Firedrake: automating the finite element method by composing abstractions

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Firedrake team

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`www.firedrakeproject.org`

Rathgeber et al. 2016 `arXiv:1501.01809 [cs.MS]`

Contact

`www.firedrakeproject.org/contact.html`

Methods

- Slack: `firedrakeproject.slack.com`
- Mail: `firedrake@imperial.ac.uk` (subscribe first)
- Github: `github.com/firedrakeproject/firedrake`

What is Firedrake?

> [...] *an automated system for the portable solution of partial differential equations using the finite element method.*

- Written in Python.
- Finite element problems specified with *embedded* domain specific language.
- *Runtime* compilation to low-level (C) code.
- Expressly *data parallel*: don't worry about MPI.

A specification of finite element problems

```
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.

$$\begin{aligned} \langle u, v\rangle + \langle \mathrm{div}\, v, p\rangle &= 0 \quad && \forall v \in V \\ \langle \mathrm{div}\, u, q\rangle &= -\langle 1, q\rangle \quad && \forall q \in Q. \end{aligned}$$

Symbolic, numerical computing

Weave together

- *symbolic* problem description

```
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
```

- with problem-specific data (which mesh, what solver?)

```
mesh = UnitSquareMesh(100, 100)
V = FunctionSpace(mesh, ”RT”, 2)
Q = FunctionSpace(mesh, ”DG”, 1)
...
solve(a == L, u, solver_parameters=...)
```

and *synthesise* efficient implementation from the symbolic problem description.

More than a pretty face

Library usability

- High-level language enables rapid model development
- Ease of experimentation
- Small model code base

Library development

- Automation of complex optimisations
- Exploit expertise across disciplines
- Small library code base

Composability of libraries that manipulate PDE solvers

`www.dolfin-adjoint.org`

Automated derivation of the discrete adjoint from forward models written using FEniCS *and Firedrake*.

```
$ cloc dolfin-adjoint/
Language  files   blank   comment   code
Python       54    2322       937   7294
$ cloc dolfin-adjoint/compatibility.py
Python        1      38        11    140
```

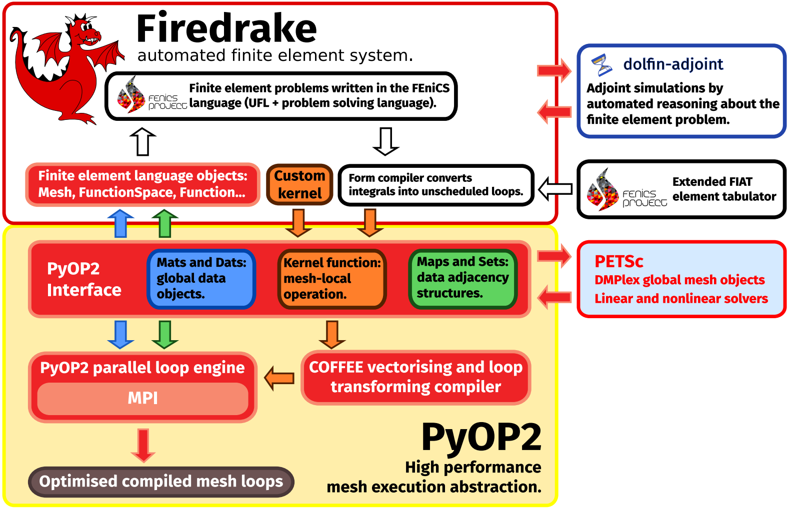
Ease of experimentation

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?

Same “easy to use” code must run fast at scale.

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

Automating expertise

- "In-person" case-by-case optimisation *does not scale*
- Code generation allows us to package expertise and provide it to everyone
- Done by a special-purpose kernel compiler

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,
- ...

COFFEE II

Vectorisation

Align and pad data structures, then use intrinsics or rely on compiler.

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

Flop reduction

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

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

`github.com/coneoproject/COFFEE`

Global iteration

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*

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”
- Lazy evaluation

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: c. 1-10 lines (+ c. 30 lines for preconditioner).

Maintainability

Core Firedrake

Component	LOC
Firedrake	11000
PyOP2	5000
TSFC	3500
COFFEE	4500
Total	24000

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
- Good vectorised performance, problem dependent, but up to 70% peak for in-cache computation.

Summary

- Firedrake provides a layered set of abstractions for finite element
- Enables automated provision of expertise to model developers
- Computational performance is good, often $> 50\%$ achievable peak.

References

Luporini, F., D. A. Ham, and P. H. J. Kelly (2016). *An algorithm for the optimization of finite element integration loops*. Submitted. arXiv: 1604.05872 [cs.MS].

Luporini, F., A. L. Varbanescu, et al. (2015). “Cross-Loop Optimization of Arithmetic Intensity for Finite Element Local Assembly”. *ACM Trans. Archit. Code Optim.* 11. doi:10.1145/2687415.

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