Firedrake

Firedrake: automating the finite element method by composing abstractions

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`www.firedrakeproject.org`

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Rathgeber et al. 2015 `arXiv:1501.01809[cs.MS]`

The right abstraction level

How do *you* solve the Poisson equation?

```
from firedrake import *
mesh = UnitSquareMesh(100, 100)
V = FunctionSpace(mesh, "RT", 2)
Q = FunctionSpace(mesh, "DG", 1)
W = V*Q
u, p = TrialFunctions(W)
v, q = TestFunctions(W)

a = dot(u, v)*dx + div(v)*p*dx + div(u)*q*dx
L = -Constant(1)*v*dx
u = Function(W)
solve(a == L, u, solver_parameters={
    "ksp_type": "gmres",
    "ksp_rtol": 1e-8,
    "pc_type": "fieldsplit",
    "pc_fieldsplit_type": "schur",
    "pc_fieldsplit_schur_fact_type": "full",
    "pc_fieldsplit_schur_precondition": "selfp",
    "fieldsplit_0_ksp_type": "preonly",
    "fieldsplit_0_pc_type": "ilu",
    "fieldsplit_1_ksp_type": "preonly",
    "fieldsplit_1_pc_type": "hypre"
})
```

Find $u \in V \times Q \subset H(\mathrm{div}) \times L^2$ s.t.

$$\langle u, v \rangle + \langle \mathrm{div}\, v, p \rangle = 0 \quad \forall\, v \in V$$

$$\langle \mathrm{div}\, u, q \rangle = -\langle 1, q \rangle \quad \forall\, q \in Q.$$

Developing models

- Choose equations
- Pick method/discretisation
- Decide on implementation language, target architecture
- Write code
- ...
- Optimise
- ...
- Profit?

Experimentation should be easy

How much code do you need to change to

- Change preconditioner (e.g. ILU to AMG)?
- Drop terms in the preconditioning operator?
- Use a completely different operator to precondition?
- Do quasi-Newton with an approximate Jacobian?
- Apply operators matrix-free?

Can we offer easy experimentation without compromising performance?

Can we offer easy experimentation without compromising performance *too much*?

FEM pseudocode

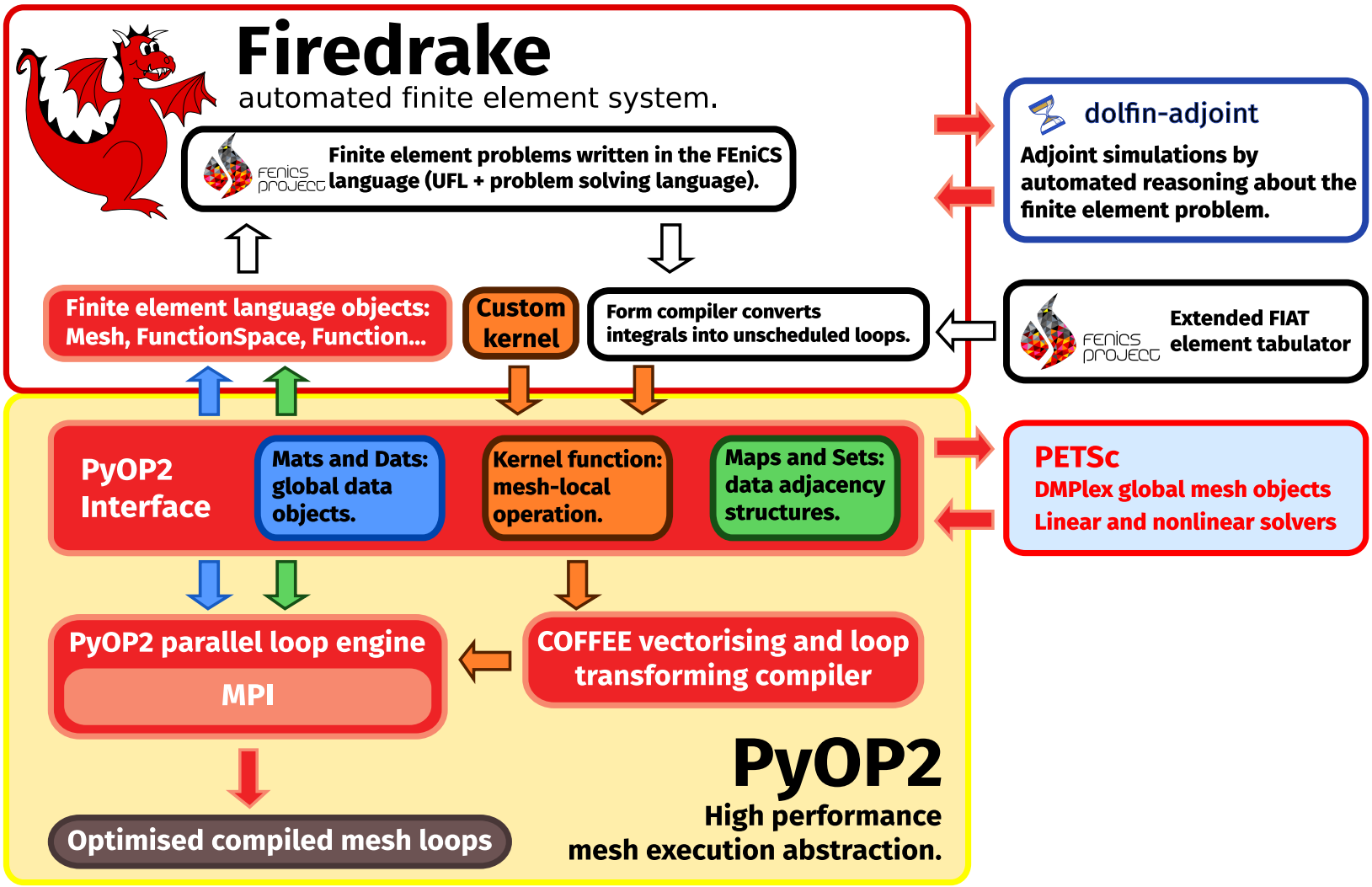
```
# x the input fields (e.g. current guess)
def form_residual(x):
    x_l <- x # global to ghosted
    for each element in mesh:
        x_e <- x_l[element] # gather through element map
        for each qp in element:
            basis_fns <- eval_basis_funs(qp)
            J <- compute_geometry(element, qp)
            for each bf in basis_fns:
                x_e_qp <- eval(x_e at qp)
                f_qp <- user_evaluation(qp, bf, x_e_qp)
            # insert into element residual
            f_e <- transform_to_physical(f_qp, J)
        f_l <- f_e # scatter through element map
    f <- f_l # ghosted to global
```

FEM pseudocode

```
f_qp <- user_evaluation(qp, bf, x_e_qp)
```

- Problem-specific variability in *innermost* loop
- Efficient implementation may need to:
  - vectorize across elements,
  - vectorize within an element,
  - exchange loop orders,
  - hoist loop-invariant code,
  - exploit structure in basis functions,
  - pre-evaluate geometry at quad points.
  - …

Say *what*, not *how*.


Firedrake
automated finite element system.
Finite element problems written in the FEniCS language (UFL + problem solving language).
Finite element language objects: Mesh, FunctionSpace, Function...
Custom kernel
Form compiler converts integrals into unscheduled loops.
dolfin-adjoint
Adjoint simulations by automated reasoning about the finite element problem.
Extended FIAT element tabulator
PyOP2 Interface
Mats and Dats: global data objects.
Kernel function: mesh-local operation.
Maps and Sets: data adjacency structures.
PETSc
DMPlex global mesh objects
Linear and nonlinear solvers
PyOP2 parallel loop engine
MPI
COFFEE vectorising and loop transforming compiler
Optimised compiled mesh loops
PyOP2
High performance mesh execution abstraction.

Local kernels

Compiling variational forms

We use UFL (Alnæs et al. 2014) from the FEniCS project for specifying variational problems.

A *form compiler* translates this to low-level executable code for evaluating the integral on an element.

An example

```
mesh = UnitTriangleMesh()
V = FunctionSpace(mesh, "CG", 2)
u = TrialFunction(V)
v = TestFunction(V)
a = u*v*dx
```

```
void integral(double A[6][6],
    const double *restrict coords[6])
{
  double t0 = (-1 * coords[0][0]);
  double t1 = (-1 * coords[3][0]);
  /* t2 ← |detJ| */
  double t2 = fabs(((t0 + (1 * coords[1][0])) *
                    (t1 + (1 * coords[5][0]))) +
                   (-1 * (t0 + (1 * coords[2][0])) *
                    (t1 + (1 * coords[4][0]))));
  static const double t3[6]    = {...};
  static const double t4[6][6] = {...};
  for (int ip = 0; ip < 6; ip += 1) {
    double t5 = (t3[ip] * t2);
    for (int j = 0; j < 6; j += 1) {
      for (int k = 0; k < 6; k += 1) {
        A[j][k] += t5 * t4[ip][j] * t4[ip][k];
      }
    }
  }
}
```

Two-stage form compilation

1. Lower finite element expressions to tensor-algebra

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`github.com/firedrakeproject/tsfc`

Lowering FE

Given, c_r, basis coefficients on a cell
Want c_q, coefficient evaluated at quad points.

$$c_q = \sum_r \mathcal{E}_{q,r} c_r$$

$\mathcal{E}_{q,r}$ provided by FIAT as tabulation of 2D array.

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Structure in $\mathcal{E}$

$$\mathcal{E}_{q,r} = \mathcal{E}_{(q_x,r_x),(q_y,r_y)}$$

$\mathcal{E}$ factorises

$$\mathcal{E}_{q,r} = \mathcal{E}^x_{q_x,r_x} \mathcal{E}^y_{q_y,r_y}$$

WIP: exploiting structure for automated sum-factorisation.

Problem

Modern optimising compilers do a bad job on finite element kernels.

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Code motion (or not?)

```
for (i = 0; i < L; i++ )
   for (j = 0; j < M; j++)
      for (k = 0; k < N; k++)
         A[j][k] += f(i, j)*g(i, k)
```

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```

Corollary

We need to spoon-feed the compiler already optimised code.

COFFEE I

No single optimal schedule for evaluation of every finite element kernel. Variability in

- polynomial degree,
- number of fields,
- kernel complexity,
- working set size,
- structure in the basis functions,
- structure in the quadrature points,
- ...

We *explore* (some of) this space using a special-purpose compiler.

COFFEE II

Vectorisation

Align and pad data structures, then use intrinsics or rely on compiler. Experience, gcc-4.X *really* doesn't want to vectorise short loops!

Luporini, Varbanescu, et al. 2015 `doi:10.1145/2687415`

Flop reduction

Exploit *linearity* in test functions to perform factorisation, code motion and CSE.

Cost model: don't introduce mesh-sized temporaries.

Luporini, Ham, and Kelly 2016 `arXiv:1604.05872[cs.MS]`

`github.com/coneoproject/COFFEE`

Global iteration

PyOP2

A library for expressing data parallel iterations

Sets	iterable entities
Dats	abstract managed arrays (data defined on a set)
Maps	relationships between elements of sets
Kernels	local computation
par_loop	Data parallel iteration over a set

Arguments to parallel loop indicate how to gather/scatter global data using *access descriptors*

```
par_loop(kernel, iterset, data1(map1, READ), data2(map2, WRITE))
```

Key ideas

Local computation

Kernels do not know about global data layout.

- Kernel defines contract on local, packed, ordering.
- Global-to-local reordering/packing appears in map.

“Implicit” iteration

Application code does not specify explicit iteration order.

- Define data structures, then just “iterate”
- Can’t write Gauss-Seidel (for example)
- Lazy evaluation

Tensions in model development I

Performance

- Keep data in cache as long as possible.
- Manually fuse kernels.
- Loop tiling for latency hiding.
- ...
- Individual components hard to test
- Space of optimisations suffers from combinatorial explosion.

Tensions in model development II

Maintainability

- Keep kernels separate
- “Straight-line” code
- …
- Testable
- Even if performance of individual kernels is good, can lose *a lot*

Lazy evaluation

- `par_loop` only executed “when you look at the data”.
- PyOP2 sees sequence of loops, can reason about them for
  - Loop fusion
  - Loop tiling
  - Communication coalescing
- Application code does not change. “What, not how”.

Another example: extruded meshes

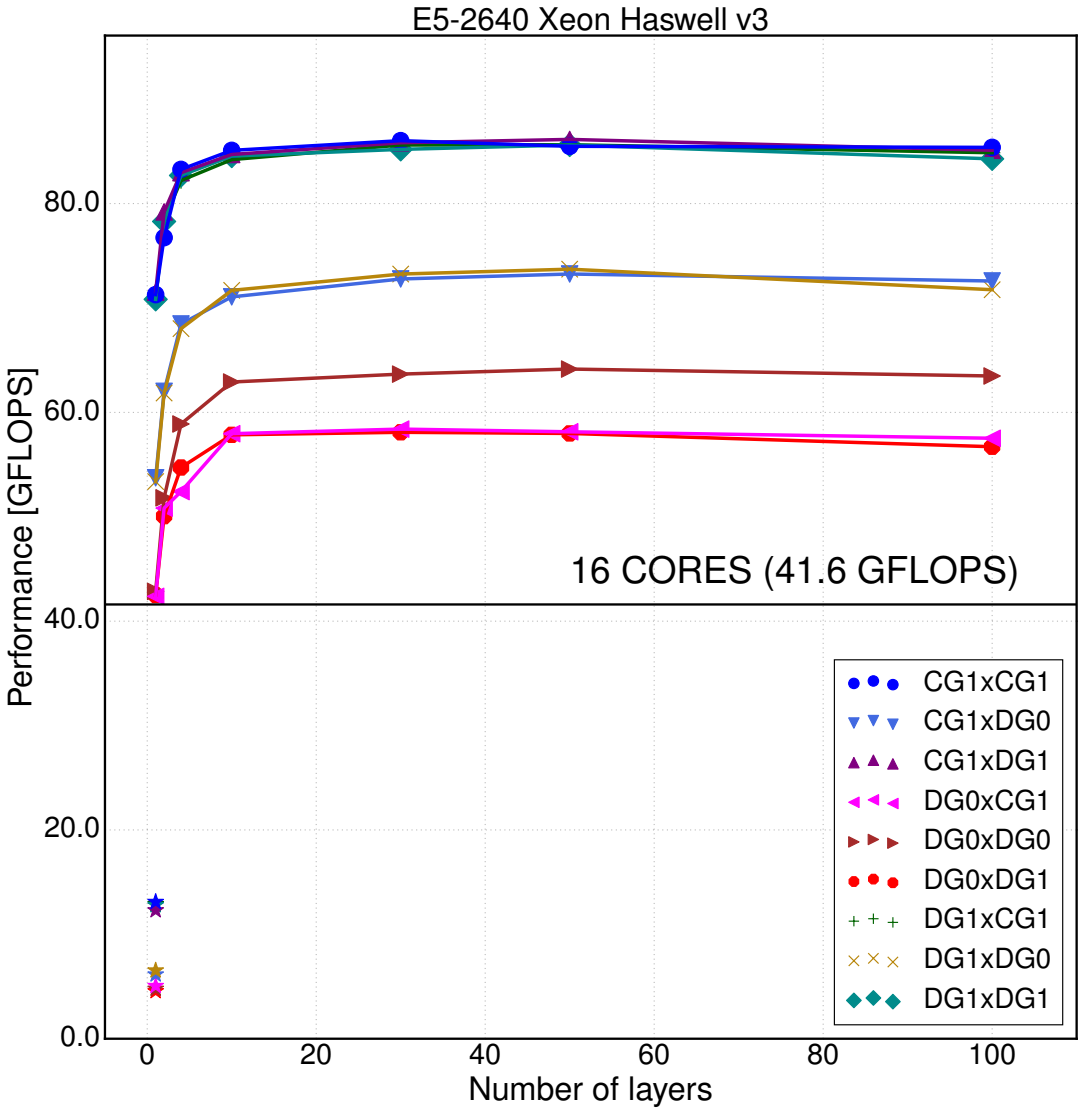
In many geophysical applications, meshes are topologically *structured* in the (short) vertical direction.

Can produce vertically structured dof-numbering, avoiding most of the indirection penalty.

Only need to annotate data structures with this extra information.

```
s = Set(100) # Unstructured set
e = ExtrudedSet(s, layers=...) # Semi-structured set
d = DataSet(...)
# values encode indirections on base set
# offsets say how to move in the structured direction
map = Map(e, d, values, offsets=[...])

par_loop(kernel, e, data(map, WRITE), ...)
```



Bercea et al. 2016 `arXiv:1604.05937[cs.MS]`

Did we succeed?

Experimentation

With model set up, experimentation is easy

- Change preconditioner: c. 1 line
- Drop terms: c. 1-4 lines
- Different operator: c. 1-10 lines
- quasi-Newton: c. 1-10 lines
- Matrix-free: XXX

Maintainability

Core Firedrake

Component	LOC
Firedrake	9000
PyOP2	5000
TSFC	2700
COFFEE	4500
Total	21200

Shared with FEniCS

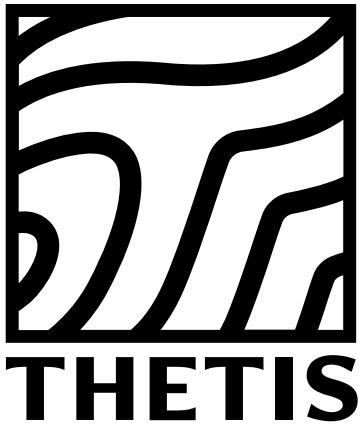
Component	LOC
FIAT	4000
UFL	13000
Total	17000

Performance I

Kernel performance

- COFFEE produces kernels that are better (operation count) than existing automated form compilers
- Provably optimal in some cases
- Also provides good vectorised performance, up to 70% peak for in-cache computation.

Performance II



Thetis

- 3D unstructured coastal ocean model in Firedrake
- Lock exchange test case

Thetis P1DG-P1DG, triangular wedges. 13s/s.

SLIM hand-coded/optimised (same discretisation), 6s/s

`github.com/thetisproject/thetis`

Abstraction degradation

Exposing PyOP2 provides means of writing mesh iterations that are not “assemble a variational form”.

Slope limiters

Vertex-based limiters need max/min over incident cells

```
par_loop("""
    for (int i=0; i<qmax.dofs; i++) {
        qmax[i][0] = fmax(qmax[i][0], centroids[0][0]);
        qmin[i][0] = fmin(qmin[i][0], centroids[0][0]);
    }
    """,
       dx,
       {'qmax': (max_field, RW),
        'qmin': (min_field, RW),
        'centroids': (centroids, READ)})
```

Coming (soon)

- Efficient high order evaluation (via tensor-products and/or Bernstein polynomials)
- Matrix-free operators and preconditioning
- Symbolic (not just algebraic) composition for multiphysics preconditioning
- Mesh adaptivity
- …

Summary

- Firedrake provides a layered set of abstractions for finite element
- Computational performance is good, often $> 50\%$ achievable peak.
- Hero-coding necessary if you want the last 10-20%
- ...but at what (person) cost.

Questions?

References I

Alnæs, M. S. et al. (2014). "Unified Form Language: A Domain-specific Language for Weak Formulations of Partial Differential Equations". *ACM Trans. Math. Softw.* **40**. doi:10.1145/2566630.

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