

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

Connor Ward

January 2023

Motivation

pyop3 interface

Final bits

Appendix

Motivation





- Domain-specific language embedded in Python for automating stencil computations
- Uses code generation to produce fast code



Features:

- ☐ Map composition
- ☐ Nesting loops (e.g. PCPATCH)
- ☐ Orientation (e.g. unstructured hexes)
- ☐ p-adaptivity
- ☐ Mixed meshes

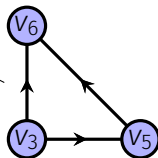
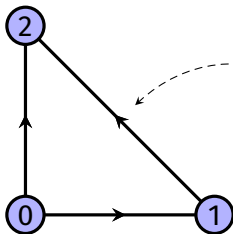
Performance:

- ☐ Mesh partial structure (e.g. extruded)¹
- ☐ Mesh numbering (e.g. DoFs up extruded columns)¹

¹Achievable in PyOP2 but very complicated and hard to extend

Claim: **pyop3**'s new data layout abstraction enables all of these.

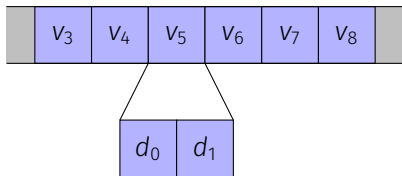
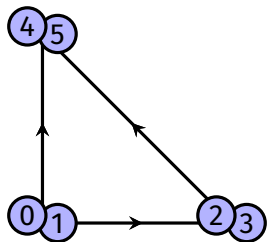
Starting simple: P1



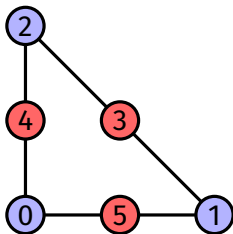
```
1 root = (  
2     MultiAxis()  
3     .add_part(AxisPart(nverts))  
4 )
```

	V ₃	V ₄	V ₅	V ₆	V ₇	V ₈	
--	----------------	----------------	----------------	----------------	----------------	----------------	--

Adding shape: vector P1



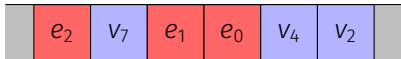
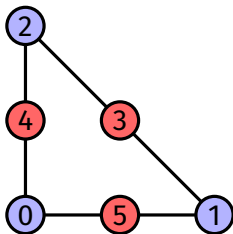
```
1 root = (  
2     MultiAxis()  
3     .add_part(AxisPart(nverts))  
4     .add_subaxis(AxisPart(2))  
5 )
```



```
1 root = (  
2   MultiAxis()  
3   .add_part(AxisPart(nedges))  
4   .add_part(AxisPart(nverts))  
5 )
```

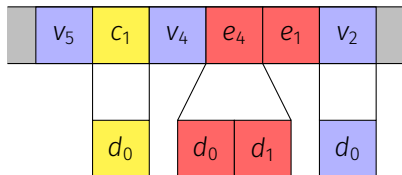
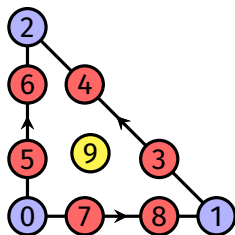


Now with renumbering

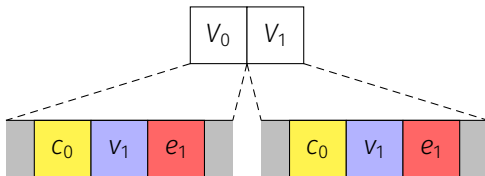


```
1 root = (  
2   MultiAxis()  
3   .add_part(AxisPart(  
4     nedges,  
5     numbering=[4,2,5,...],  
6   ))  
7   .add_part(AxisPart(  
8     nverts,  
9     numbering=[3,0,1,...],  
10  ))  
11 )
```

More complicated inner shape: P3



```
1 root = (  
2   MultiAxis()  
3   .add_part(AxisPart(ncells, "cells"))  
4   .add_part(AxisPart(nedges, "edges"))  
5   .add_part(AxisPart(nverts, "verts"))  
6   .add_subaxis("edges", AxisPart(2))  
7 )
```



```
1 root = (  
2     MultiAxis()  
3     .add_part(AxisPart(1, "v0"))  
4     .add_part(AxisPart(1, "v1"))  
5     .add_subaxis("v0", ...)  
6     .add_subaxis("v1", ...)  
7 )
```









Something really crazy



pyop3 interface







Some examples: Interior facet integrals



Some examples: Patches



Final bits





Appendix





