Compiler technology for solving PDEs with performance portability

Paul H J Kelly
Group Leader, Software Performance Optimisation
Co-Director, Centre for Computational Methods in Science and Engineering
Department of Computing, Imperial College London

Joint work with :

David Ham (Imperial Computing/Maths/Grantham Inst for Climate Change)
Gerard Gorman, (Imperial Earth Science Engineering – Applied Modelling and Computation Group)
Mike Giles, Gihan Mudalige, Istvan Reguly (Mathematical Inst, Oxford)
Doru Bercea, Fabio Luporini, Graham Markall, Lawrence Mitchell, Florian Rathgeber, George Rokos (Software Perf Opt Group, Imperial Computing)
Spencer Sherwin (Aeronautics, Imperial), Chris Cantwell (Cardio-mathematics group, Mathematics, Imperial)
Michelle Mills Strout, Chris Krieger, Cathie Olschanowsky (Colorado State University)
Carlo Bertolli (IBM Research)
Ram Ramanujam (Louisiana State University)

Imperial College London

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What do we actually gain from domain-specificity?

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Doru Thom Popovici, Franz Franchetti (CMU), Karl Wilkinson (Capetown), Chris–Kriton Skylaris (Southampton)

Have your cake and eat it too

This talk is about the following idea:

- can we simultaneously
  - raise the level at which programmers can reason about code,
  - provide the compiler with a model of the computation that enables it to generate faster code than you could reasonably write by hand?

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Have your cake and eat it too

This talk is about the following idea:

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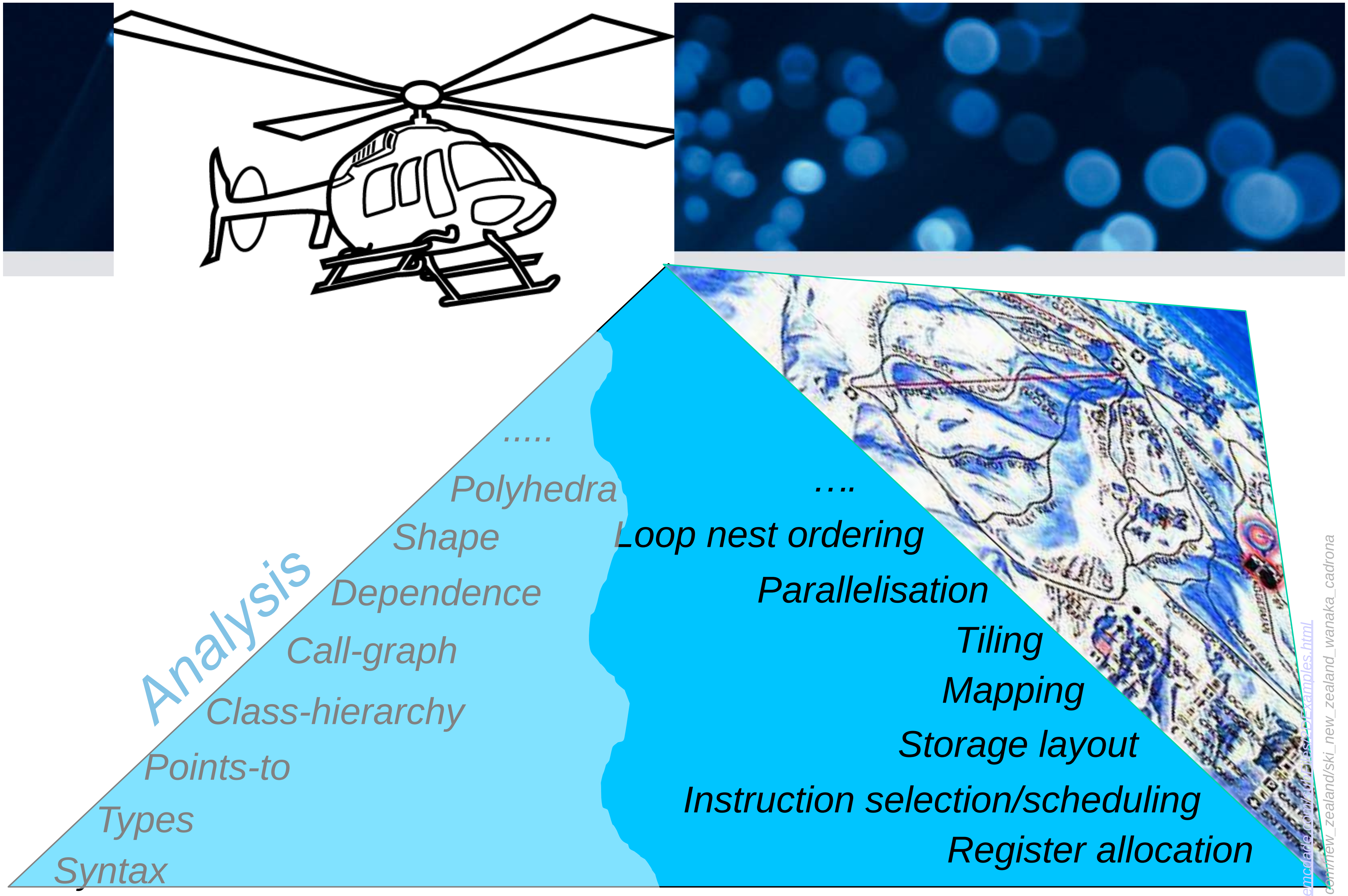


Analysis

.....

Polyhedra

Shape

Dependence

Call-graph

Class-hierarchy

Points-to

Types

Syntax

....

Loop nest ordering

Parallelisation

Tiling

Mapping

Storage layout

Instruction selection/scheduling

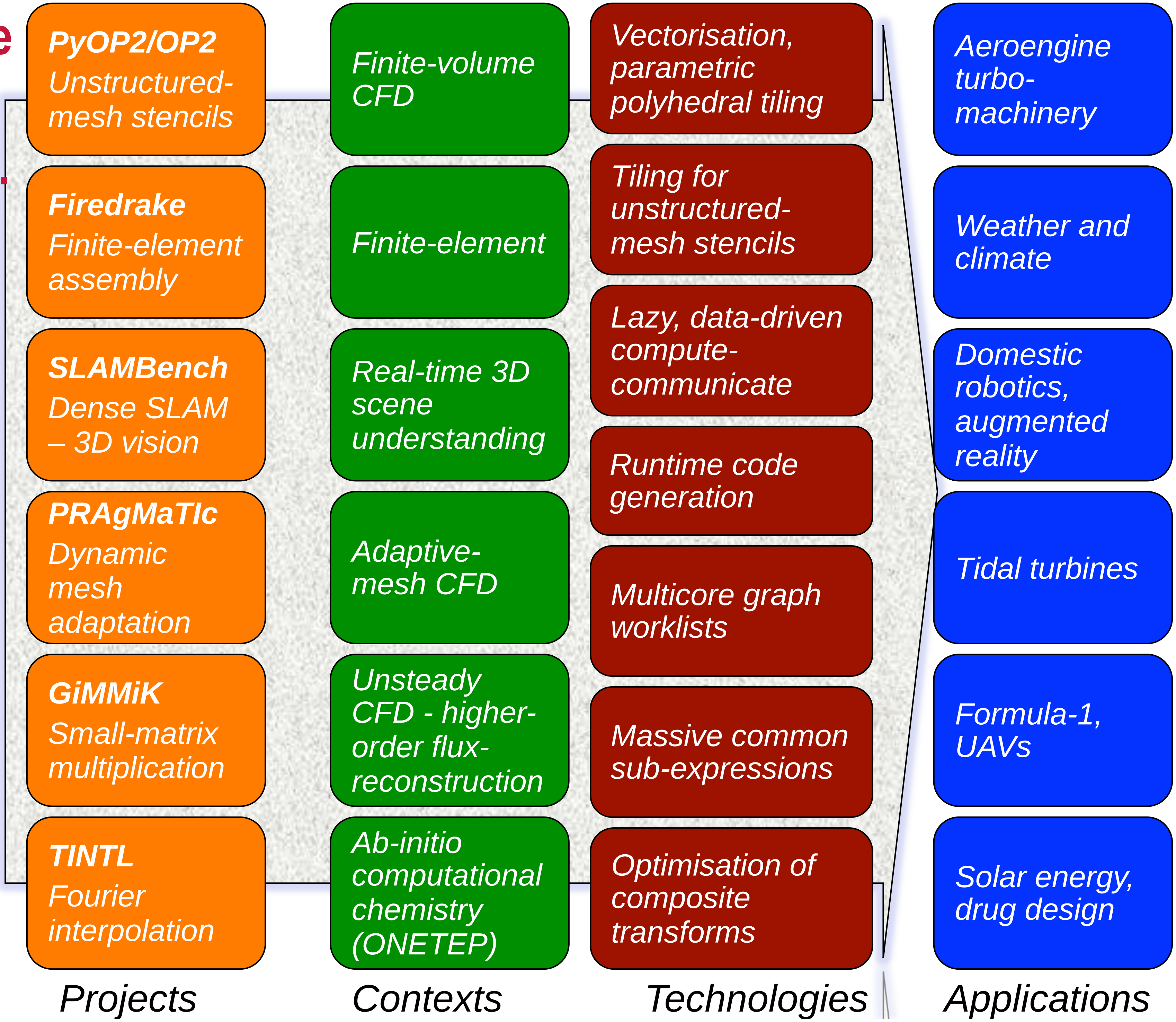
Register allocation

http://www.nikkiemcdade.com/subFiles/2DExamples.html

http://www.ginz.com/new_zealand/ski_new_zealand_wanaka_cadrona

- Compilation is like skiing
- Analysis is not always the interesting part....

What we are doing….



PyOP2/OP2
Unstructured-mesh stencils

Firedrake
Finite-element assembly

SLAMBench
Dense SLAM – 3D vision

PRAgMaTIc
Dynamic mesh adaptation

GiMMiK
Small-matrix multiplication

TINTL
Fourier interpolation

Projects

Finite-volume CFD

Finite-element

Real-time 3D scene understanding

Adaptive-mesh CFD

Unsteady CFD - higher-order flux-reconstruction

Ab-initio computational chemistry (ONETEP)

Contexts

Vectorisation, parametric polyhedral tiling

Tiling for unstructured-mesh stencils

Lazy, data-driven compute-communicate

Runtime code generation

Multicore graph worklists

Massive common sub-expressions

Optimisation of composite transforms

Technologies

Aeroengine turbo-machinery

Weather and climate

Domestic robotics, augmented reality

Tidal turbines

Formula-1, UAVs

Solar energy, drug design

Applications

Targetting MPI, OpenMP, OpenCL, Dataflow/ FPGA, from supercomputers to mobile, embedded and wearable

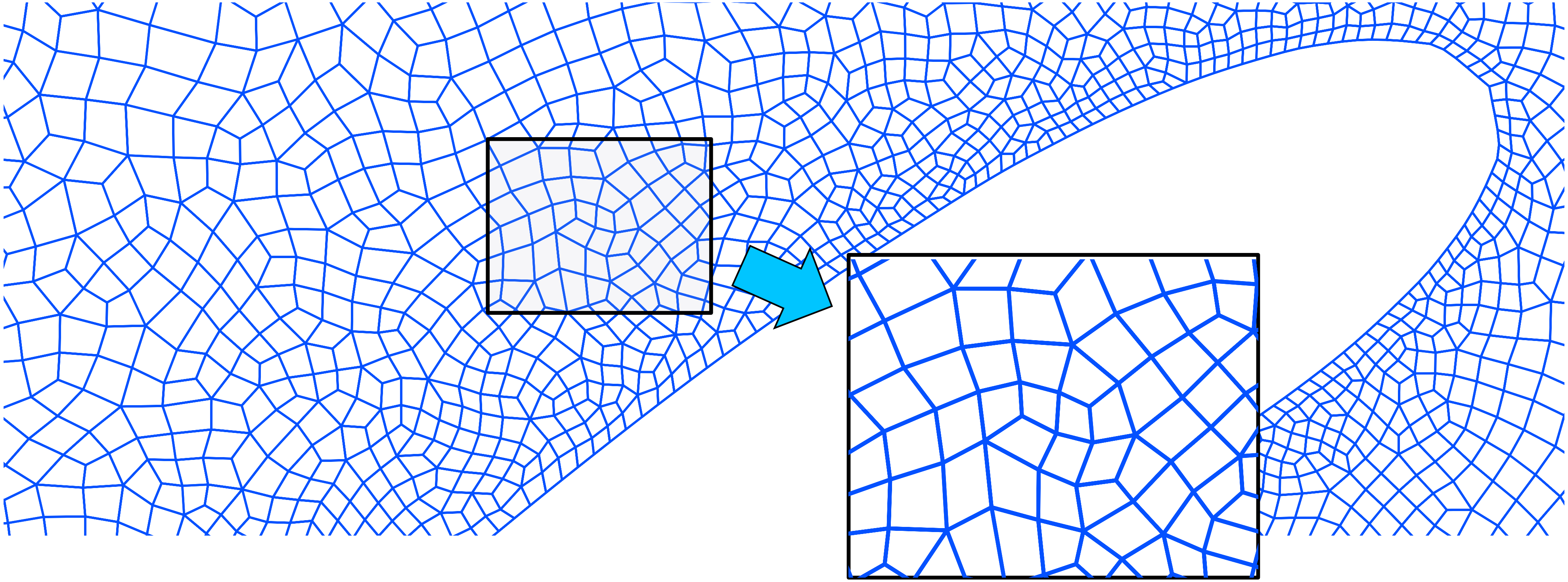
This talk

- Some examples of domain-specific optimisations
  - BLINK: visual effects filters – fusion, vectorisation, CUDA
  - DESOLA: runtime fusion for linear algebra
  - OP2: (among many) staging for CUDA shared memory
  - PyOP2: (ditto) fusion and tiling for unstructured meshes
  - COFFEE: (ditto) generalised loop-invariant code motion
  - GiMMiK: tiling & full unrolling for block-panel matrix multiply
  - TINTL: Fourier interpolation for density functional theory
- **This talk's question:**
  - **What do we actually gain by building domain-specific tools? Where does the advantage come from?**

This talk

- The standard DSL message:
  - Avoid analysis for transformational optimisation
  - Transform at the right level of abstraction
  - Get the abstraction right

- But what do we actually gain by building domain-specific compiler tools?

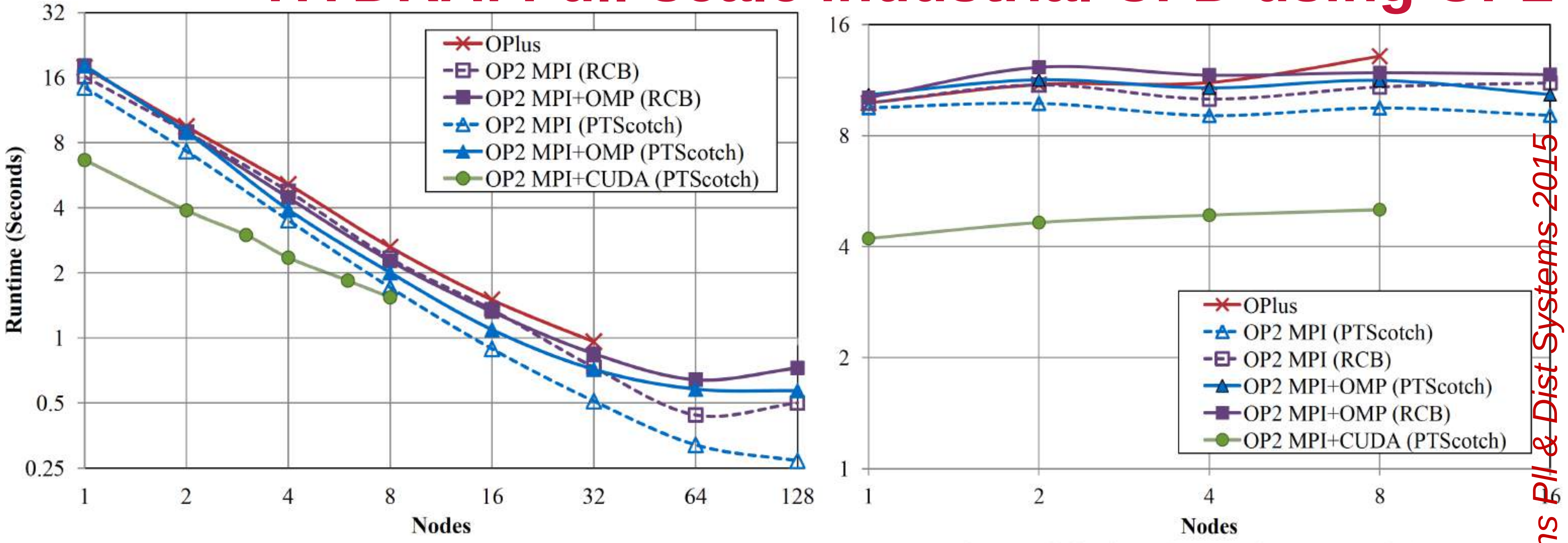


- Unstructured meshes require pointers/indirection because adjacency lists have to be represented explicitly
- A controlled form of pointers

- **OP2** is a C++ and Fortran library for parallel loops over the mesh implemented by source-to-source transformation
- **PyOP2** is an major extension implemented in Python using runtime code generation

- Generates highly-optimised CUDA, OpenMP and MPI code

HYDRA: Full-scale industrial CFD using OP2



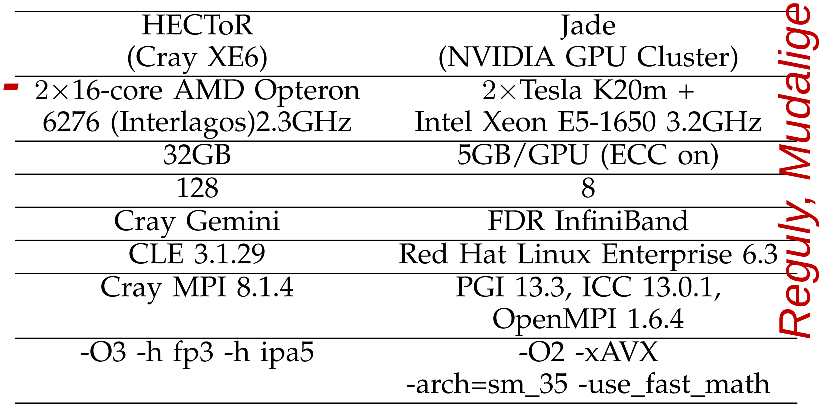
(a) Strong Scaling (2.5M edges)

(b) Weak Scaling (0.5M edges per node)

- ***Unmodified Fortran OP2 source code exploits inter-node parallelism using MPI, and intra-node parallelism using OpenMP and CUDA***
- ***Application is a proprietary, full-scale, in-production fluids dynamics package***
- ***Developed by Rolls Royce plc and used for simulation of aeroplane engines***

(joint work with Mike Giles, Istvan Reguly, Gihan Mudalige at Oxford)

- ***"Performance portability"***



HECToR (Cray XE6)	Jade (NVIDIA GPU Cluster)
2×16-core AMD Opteron 6276 (Interlagos)2.3GHz	2×Tesla K20m + Intel Xeon E5-1650 3.2GHz
32GB	5GB/GPU (ECC on)
128	8
Cray Gemini	FDR InfiniBand
CLE 3.1.29	Red Hat Linux Enterprise 6.3
Cray MPI 8.1.4	PGI 13.3, ICC 13.0.1, OpenMPI 1.6.4
-O3 -h fp3 -h ipa5	-O2 -xAVX -arch=sm_35 -use_fast_math

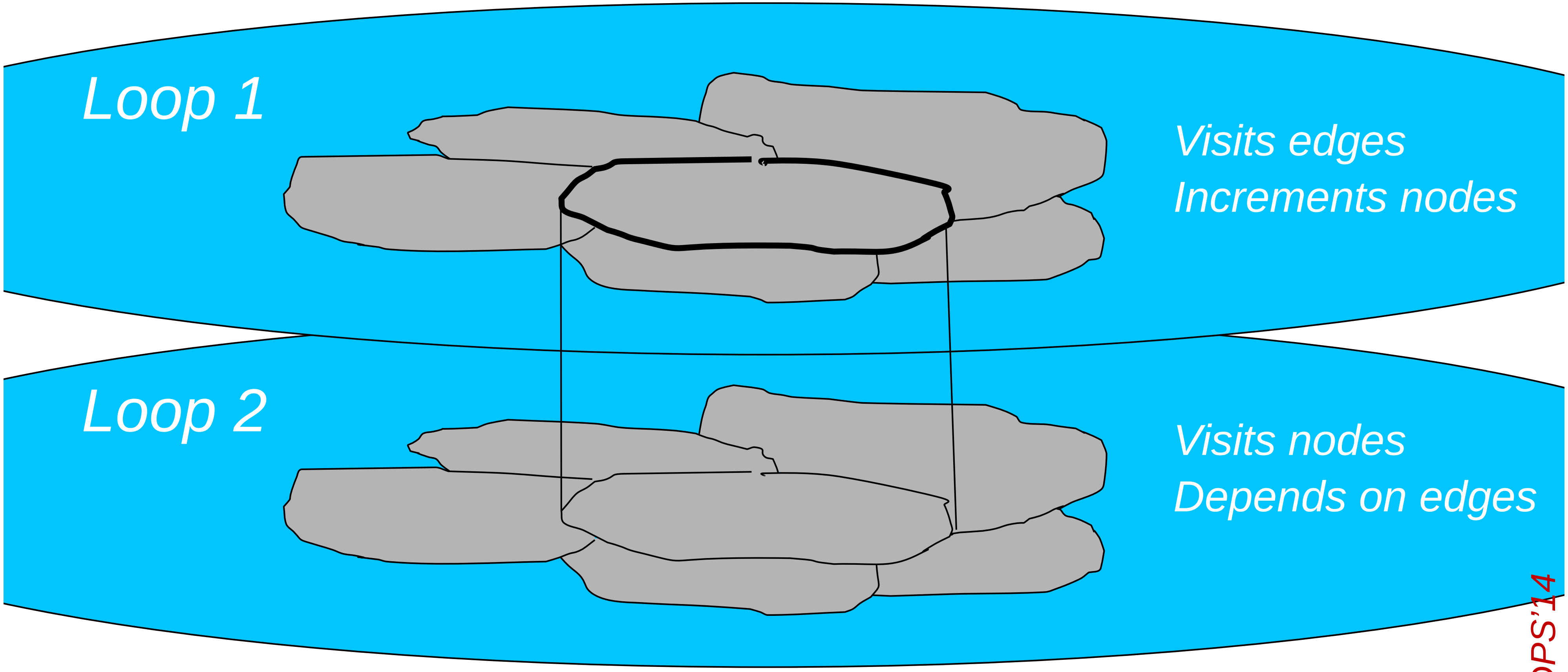
Reguly, Mudalige et al, IEEE Trans Pll & Dist Systems 2015

HYDRA: Full-scale industrial CFD using OP2

- **Where did the domain-specific advantage come from?**
  - Automatic code synthesis, for MPI, OpenMP, CUDA, OpenCL – single source code, clean API
  - Inspector-executor scheme: we know we will iterate over the mesh many times, so we can invest in partitioning, colouring etc
  - Code synthesis templates to deliver optimised implementations, eg:
    - Colouring to avoid read-increment-write conflicts
    - Staging of mesh data into CUDA shared memory
    - Splitting push loops (that increment via a map) to reduce register pressure (LCPC2012)

Reguly, Mudalige et al, IEEE Trans PII & Dist Systems 2015

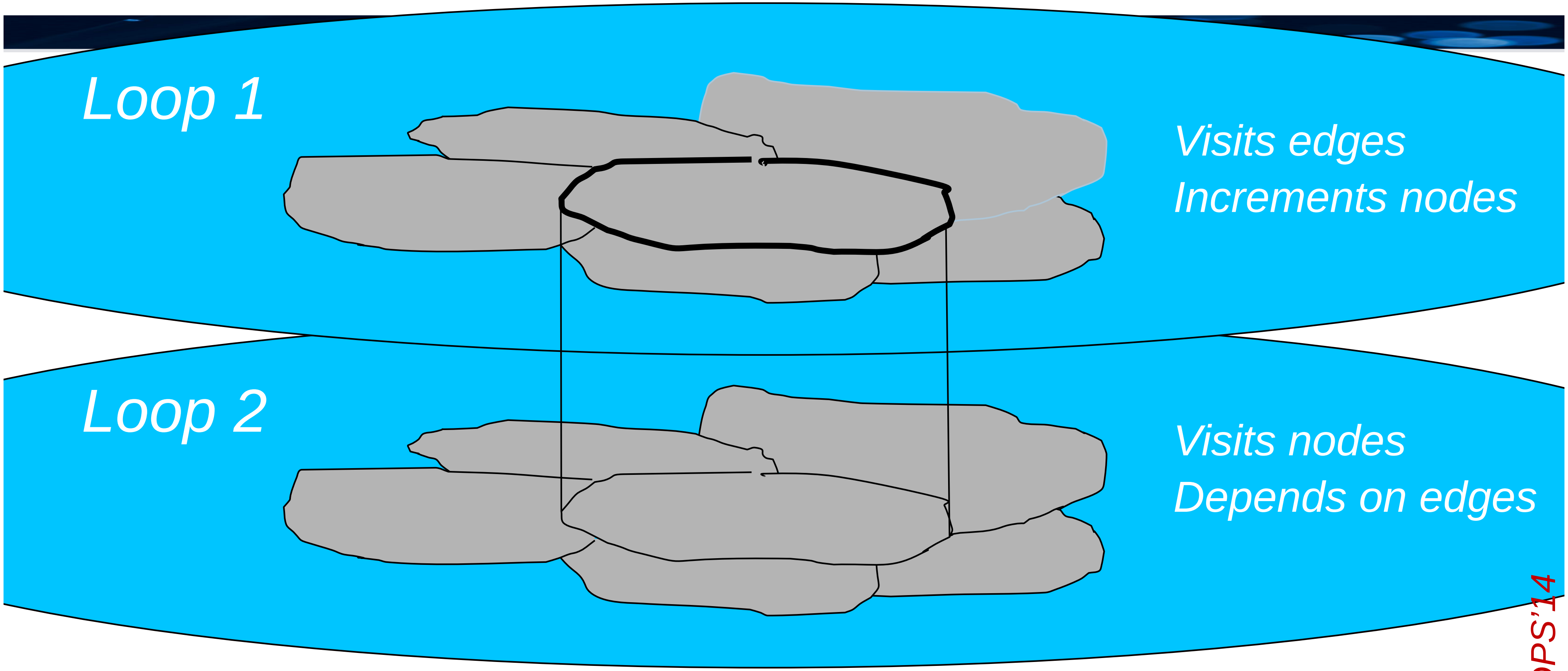
Sparse split tiling on an unstructured mesh, for locality



- How can we fuse two loops, when there is a “halo” dependence?
- I.e. load a block of mesh and do the iterations of loop 1, then the iterations of loop 2, before moving to the next block
- If we could, we could dramatically improve the memory access behaviour!

Strout, Luporini et al, IPDPS’14

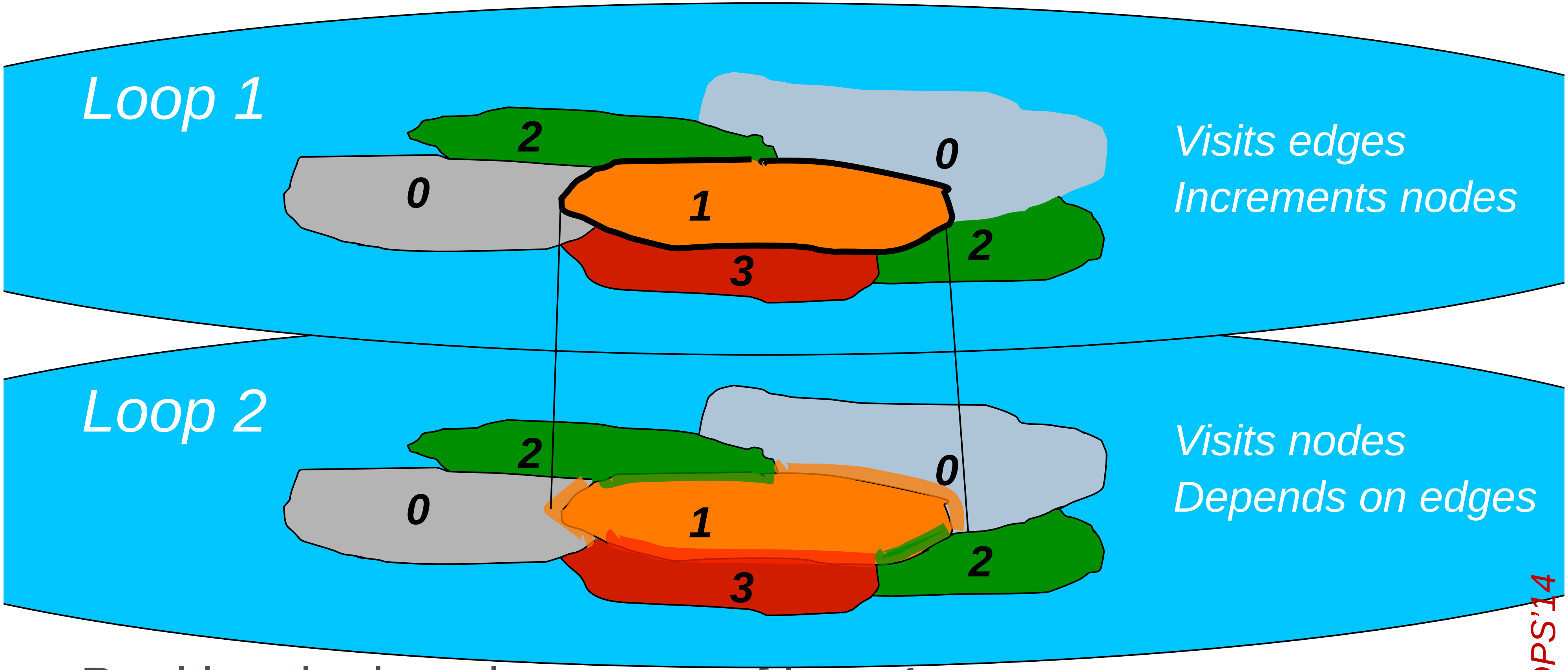
Sparse split tiling



- Partition the iteration space of loop 1

Strout, Luporini et al, IPDPS'14

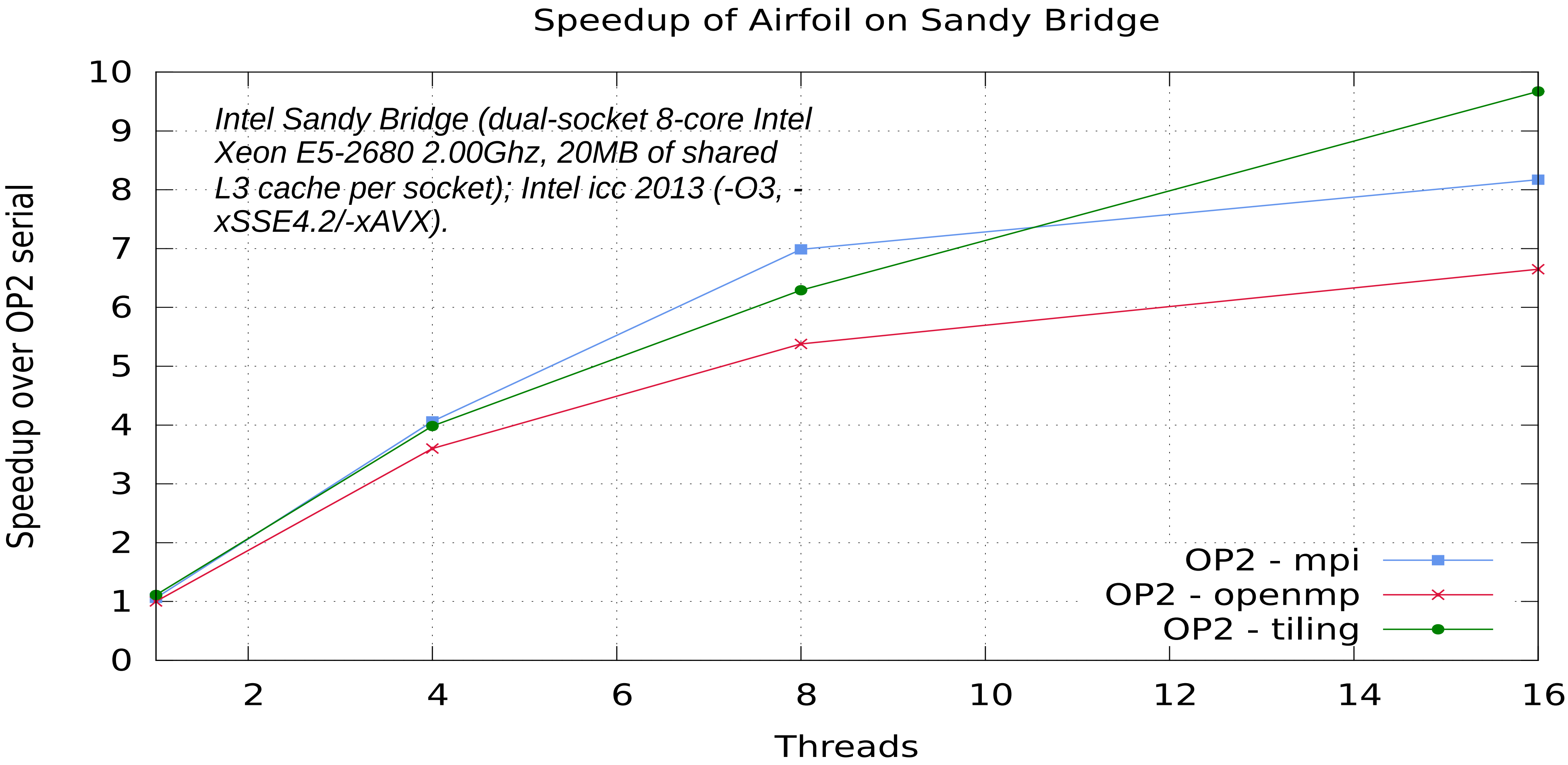
Sparse split tiling



- Partition the iteration space of loop 1
- Colour the partitions
- Project the tiles, using the knowledge that colour n can use data produced by colour n-1
- Thus, the tile coloured #1 *grows* where it meets colour #0
- And *shrinks* where it meets colours #2 and #3

Strout, Luporini et al, IPDPS'14

OP2 loop fusion in practice



Intel Sandy Bridge (dual-socket 8-core Intel Xeon E5-2680 2.00Ghz, 20MB of shared L3 cache per socket); Intel icc 2013 (-O3, -xSSE4.2/-xAVX).

- *Mesh size = 1.5M edges*
- *# Loop chain = 6 loops*
- *No inspector/plans overhead*

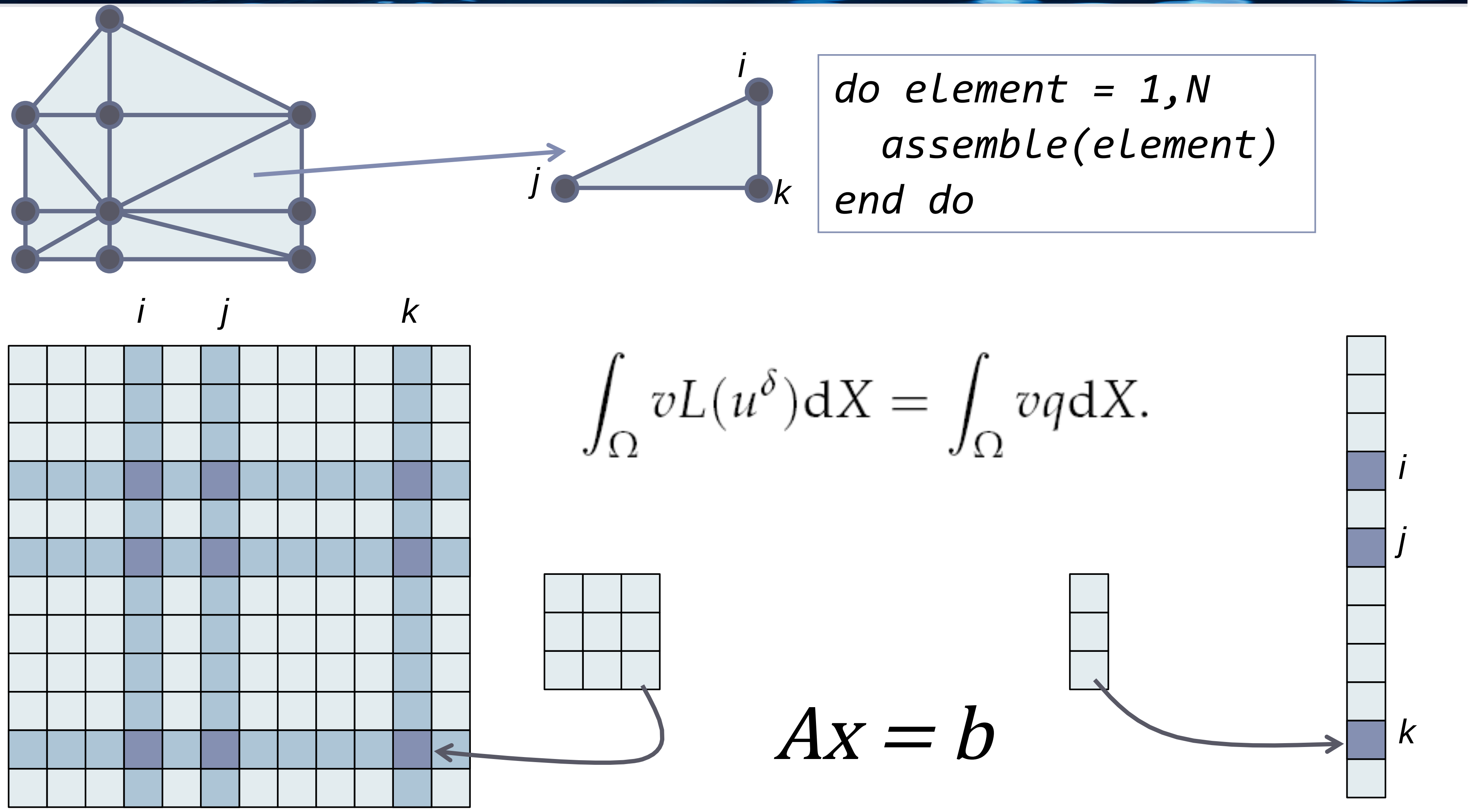
- *Airfoil test problem*
- *Unstructured-mesh finite-volume*

Sparse split tiling

- **Where did the domain-specific advantage come from?**
  - OP2's access descriptors provide precise dependence iteration-to-iteration information
  - We "know" that we will iterate many times over the same mesh – so it's worth investing in an expensive "inspector-executor" scheme
  - We capture chains of loops over the mesh
    - We *could* get our compiler to find adjacent loops
    - We *could* extend the OP2 API with "loop chains"
  - What we actually do?
    - We delay evaluation of parallel loops
    - We build a chain (DAG) of parallel loops at runtime
    - We generate code at runtime for the traces that occur

Strout, Luporini et al IPDPS 2014

The finite element method in outline



```
do element = 1,N
  assemble(element)
end do
```

$$\int_\Omega v L(u^\delta)\mathrm{d}X = \int_\Omega vq\mathrm{d}X.$$

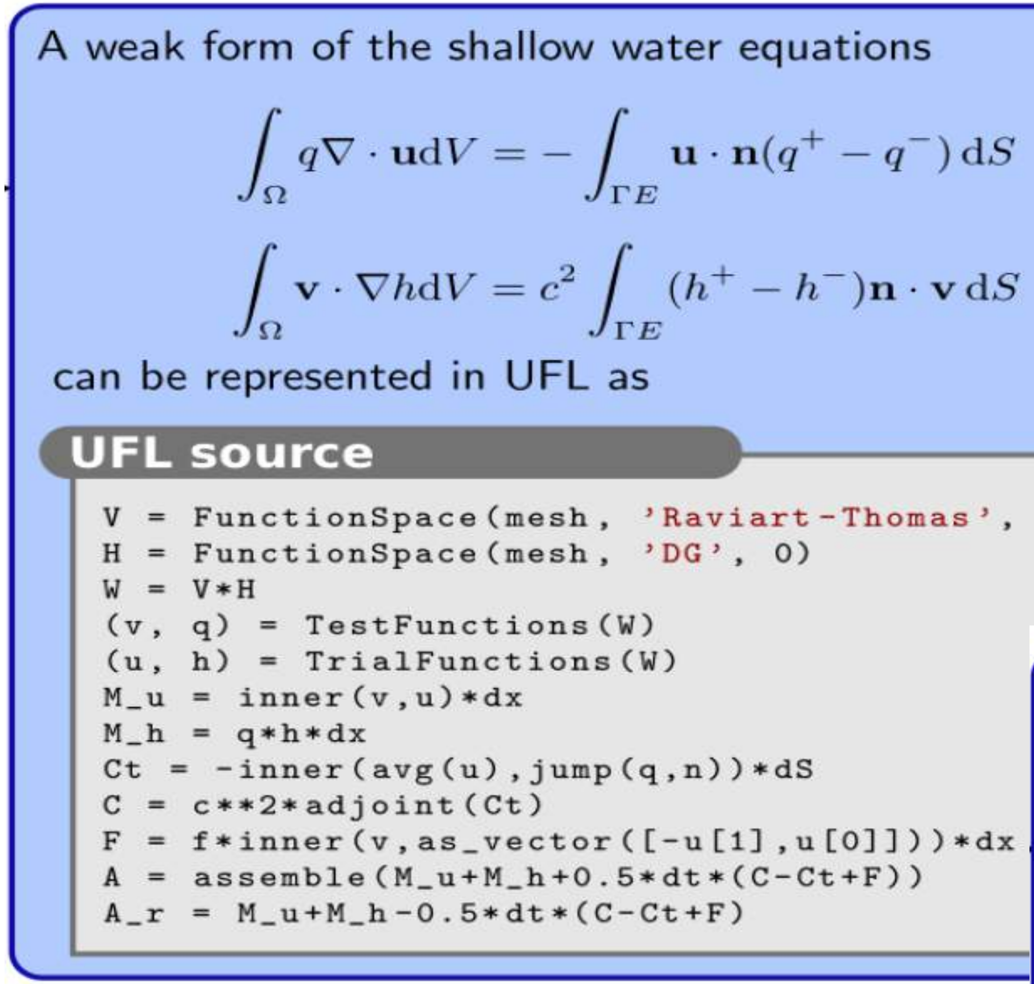
$$Ax = b$$

- Key data structures: Mesh, dense local assembly matrices, sparse global system matrix, and RHS vector

Multilayered abstractions for FE

- Local assembly:
  - Specified using the FEniCS project’s DSL, UFL (the “Unified Form Language”)
  - Computes local assembly matrix
  - Key operation is evaluation of expressions over basis function representation of the element
- Mesh traversal:
  - *OP2*
  - *Loops over the mesh*
  - *Key is orchestration of data movement*
- Solver:
  - Interfaces to standard solvers, such as PetSc

The FEniCS project's Unified Form Language (UFL)



A weak form of the shallow water equations

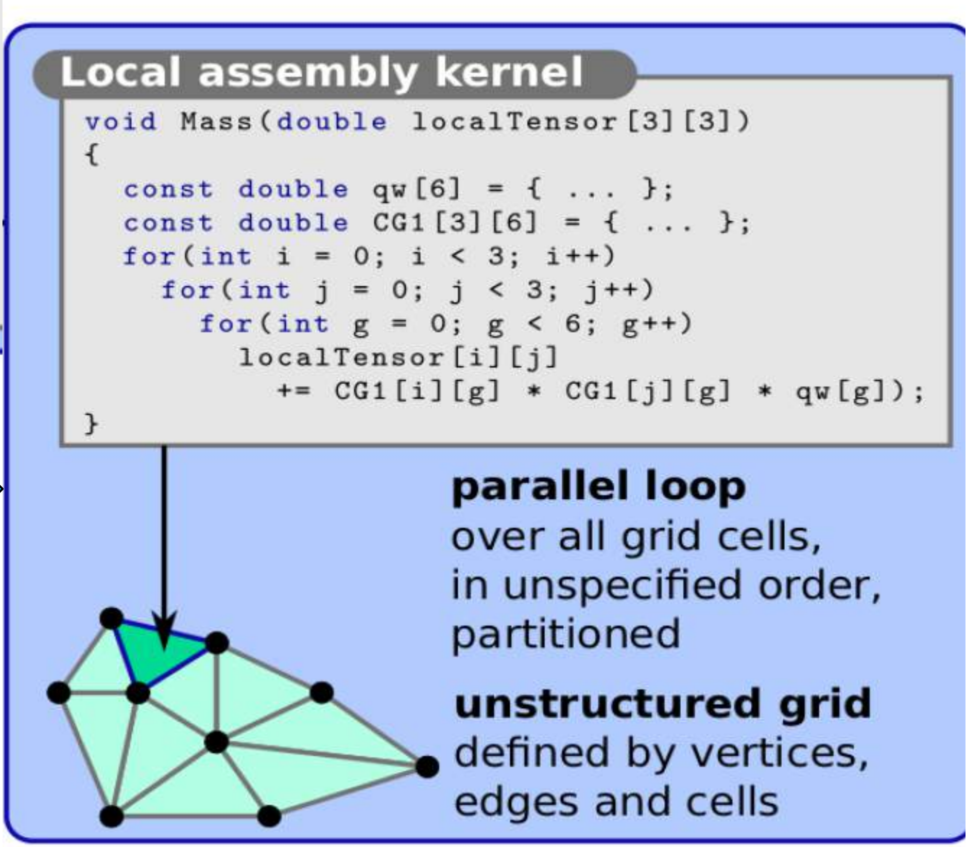
$$\int_{\Omega} q\nabla\cdot\mathbf{u}\mathrm{d}V = -\int_{\Gamma E}\mathbf{u}\cdot\mathbf{n}(q^{+}-q^{-})\,\mathrm{d}S$$

$$\int_{\Omega} \mathbf{v}\cdot\nabla h\mathrm{d}V = c^{2}\int_{\Gamma E}(h^{+}-h^{-})\mathbf{n}\cdot\mathbf{v}\,\mathrm{d}S$$

can be represented in UFL as

UFL source

```
V = FunctionSpace(mesh, 'Raviart-Thomas', 1)
H = FunctionSpace(mesh, 'DG', 0)
W = V*H
(v, q) = TestFunctions(W)
(u, h) = TrialFunctions(W)
M_u = inner(v,u)*dx
M_h = q*h*dx
Ct = -inner(avg(u),jump(q,n))*dS
C = c**2*adjoint(Ct)
F = f*inner(v,as_vector([-u[1],u[0]]))*dx
A = assemble(M_u+M_h+0.5*dt*(C-Ct+F))
A_r = M_u+M_h-0.5*dt*(C-Ct+F)
```



Local assembly kernel

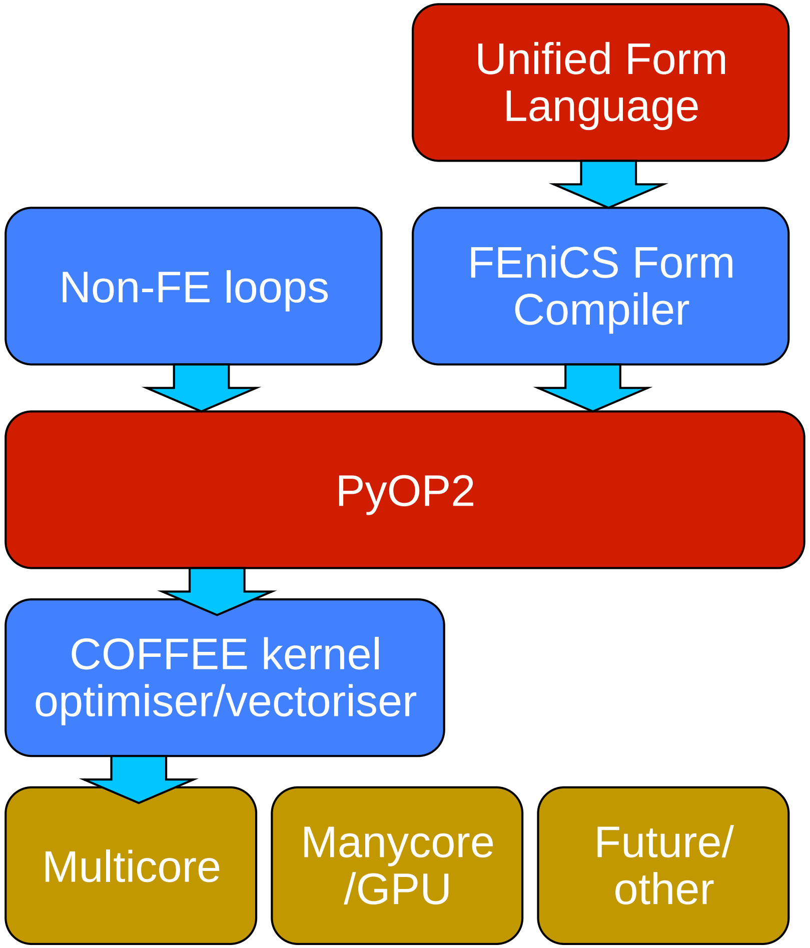
```
void Mass(double localTensor[3][3])
{
  const double qw[6] = { ... };
  const double CG1[3][6] = { ... };
  for(int i = 0; i < 3; i++)
    for(int j = 0; j < 3; j++)
      for(int g = 0; g < 6; g++)
        localTensor[i][j]
          += CG1[i][g] * CG1[j][g] * qw[g]);
}
```

parallel loop
over all grid cells,
in unspecified order,
partitioned

unstructured grid
defined by vertices,
edges and cells

Firedrake: a finite-element framework

- An alternative implementation of the FEniCS language
- Using PyOP2 as an intermediate representation of parallel loops
- All embedded in Python



- The FEniCS project's UFL – DSL for finite element discretisation
- Compiler generates PyOP2 kernels and access descriptors

- Stencil DSL for *unstructured-mesh*
- Explicit *access descriptors* characterise access footprint of kernels
- Runtime code generation

Rathgeber, Ham, Mitchell et al, http://arxiv.org/abs/1501.01809

- **The advection-diffusion problem:**

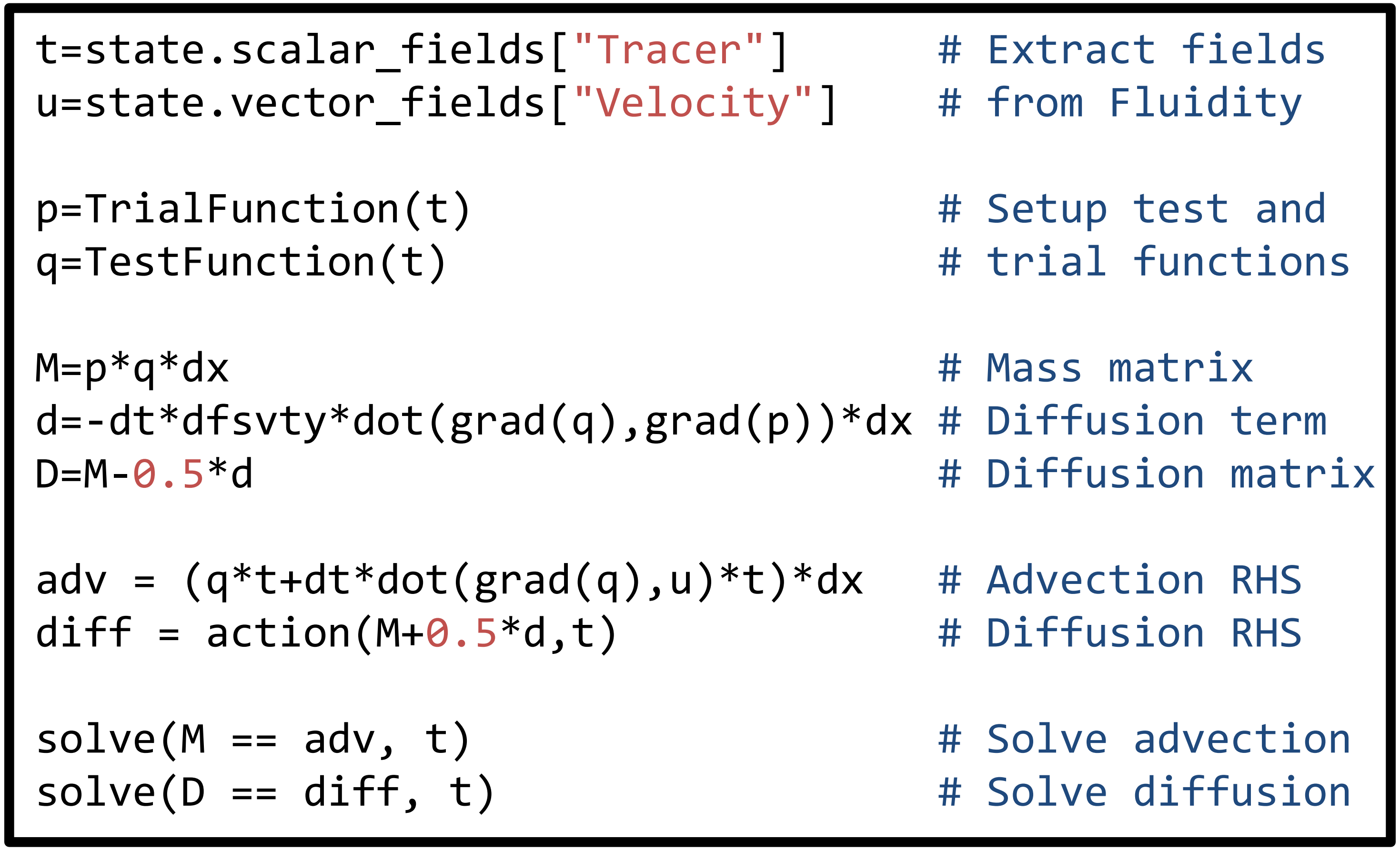
$$\frac{\partial T}{\partial t} = \underbrace{D\nabla^2 T}_{\text{Diffusion}} - \underbrace{\mathbf{u}\cdot\nabla T}_{\text{Advection}}$$

- Weak form:

$$\int_\Omega q\frac{\partial T}{\partial t}\,\mathrm{d}X = \int_{\partial\Omega} q(\nabla T - \mathbf{u}T)\cdot\mathbf{n}\,\mathrm{d}s - \int_\Omega \nabla q\cdot\nabla T\,\mathrm{d}X + \int_\Omega \nabla q\cdot\mathbf{u}T\,\mathrm{d}X$$

- This is the entire specification for a solver for an advection-diffusion test problem

- Same model implemented in FEniCS/ Dolfin, and also in Fluidity – hand-coded Fortran



```
t=state.scalar_fields["Tracer"]         # Extract fields
u=state.vector_fields["Velocity"]       # from Fluidity

p=TrialFunction(t)                      # Setup test and
q=TestFunction(t)                       # trial functions

M=p*q*dx                                # Mass matrix
d=-dt*dfsvty*dot(grad(q),grad(p))*dx # Diffusion term
D=M-0.5*d                               # Diffusion matrix

adv = (q*t+dt*dot(grad(q),u)*t)*dx      # Advection RHS
diff = action(M+0.5*d,t)                # Diffusion RHS

solve(M == adv, t)                      # Solve advection
solve(D == diff, t)                     # Solve diffusion
```

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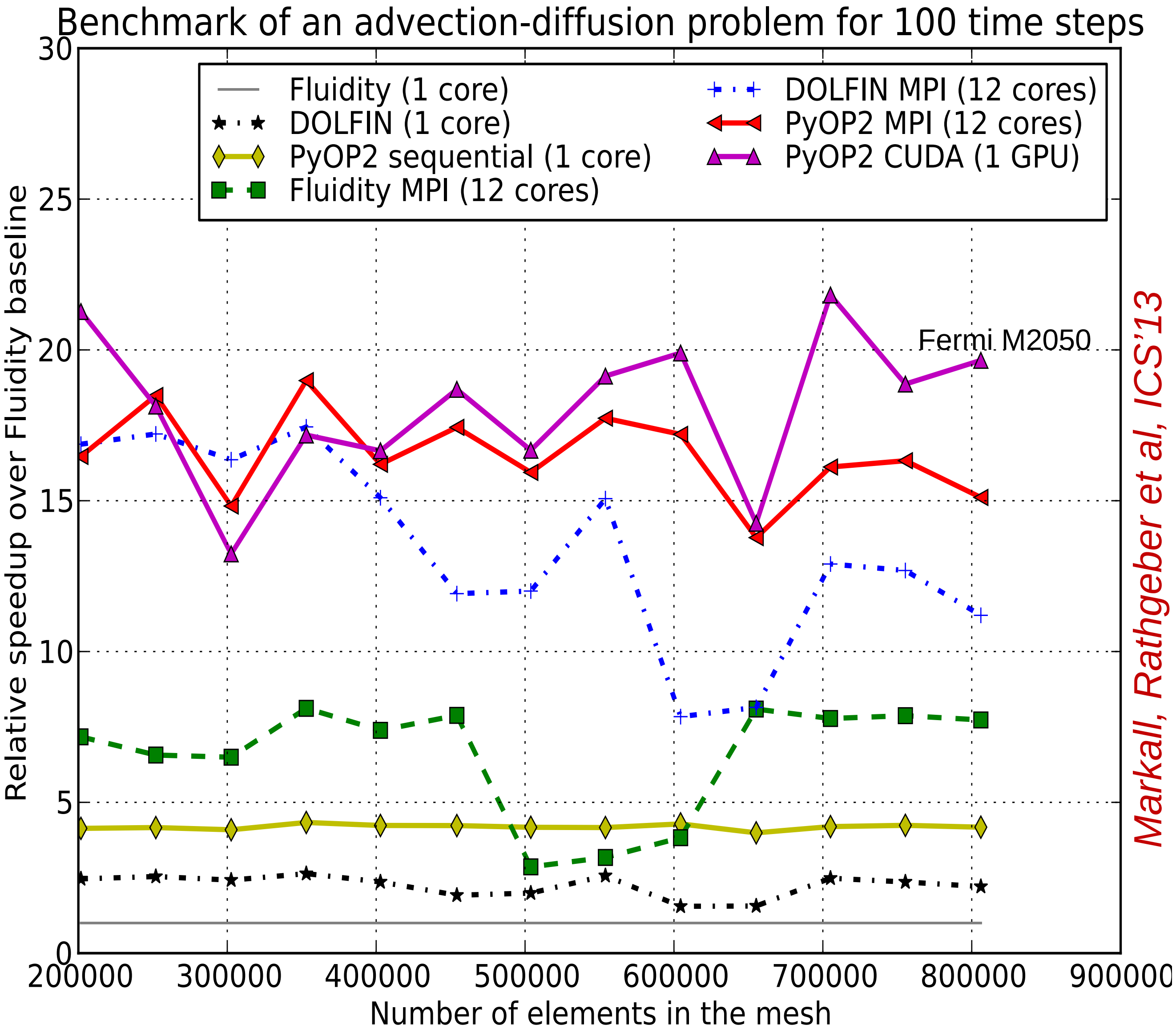
Firedrake – single-node performance

- Here we compare performance against two production codes solving the same problem on the same mesh:
  - Fluidity: Fortran/ C++
  - DOLFIN: the FEniCS project's implementation of UFL

These results are preliminary and are presented for discussion purposes – see Rathgeber, Ham, Mitchell et al, http://arxiv.org/abs/1501.01809 for more systematic evaluation



Markall, Rathgeber et al, ICS'13

- Graph shows speedup over Fluidity on one core of a 12-core Westmere node

Firedrake

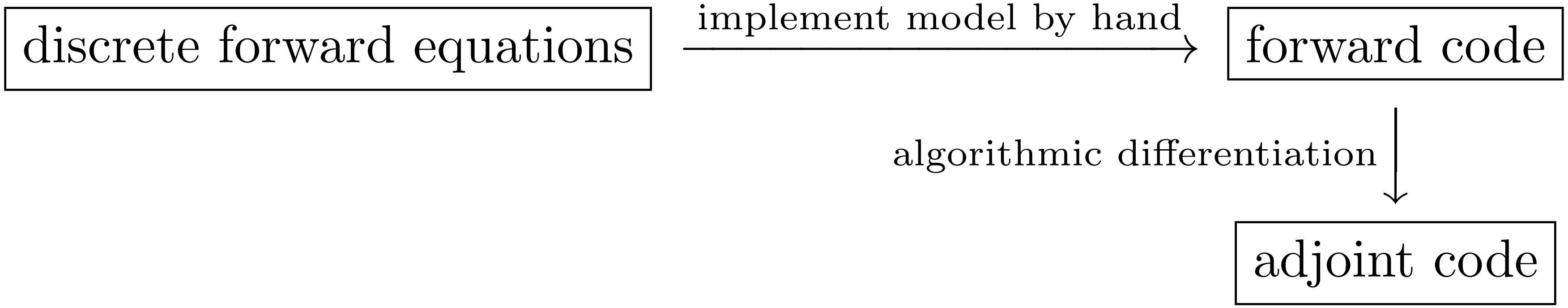
- **Where did the domain-specific advantage come from?**
  - UFL (the Unified Form Language, inherited from the FEniCS Project)
    - Delivers spectacular expressive power
    - Reduces scope for coding errors
    - Supports flexible exploration of different models, different PDEs, different solution schemes
  - Building on PyOP2
    - Handles MPI, OpenMP, CUDA, OpenCL
    - Completely transparently

    - PyOP2 uses runtime code generation
    - So we don't need to do static analysis
    - So the layers above can freely exploit unlimited abstraction

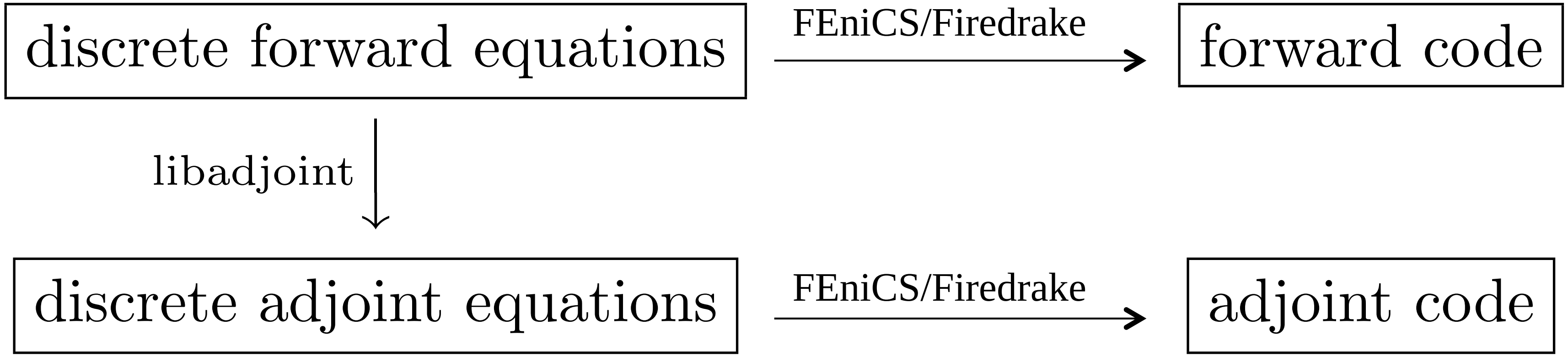
Rathgeber, Ham, Mitchell et al, http://arxiv.org/abs/1501.01809

Firedrake

- **Where did the domain-specific advantage come from?**
  - The adjoint of the PDE characterises the sensitivity of the PDE’s solution to input variables; it is usually derived by automatic differentiation of the solver code:



  - With UFL we have access to the PDE so we can *generate* the adjoint solver directly:



Farrell, Ham, Funke, Rognes, SIAM J. Sci Comp. 2013

COFFEE: Optimisation of kernels

```
void helmholtz(double A[3][3], double **coords) {
  // K, det = Compute Jacobian (coords)

  static const double W[3] = {...}
  static const double X_D10[3][3] = {{...}}
  static const double X_D01[3][3] = {{...}}

  for (int i = 0; i<3; i++)
    for (int j = 0; j<3; j++)
      for (int k = 0; k<3; k++)
        A[j][k] += ((Y[i][k]*Y[i][j]+
           +((K1*X_D10[i][k]+K3*X_D01[i][k])*(K1*X_D10[i][j]+K3*X_D01[i][j]))+
           +((K0*X_D10[i][k]+K2*X_D01[i][k])*(K0*X_D10[i][j]+K2*X_D01[i][j])))*
           *det*W[i]);
}
```

- Local assembly code generated by Firedrake for a Helmholtz problem on a 2D triangular mesh using Lagrange p = 1 elements.
- The local assembly operation computes a small dense submatrix
- Essentially computing (for example) integrals of flows across facets
- These are combined to form a global system of simultaneous equations capturing the discretised conservation laws expressed by the PDE

Luporini, Varbenescu et al, ACM TACO/HiPEAC 2015

COFFEE: Optimisation of kernels

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  static const double W[3] = {...}
  static const double X_D10[3][3] = {{...}}
  static const double X_D01[3][3] = {{...}}

  for (int i = 0; i<3; i++)
    for (int j = 0; j<3; j++)
      for (int k = 0; k<3; k++)
        A[j][k] += ((Y[i][k]*Y[i][j]+
           +((K1*X_D10[i][k]+K3*X_D01[i][k])*(K1*X_D10[i][j]+K3*X_D01[i][j]))+
           +((K0*X_D10[i][k]+K2*X_D01[i][k])*(K0*X_D10[i][j]+K2*X_D01[i][j])))*
           *det*W[i]);
}
```

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Luporini, Varbenescu et al, AC TACO/HiPEAC 2015

COFFEE: Optimisation of kernels

```
void helmholtz(double A[3][4], double **coords) {
  #define ALIGN __attribute__((aligned(32)))
  // K, det = Compute Jacobian (coords)

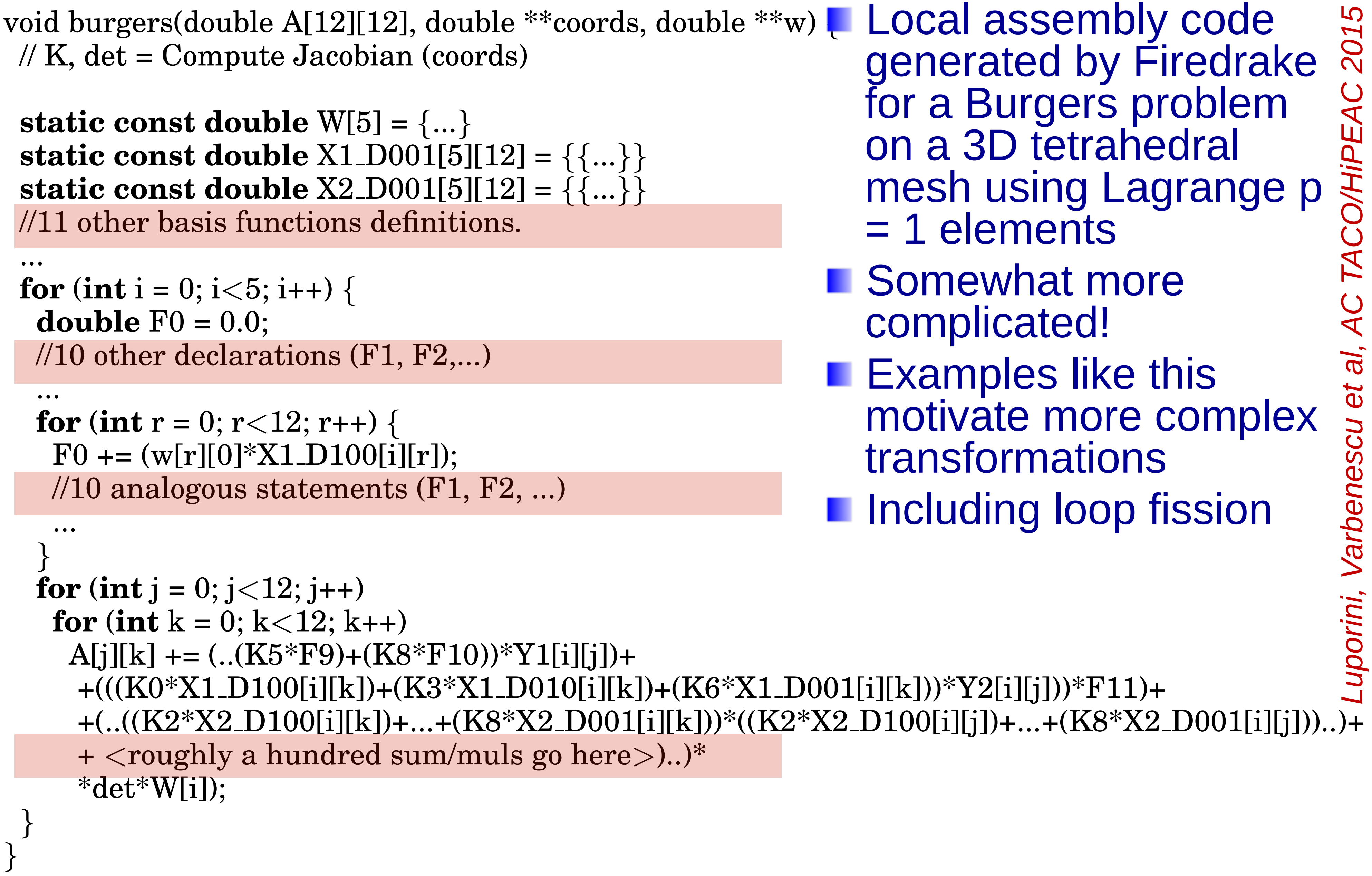
  static const double W[3] ALIGN = {...}
  static const double X_D10[3][4] ALIGN = {{...}}
  static const double X_D01[3][4] ALIGN = {{...}}

  for (int i = 0; i<3; i++) {
    double LI_0[4] ALIGN;
    double LI_1[4] ALIGN;
    for (int r = 0; r<4; r++) {
      LI_0[r] = ((K1*X_D10[i][r])+(K3*X_D01[i][r]));
      LI_1[r] = ((K0*X_D10[i][r])+(K2*X_D01[i][r]));
    }
    for (int j = 0; j<3; j++)
      #pragma vector aligned
      for (int k = 0; k<4; k++)
        A[j][k] += (Y[i][k]*Y[i][j]+LI_0[k]*LI_0[j]+LI_1[k]*LI_1[j])*det*W[i]);
  }
}
```

- Local assembly code for the Helmholtz problem after application of
  - padding,
  - data alignment,
  - Loop-invariant code motion
- In this example, sub-expressions invariant to j are identical to those invariant to k, so they can be precomputed once in the r loop

Luporini, Varbenescu et al, AC TACO/HiPEAC 2015

Kernels are often a lot more complicated



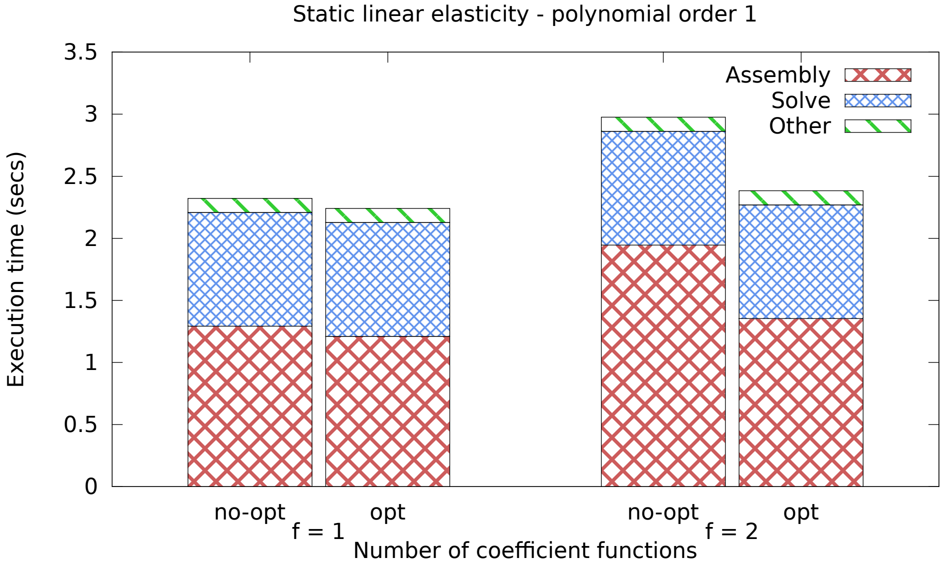
```
void burgers(double A[12][12], double **coords, double **w) {
  // K, det = Compute Jacobian (coords)

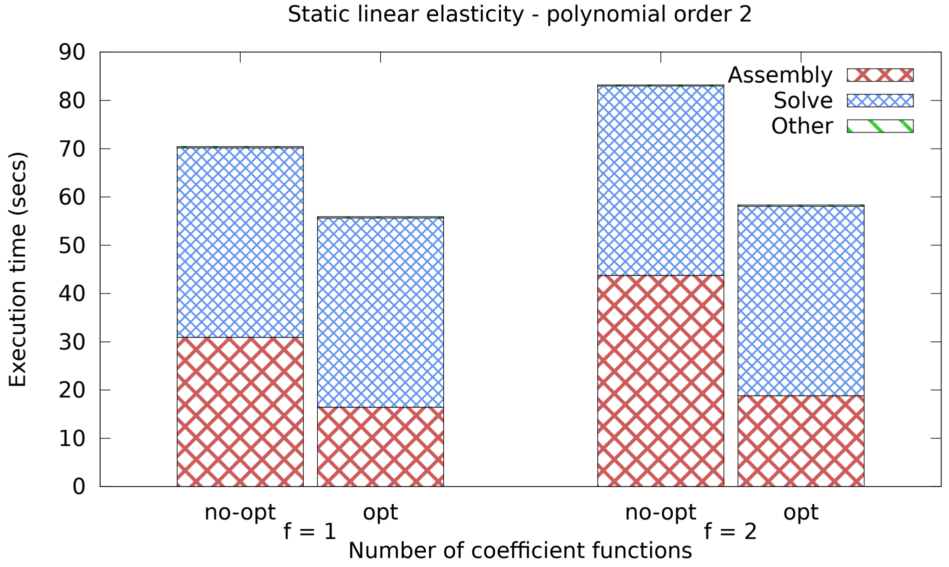
  static const double W[5] = {...}
  static const double X1_D001[5][12] = {{...}}
  static const double X2_D001[5][12] = {{...}}
  //11 other basis functions definitions.
  ...
  for (int i = 0; i<5; i++) {
    double F0 = 0.0;
    //10 other declarations (F1, F2,...)
    ...
    for (int r = 0; r<12; r++) {
      F0 += (w[r][0]*X1_D100[i][r]);
      //10 analogous statements (F1, F2, ...)
      ...
    }
    for (int j = 0; j<12; j++)
      for (int k = 0; k<12; k++)
        A[j][k] += (..(K5*F9)+(K8*F10))*Y1[i][j])+
         +(((K0*X1_D100[i][k])+(K3*X1_D010[i][k])+(K6*X1_D001[i][k]))*Y2[i][j]))*F11)+
         +(..((K2*X2_D100[i][k])+...+(K8*X2_D001[i][k]))*((K2*X2_D100[i][j])+...+(K8*X2_D001[i][j]))..)+
         + <roughly a hundred sum/muls go here>)..)*
         *det*W[i]);
  }
}
```

- Local assembly code generated by Firedrake for a Burgers problem on a 3D tetrahedral mesh using Lagrange p = 1 elements
- Somewhat more complicated!
- Examples like this motivate more complex transformations
- Including loop fission

Luporini, Varbenescu et al, AC TACO/HiPEAC 2015

COFFEE: Performance impact





- Fairly serious, realistic example: static linear elasticity, p=2 tetrahedral mesh, 196608 elements
- Including both assembly time and solve time
- Single core of Intel Sandy Bridge
- Compared with Firedrake loop nest compiled with Intel’s icc compiler version 13.1
- At low p, matrix insertion overheads dominate assembly time
- At higher p, and with more coefficient functions (f=2), we get up to 1.47x overall application speedup

Luporini, Varbenescu et al, AC TACO/HiPEAC 2015

COFFEE

- **Where did the domain-specific advantage come from?**
  - Finite-element assembly kernels have complex structure
  - With rich loop-invariant expression structure
  - And simple dependence structure

  - COFFEE generates C code that we feed to the best available compiler
  - COFFEE's transformations make this code run faster
  - COFFEE does not use any semantic information not available to the C compiler
    - But it does make better decisions
    - For the loops we're interested in

Luporini, Varbenescu et al, AC TACO/HiPEAC 2015

Where did the domain-specific advantage come from?

```
int A[100];
int x=0, y=0;
for (int i=0; i<100; i++) {
  for (int j=0; j<100; j++) {
    x+=A[i][i]*A[n-i][n-i];
    y+=A[j][n-j]*A[n-j][j];
  }
}
```

y is variant in j, but recomputed on each i iteration

```
int A[100];
int x=0, y=0;
int t1[100];
for (int j=0; j<100; j++) {
  t1[j]=A[j][n-j]*A[n-j][j];
}
for (int i=0; i<100; i++) {
  int t2 = A[i][i]*A[n-i][n-i];
  for (int j=0; j<100; j++) {
    x+=t2;
    y+=t1;
  }
}
```

x is invariant in j – interchange doesn't help

Paul Colea, MSc thesis, Imperial

- COFFEE does “generalised” loop-invariant code motion (GLICM)
- *“an expression in a loop L is invariant with respect to a parent loop P if each of its operands is*
  - *defined outside of P,*
  - *or is the induction variable of L,*
  - *or is the induction variable of a superloop of L which is also a subloop of P.”*
- We have an implementation for LLVM… preliminary evaluation suggests rather few general C programs benefit from GLICM

Conclusions

- Where do DSO opportunities come from?
  - Domain semantics (eg in SPIRAL)
  - Domain expertise (eg we know that inspector-executor will pay off)
  - Domain idiosyncracies (eg for GLICM)
  - Transforming at the right representation
    - Eg fusing linear algebra ops instead of loops
  - Data abstraction (eg AoS vs SoA)
    - Or whether to build the global system matrix (in instead to use a matrix-free or local-assembly scheme)
- Runtime code generation is liberating
  - **We do not try to do static analysis on client code**
  - **We encourage client code to use powerful abstractions**

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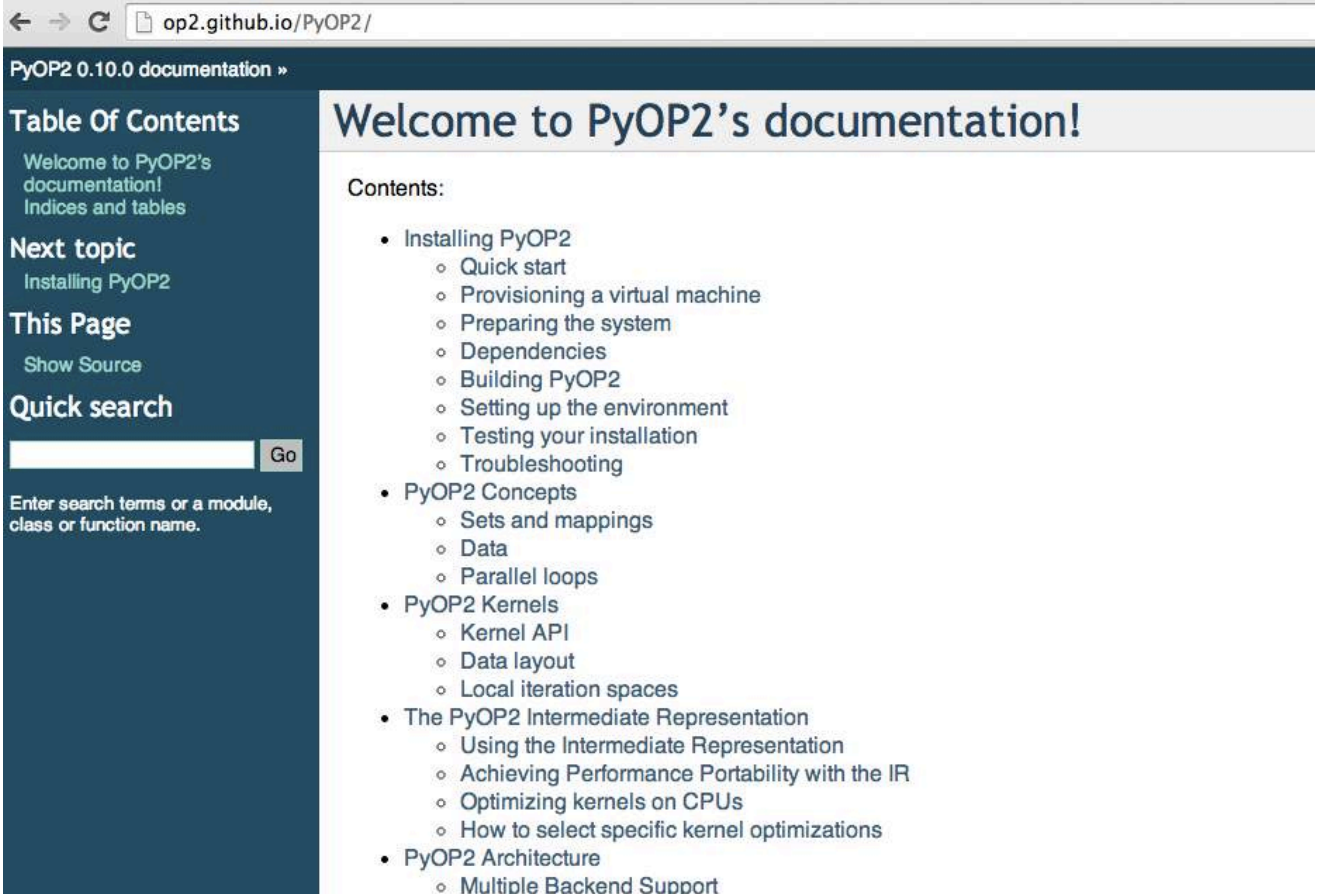
- EPSRC “Custom Computing” Platform Grant (EP/I012036/1)
- AMD, Codeplay, Maxeler Technologies

- Code:
  - http://www.firedrakeproject.org/
  - http://op2.github.io/PyOP2/

Imperial College
London

PyOP2 is on github



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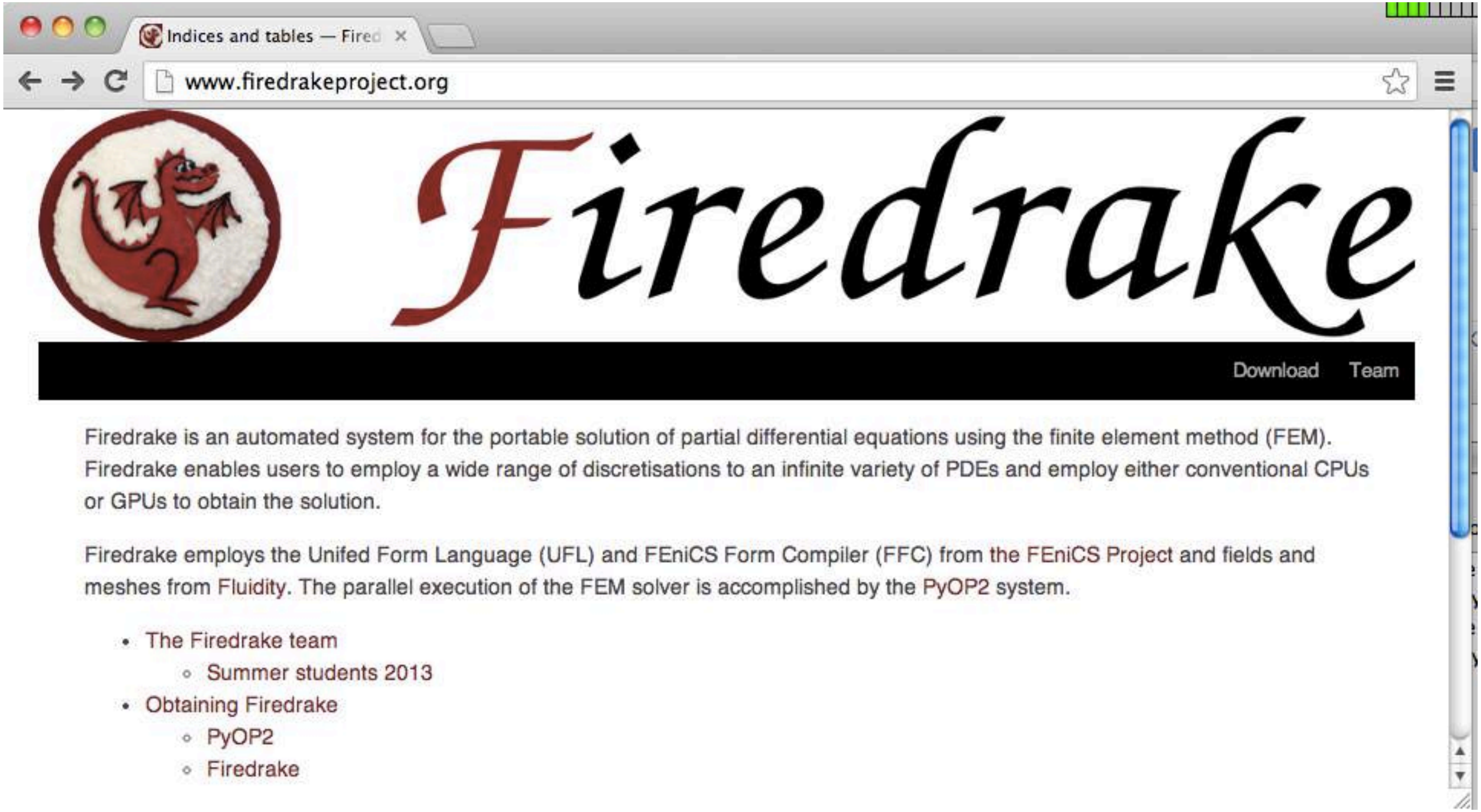
Firedrake is on github



Firedrake is an automated system for the portable solution of partial differential equations using the finite element method (FEM). Firedrake enables users to employ a wide range of discretisations to an infinite variety of PDEs and employ either conventional CPUs or GPUs to obtain the solution.

Firedrake employs the Unifed Form Language (UFL) and FEniCS Form Compiler (FFC) from the FEniCS Project and fields and meshes from Fluidity. The parallel execution of the FEM solver is accomplished by the PyOP2 system.

- The Firedrake team
  - Summer students 2013
- Obtaining Firedrake
  - PyOP2
  - Firedrake

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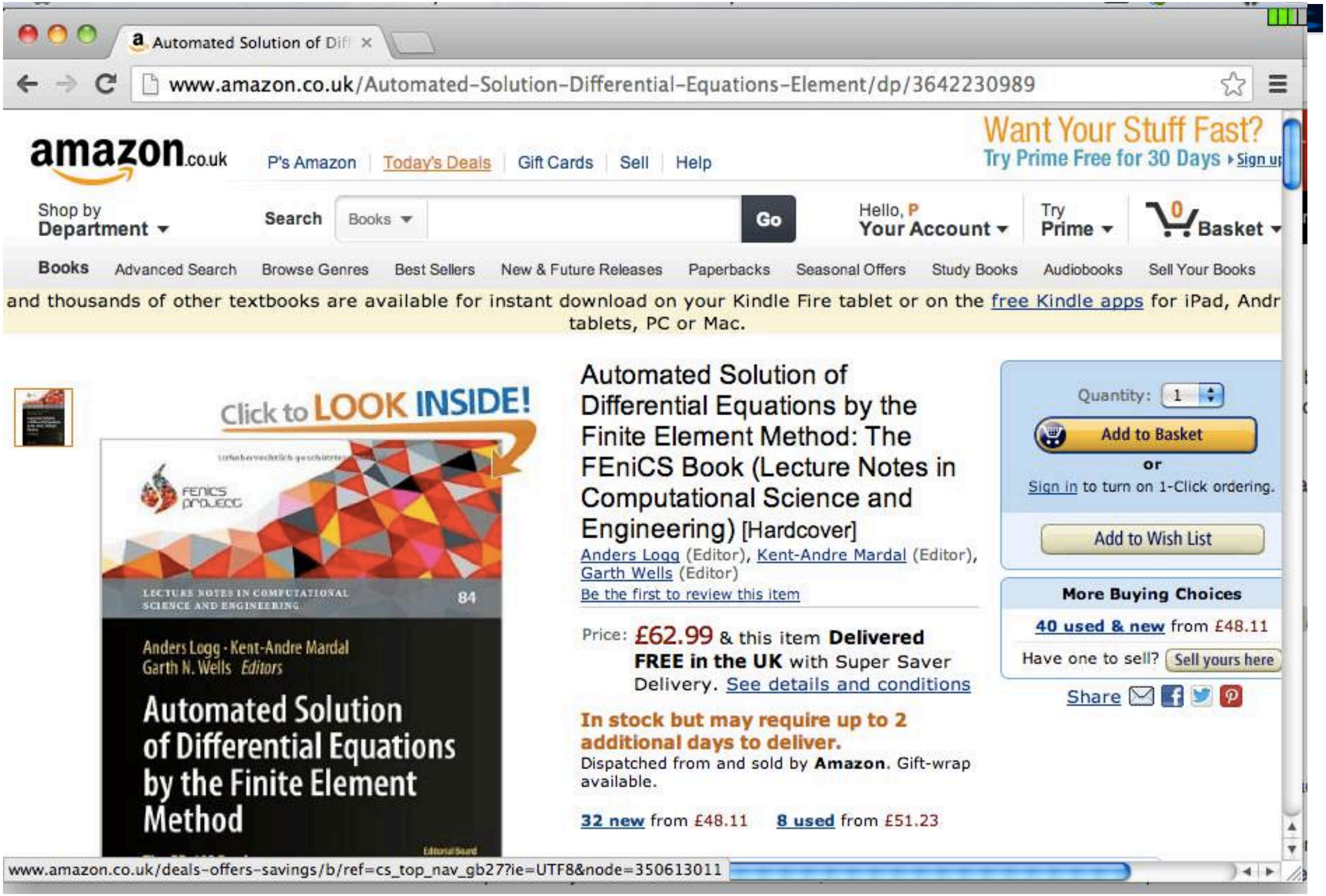
The FEniCS project... The book



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Abstraction…

- computer science is a science of abstraction — creating the right model for thinking about a problem and devising the appropriate mechanizable techniques to solve it

(Aho and Ullman, Foundations of Computer Science, Ch1, http://infolab.stanford.edu/~ullman/focs.html)