Firedrake: a multilevel domain specific language approach to unstructured mesh stencil computations

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What are we interested in?

- (Predominantly) finite element simulations
  - primary application areas in geophysical fluids (ocean and atmosphere)
  - simulations on unstructured and semi-structured meshes
- Providing high-level interfaces for users, with performance

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- Providing high-level interfaces for users, with performance
- the moon, on a stick

What are the elementary operations?

- Numerics tell us the elementary operation we apply everywhere in the mesh (a "kernel")
- Mesh topology gives us the "stencil" pattern
- Our job: efficiently apply the kernel over the whole mesh

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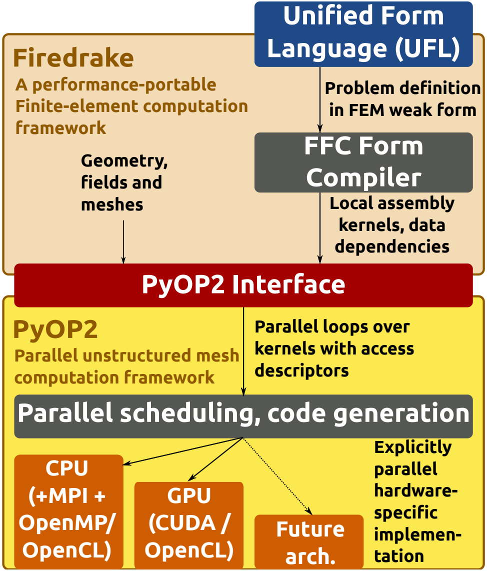
Express what, not how

- User code should make as few decisions about implementation as possible
- FE discretisations expressed symbolically using the Unified Form Language
  - developed in the FEniCS project (`http://www.fenicsproject.org`)
  - symbolic representation compiled to a C kernel
- Data to feed to kernel (and interface to solvers) provided by Firedrake (`http://www.firedrakeproject.org`)
- Execution of kernel over entire domain expressed as parallel loop with access descriptors
  - uses PyOP2 unstructured mesh library (`http://github.com/OP2/PyOP2`)


Unified Form Language (UFL)
Firedrake
A performance-portable Finite-element computation framework
Problem definition in FEM weak form
FFC Form Compiler
Geometry, fields and meshes
Local assembly kernels, data dependencies
PyOP2 Interface
PyOP2
Parallel unstructured mesh computation framework
Parallel loops over kernels with access descriptors
Parallel scheduling, code generation
CPU (+MPI + OpenMP/ OpenCL)
GPU (CUDA / OpenCL)
Future arch.
Explicitly parallel hardware-specific implemen-tation

An example

```
from firedrake import *
m = UnitSquareMesh(32, 32)
V = FunctionSpace(m, 'Lagrange', 2)
u = Function(V)
v = TestFunction(V)
# F(u; v) = ∫ ∇u · ∇v + uv dx
F = inner(grad(u), grad(v))*dx + u*v*dx
solve(F == 0, u)
```

- Kernels produced for residual and jacobian evaluation
  - jacobian computed by symbolic differentiation of residual form
- Kernels executed over mesh using PyOP2
  - http://github.com/OP2/PyOP2

PyOP2 data model

- Data types

Set	e.g. cells, degrees of freedom (dofs)
Dat	data defined on a `Set` (one entry per set element)
Map	a mapping between two sets (e.g. cells to dofs), a "stencil"
Global	global data (one entry)
Kernel	a piece of code to execute over the mesh (in C)

- access descriptors
  - READ, RW, WRITE, INC, ...
- iteration construct

`par_loop`	execute a Kernel over every element in a `Set`

Example

```
elements = Set(...)
nodes = Set(...)
elem_node = Map(elements, nodes, 3, ...) # 3 nodes per element
node_data = Dat(nodes, ...)
element_data = Dat(elements, ...)
count = Global(...)                    # no set (global value)
par_loop(kernel, elements,
         element_data(READ),           # direct read
         node_data(INC, elem_node),    # indirect increment
         count(INC))                   # global increment
```

- executes kernel for each ele in elements
- runtime knows it has to care about data dependencies for
  - increments into node_data
  - increment into count

Synthesis, not analysis

- Low level code is generated at runtime for parallel loops
- Access descriptors on parallel loops mean:
  - code generation requires synthesis, not analysis
  - determination of when halo exchanges need to occur is automatic
  - colouring for shared memory parallelisation can be computed automatically

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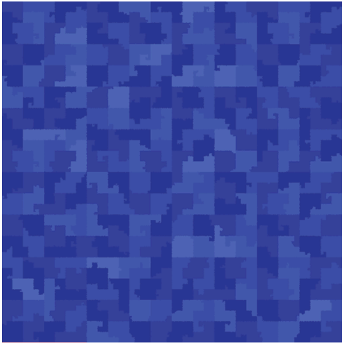
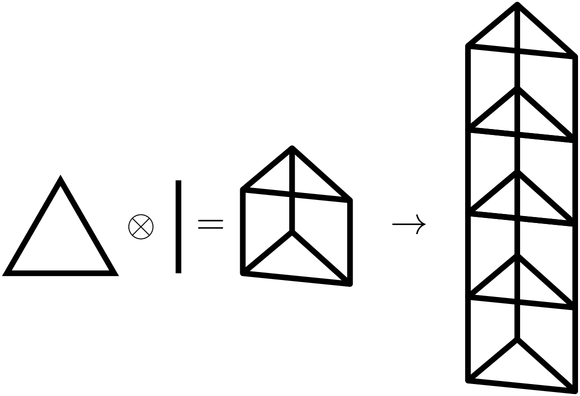


Semi-structured meshes

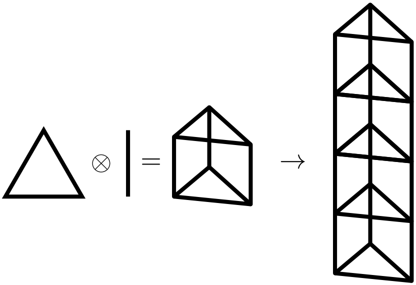
- Many application areas have a "short" direction
  - ocean and atmosphere
  - thin shells
- Numerics dictate we should do something different in short direction
- Use semi-structured meshes
  - unstructured in "long" directions, structured in short
  - can we exploit this structure?

A picture of triangles



Admits a fast implementation

- Exploit structure in mesh to amortize indirect lookups
  - arrange for iteration over short direction to be innermost loop
  - pay one indirect lookup per mesh column
  - walk up column directly



A bandwidth bound test

- Walk over mesh, read from vertices and cells, sum into global

```
void kernel(double *a, double *x[], double *y[]) {
    const double area = fabs(x[0][0]*(x[2][1]-x[4][1])
                             + x[2][0]*(x[4][1]-x[0][1])
                             + x[4][0]*(x[0][1]-x[2][1]));
    *a += area * 0.5 * y[0][0];
}
```

- Can we sustain an appreciable fraction of memory bandwidth?

Measuring throughput

- "Effective" data volume
  - assume every piece of data is touched exactly once (in perfect order)
  - don't count data movement for indirection maps
- "Valuable" bandwidth
  - effective data volume per second
- Actual memory bandwidth will be higher (reading indirection maps)
  - but this is not "useful"

Benchmark setup

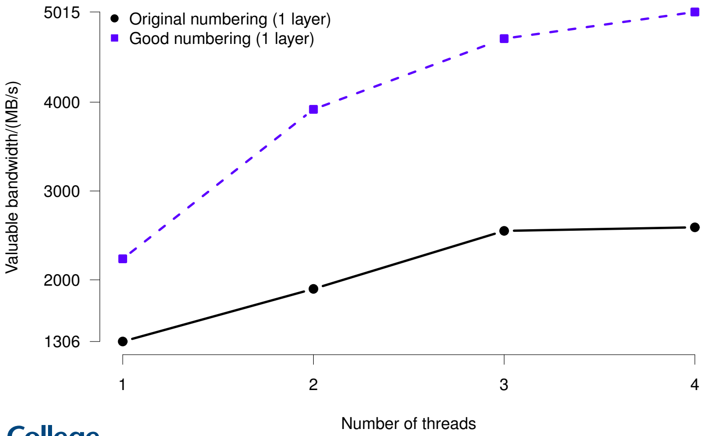
- 2D unstructured mesh: 806110 cells, 403811 vertices.
  - 2D coordinate field located at vertices (implicit 3rd coordinate)
  - scalar field stored at cell centres
- Run with increasing number of extruded cell layers (n_{layer})
  - data volume $(806110 * n_{layer}) + 403811 * 2\ (n_{layer} + 1)$ doubles
  - 1 layer: 18.4MB
  - 200 layers: 2468MB
- Execute kernel over mesh 100 times

Single node

- Intel Sandybridge 4 cores (2 way hyperthreading)
  - 32kB L1 cache (per core)
  - 256 kB L2 cache (per core)
  - 8 MB L3 cache (shared)
- Measured STREAM bandwidth (8 threads)
  - 11341 MB/s

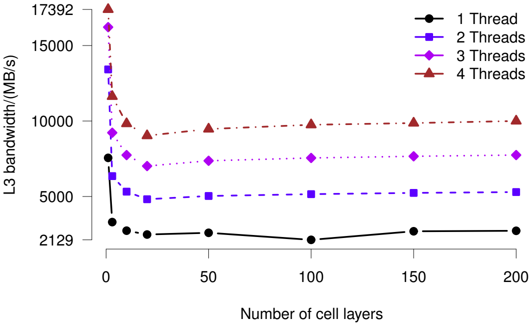
Effect of good base numbering

- Being completely unstructured hurts a lot
- Compare default (mesh generator) numbering with renumbered mesh using 2D space filling curve



Adding layers amortizes indirection cost

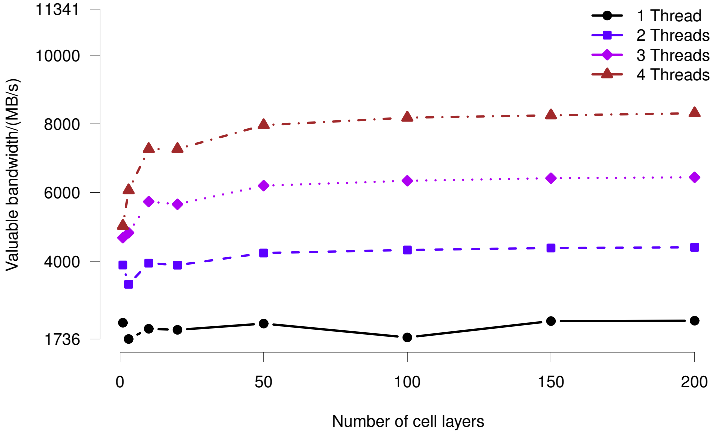
- L3 cache bandwidth
  - low layer numbers hit the L3 more often (indirection lookups)



- What about actual throughput though?

Valuable bandwidth

- Above ~20 layers, indirection cost "hidden"



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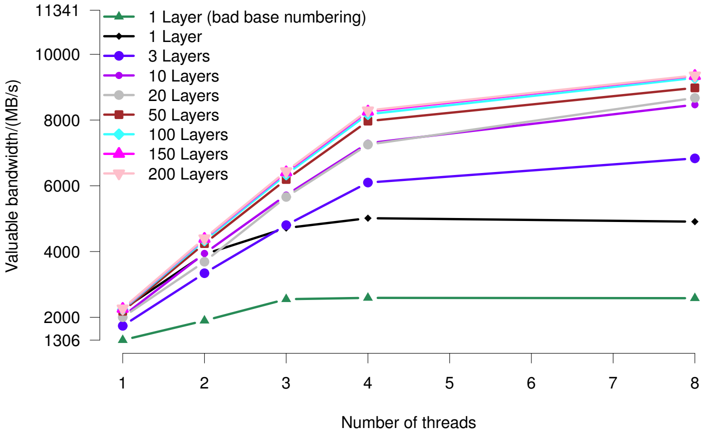
More threads

- Hyperthreading gives some further gains (82% STREAM bandwidth)



Possible to be unstructured and fast

- A good numbering gets you a reasonable way there
- If there is structure in your problem, use it!
- High level abstractions need not kill performance

Work with us

- All code is open source, and online:

  Firedrake http://www.firedrakeproject.org and http://github.com/firedrakeproject/firedrake

  PyOP2 http://github.com/OP2/PyOP2 (documentation at http://op2.github.io/PyOP2)
- Postdoc positions in this area are available
  - contact: me (lawrence.mitchell@imperial.ac.uk) or David Ham (david.ham@imperial.ac.uk)

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