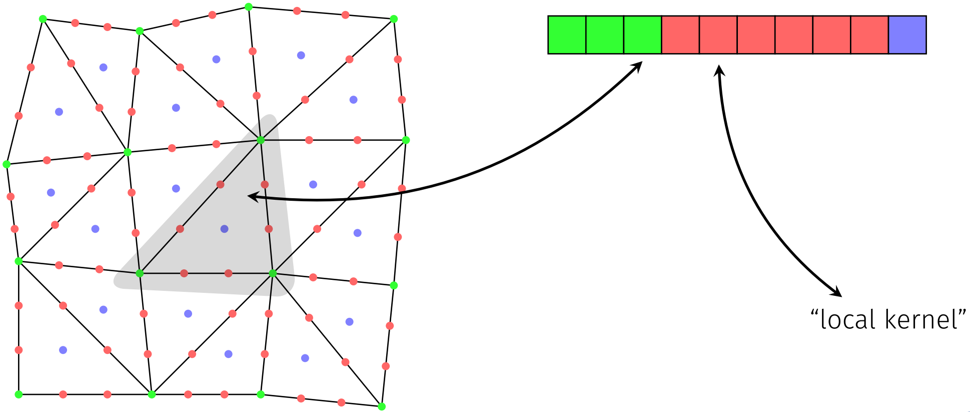
Now let's do a loop



Residual assembly in pyop3

```
for every cell in the mesh:
  collect DoFs found in the cell's closure
  call a local kernel with these DoFs
  scatter the result to a global vector
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```
loop(
  c := mesh.cells.index(),
  kernel(func0[closure(c)], ...)
)
```

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Code generation!

```
void my_loop(double *func0, int *map0, int *map1, int *layout0, int *layout1, int *layout2, ...) {
  double t_0[10];  // to store the "packed" data

  for (int32_t i_0 = 0; i_0 < 2; ++i_0) {                     // loop over cells
    // pack cell DoFs
    t_0[0] = func0[layout0[i_0]];

    // pack edge DoFs
    for (int32_t i_5 = 0; i_5 < 3; ++i_5) {                   // loop over edges
      for (int32_t i_6 = 0; i_6 < 2; ++i_6) {                 // loop over edge DoFs
        j_3 = map0[i_0 * 3 + i_5];                            // select the right edge
        t_0[i_5*2 + i_6 + 1] = func0[layout1[j_3] + i_6];   // pack DoF
      }
    }

    // pack vertex DoFs
    for (int32_t i_7 = 0; i_7 < 3; ++i_7) {                   // loop over vertices
      j_5 = map1[i_0 * 3 + i_7];                              // select the right vertex
      t_0[i_7 + 7] = func0[layout2[j_5]];                     // pack DoF
    }

    // execute the local kernel and unpack the result
    kernel(t_0, ...);
    ...
  }
}
```

What’s the point?

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Is it faster than PyOP2?

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Composability!

Why is composability important?

- Performance optimisation is not the main priority, expressibility is
- PyOP2 has limitations:
  - Single loop
  - Single kernel
  - No map composition
  - Extruded meshes require invasive code changes
- Can do more in fewer lines of code
  - `pyop3` compiler is $\sim$ 1000 lines of code, PyOP2's is $\sim$ 2500
  - No special casing for extruded

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Map composition

- Interior facet integrals:

```
loop(facet := mesh.interior_facets, kernel(func0[closure(support(facet))]))
```

- Multigrid:

```
closure(fine2coarse(fine_cell))
```

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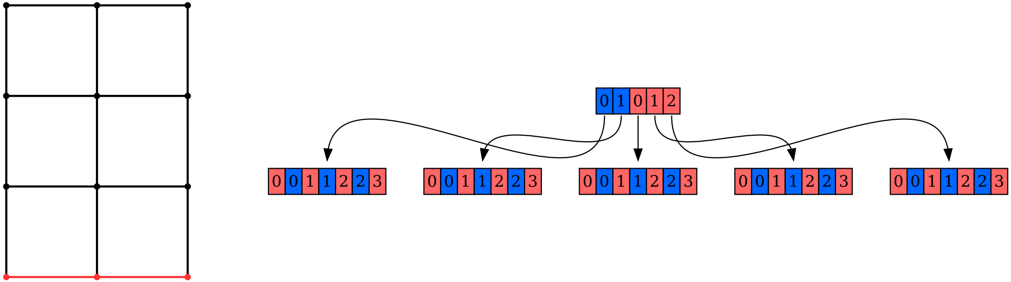
Loop and kernel composition: PCPATCH

```
loop(v := mesh.vertices.index, [
  loop(c := star(v).index, [
    kernel1(dat1[closure(c)], "mat"),
    kernel2(dat2[closure(c)], "vec")
  ]),
  solve("mat", "vec", dat3[v])
])
```

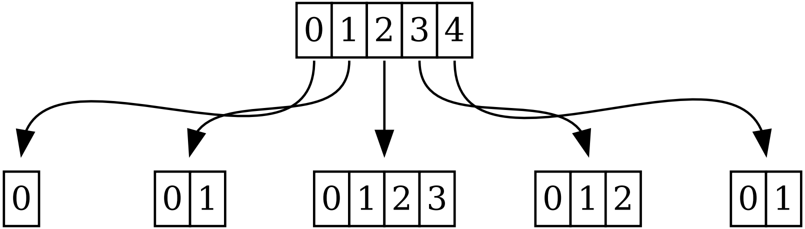
- We could also try to rewrite SLATE
- Loop composition can enable certain tiling optimisations

And this composability will work with LOADS of data structures...

Example 1: extruded



Example 2: ragged

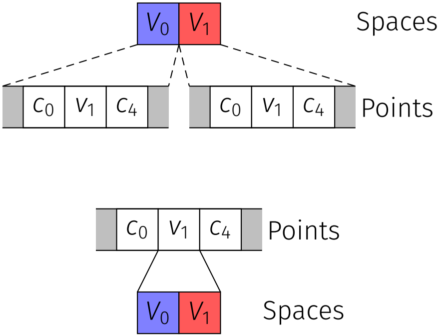


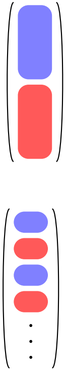
Useful for variable-layer extrusion and PIC.

Example 3: sparse

- Like ragged (no picture sorry)
- Arbitrary sparsity is completely possible

Example 4: “swapping” axes





Summary

- pyop3 is a DSL/compiler framework for writing kernels with non-trivial access patterns
- It can do everything PyOP2 can do, and more!
- WIP

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