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Synthesis versus analysis: what do we actually gain from domain-specificity?

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Doru Bercea, Fabio Luporini, Graham Markall, Lawrence Mitchell, Florian Rathgeber, Francis Russell, George Rokos, Paul Colea (Software Perf Opt Group, Imperial Computing)
Spencer Sherwin (Aeronautics, Imperial), Chris Cantwell (Cardio-mathematics group, Mathematics, Imperial)
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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?

Have your cake and eat it too

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  - raise the level at which programmers can reason about code,
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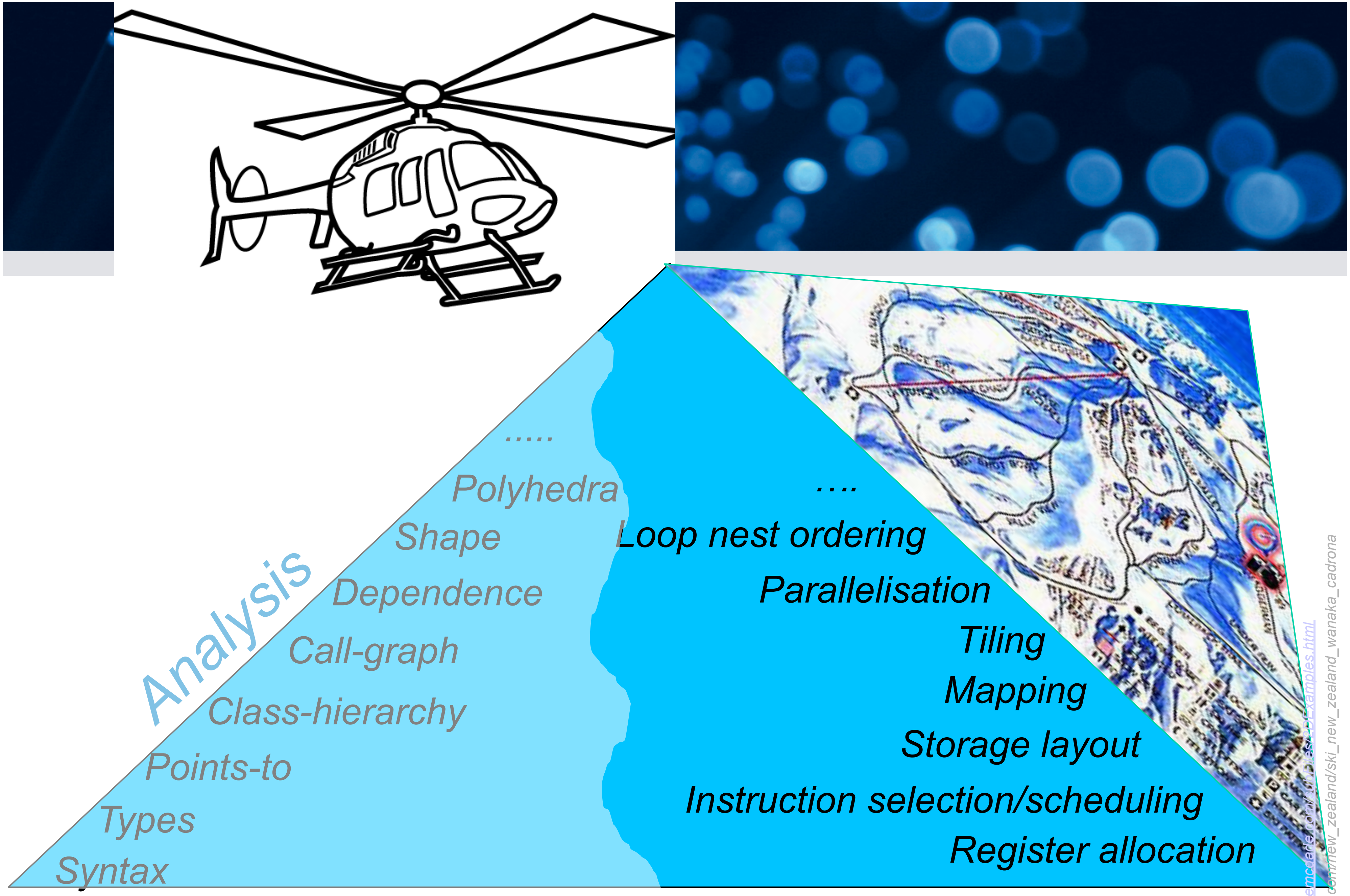
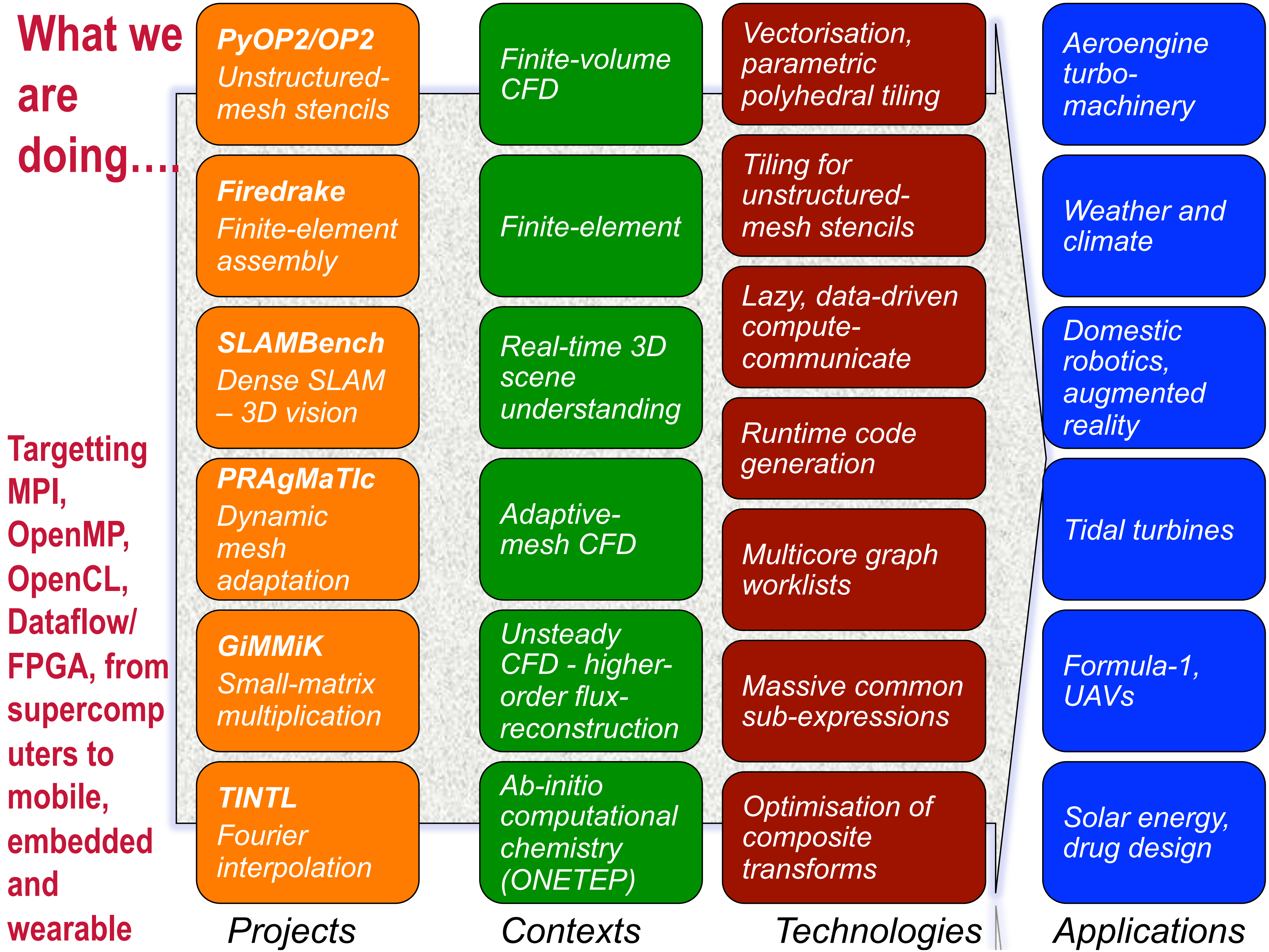


- Compilation is like skiing
- Analysis is not always the interesting part....

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



What we are doing….
Targetting MPI, OpenMP, OpenCL, Dataflow/ FPGA, from supercomputers to mobile, embedded and wearable
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
Finite-volume CFD
Finite-element
Real-time 3D scene understanding
Adaptive-mesh CFD
Unsteady CFD - higher-order flux-reconstruction
Ab-initio computational chemistry (ONETEP)
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
Aeroengine turbo-machinery
Weather and climate
Domestic robotics, augmented reality
Tidal turbines
Formula-1, UAVs
Solar energy, drug design
Projects
Contexts
Technologies
Applications

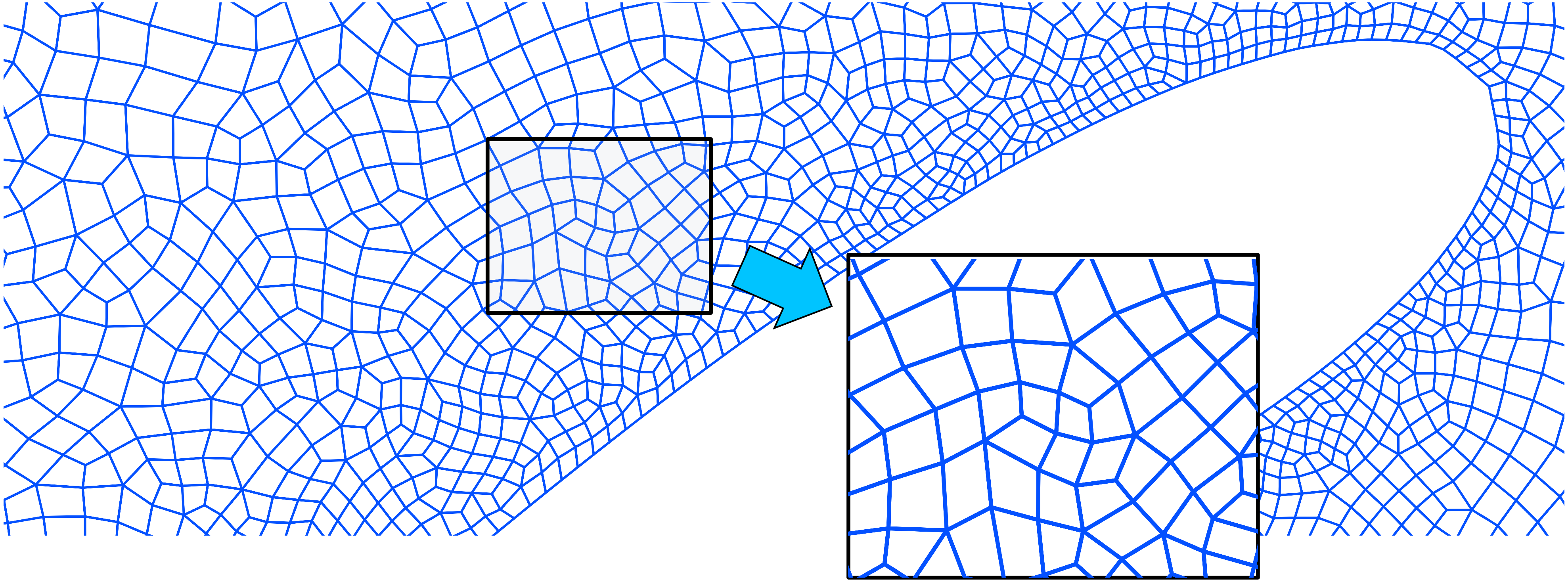
This talk

- 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?

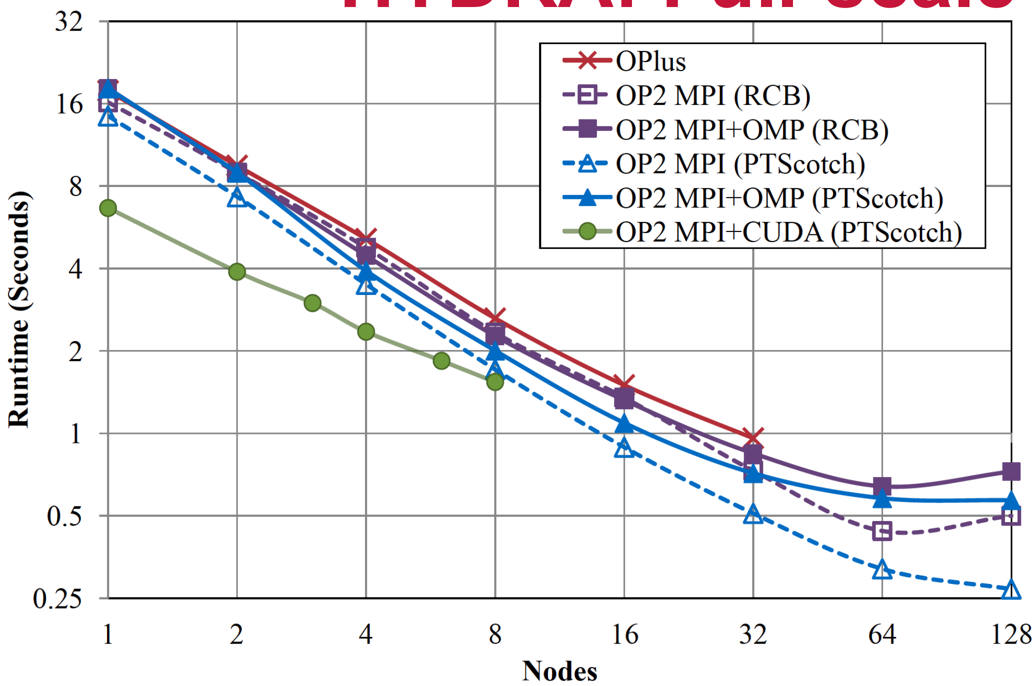


- Unstructured meshes require pointers/indirection because adjacency lists have to be represented explicitly
- A controlled form of pointers

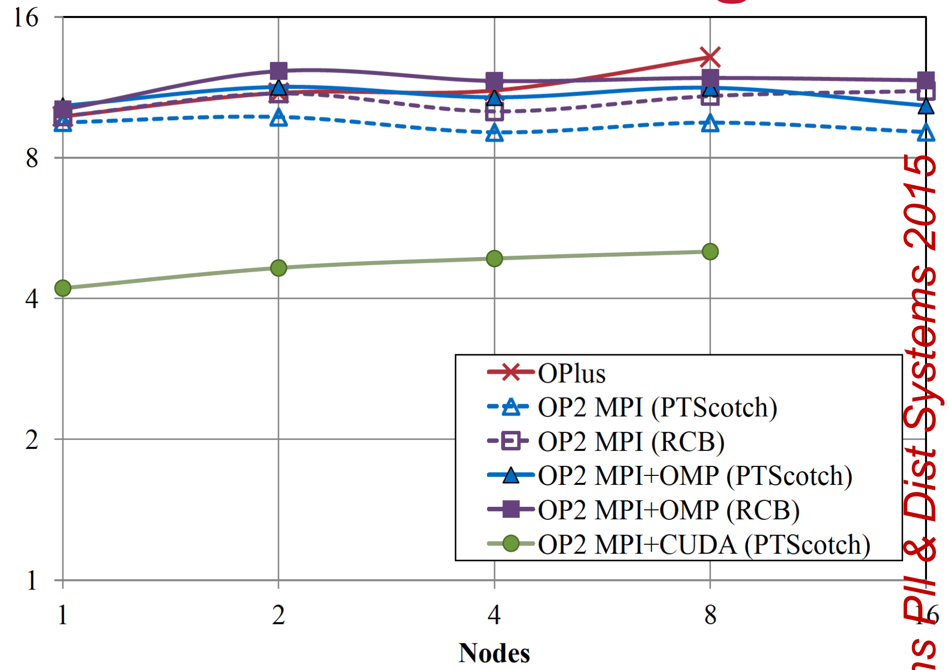
- **OP2** is a C++ and Fortran library for parallel loops over the mesh implemented by source-to-source transformation
- **PyOP2** is an major extension implemented in Python using runtime code generation

- 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

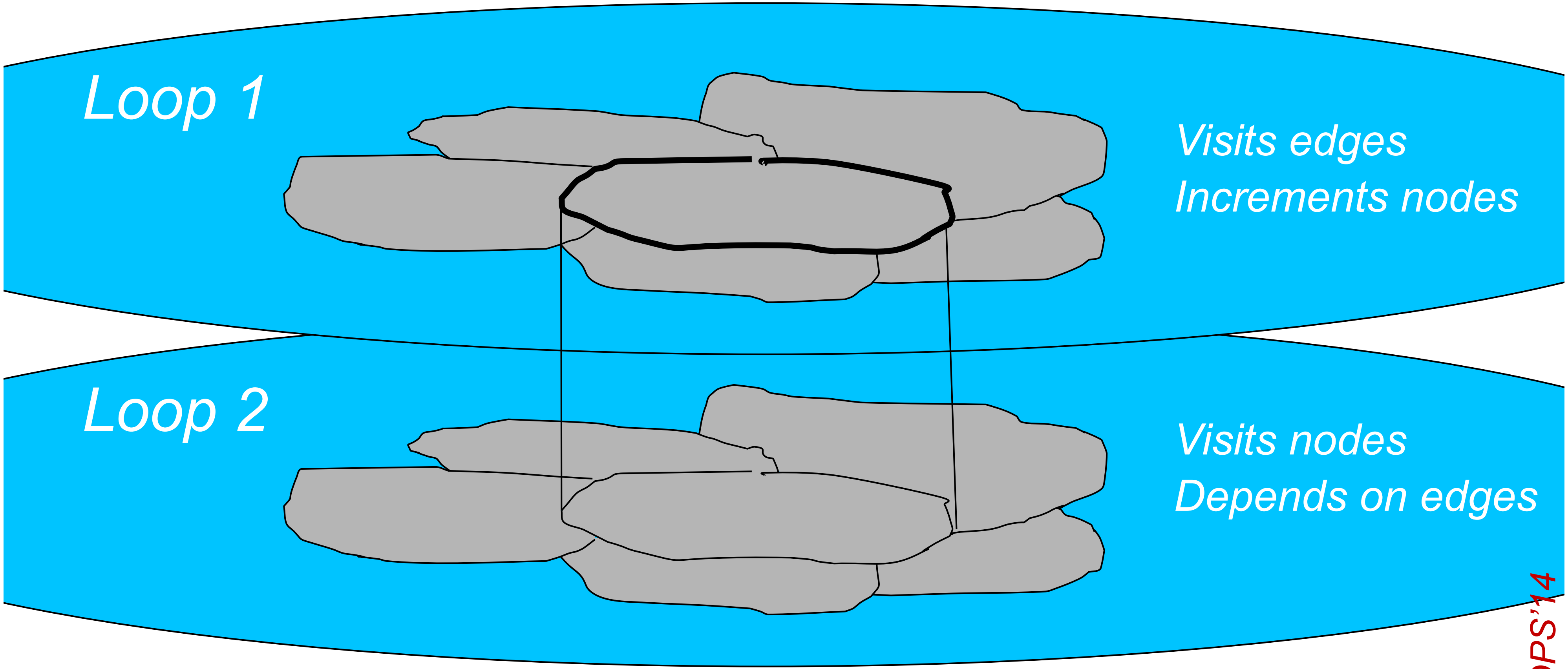
Reguly, Mudalige et al, IEEE Trans PDS 2015

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

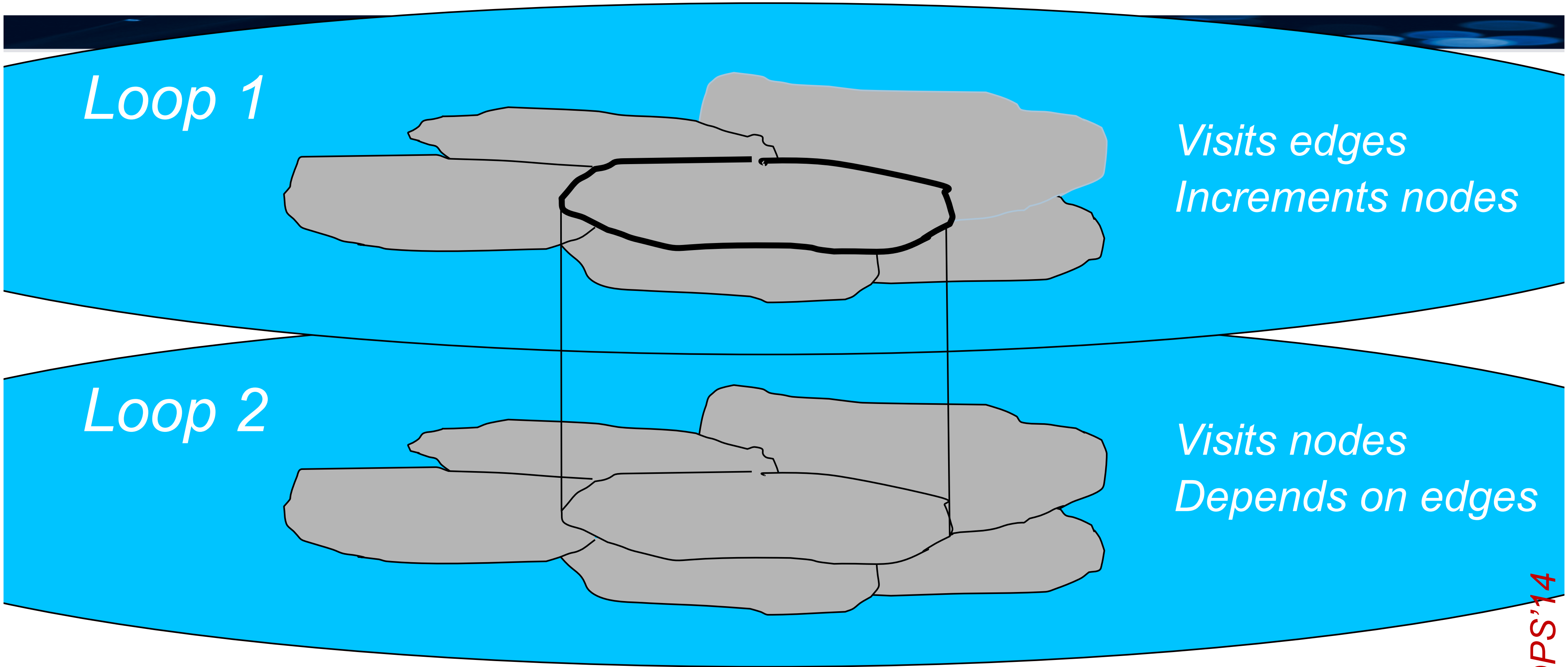
Sparse split tiling on an unstructured mesh, for locality



- 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

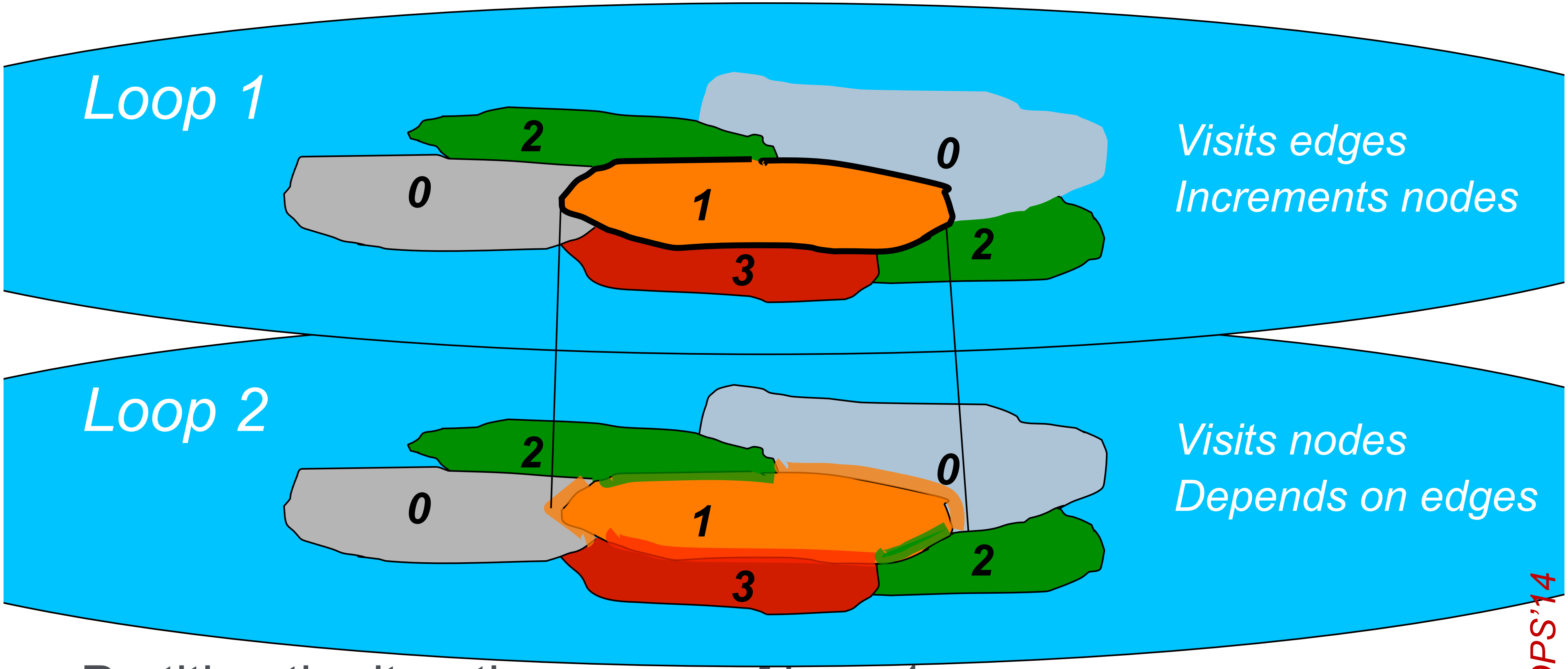
Sparse split tiling



- Partition the iteration space of loop 1

Strout, Luporini et al, IPDPS'14

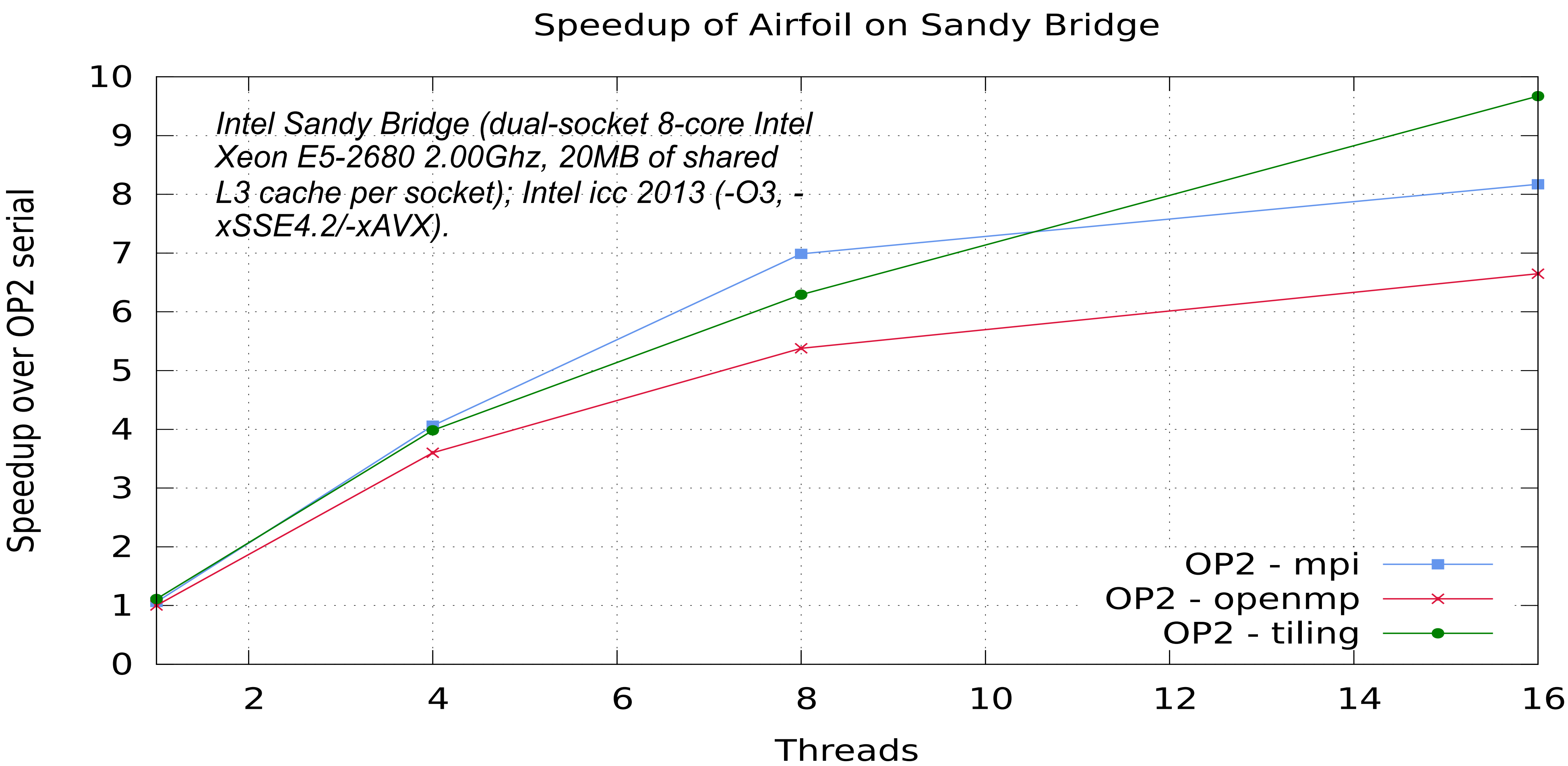
Sparse split tiling



- 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



- *Mesh size = 1.5M edges*
- *# Loop chain = 6 loops*
- *No inspector/plans overhead*
- *Airfoil test problem*
- *Unstructured-mesh finite-volume*

- **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

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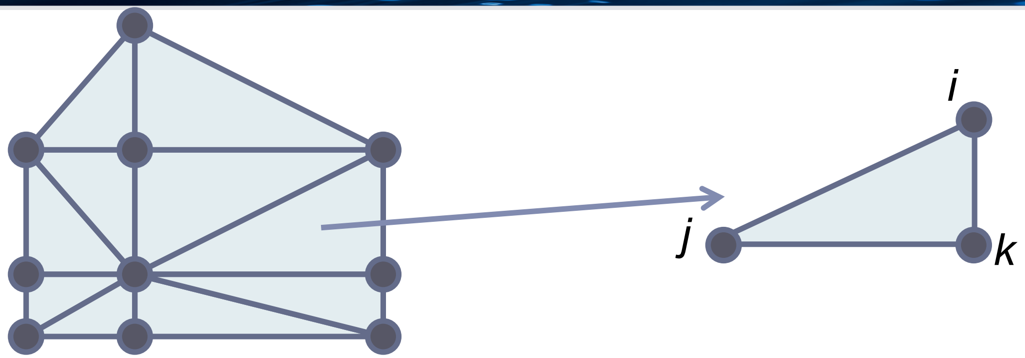
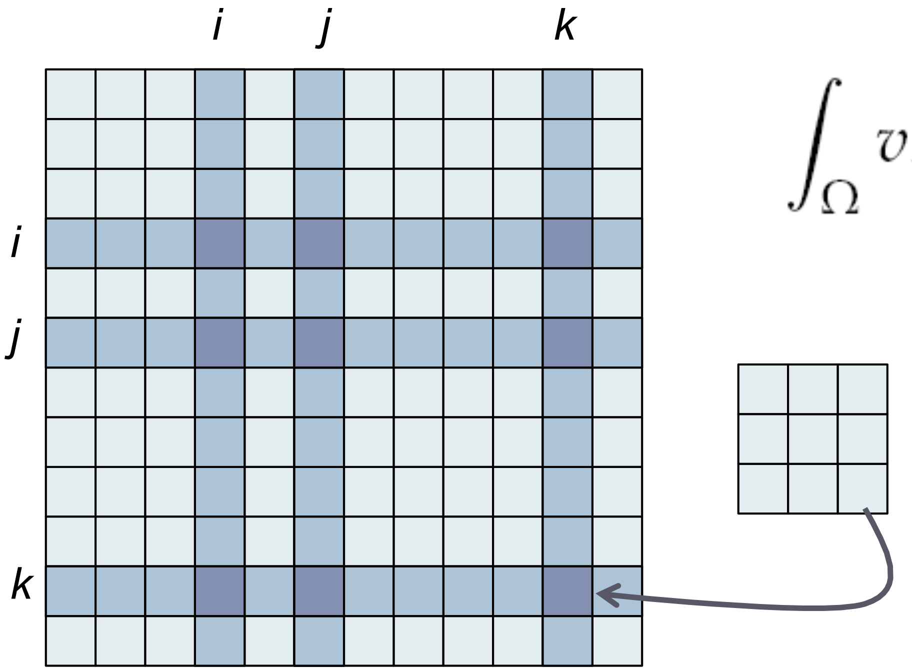
The finite element method in outline

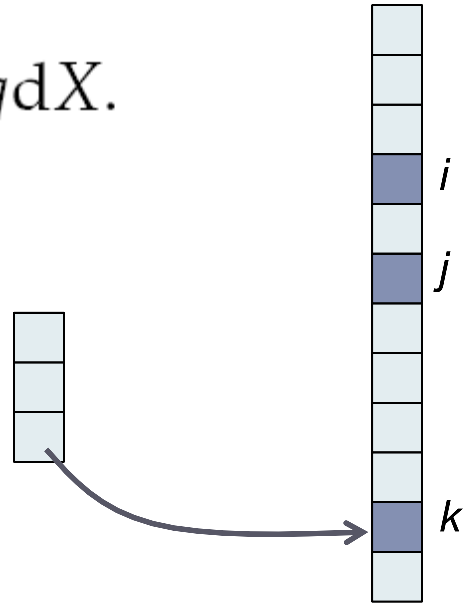



```
do element = 1,N
  assemble(element)
end do
```



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

$$Ax = b$$



- 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

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

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

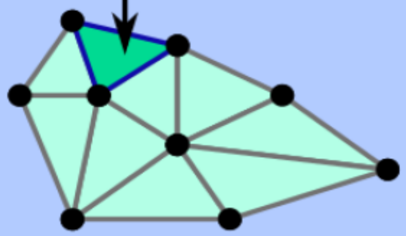
can be represented in UFL as

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]);
}
```

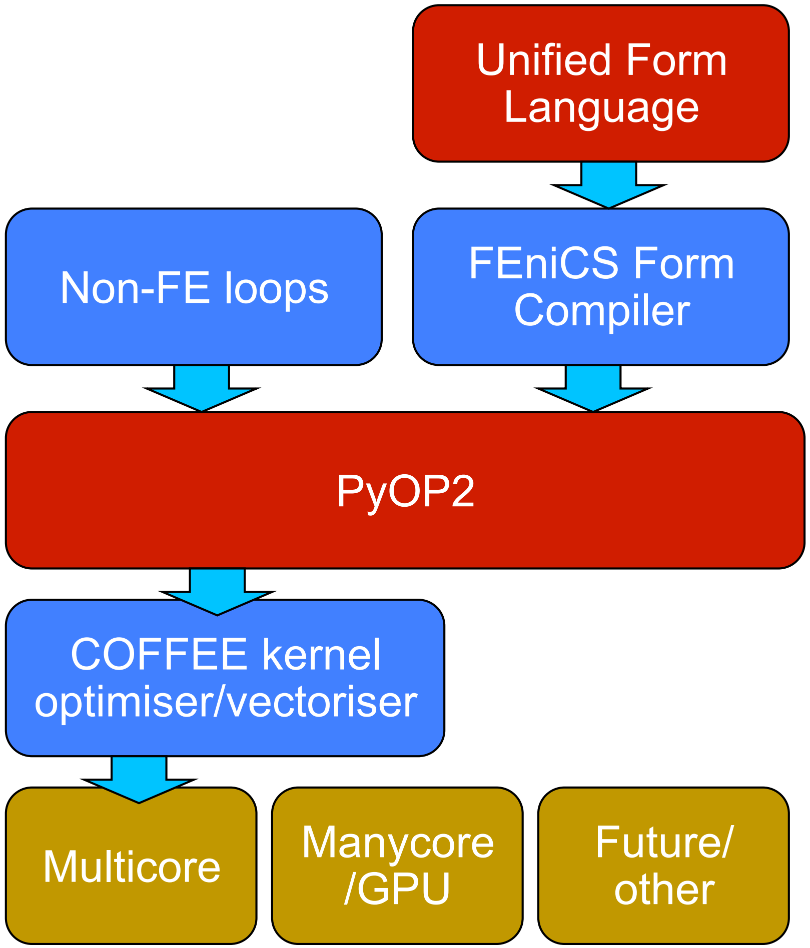


parallel loop
over all grid cells,
in unspecified order,
partitioned

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

```
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

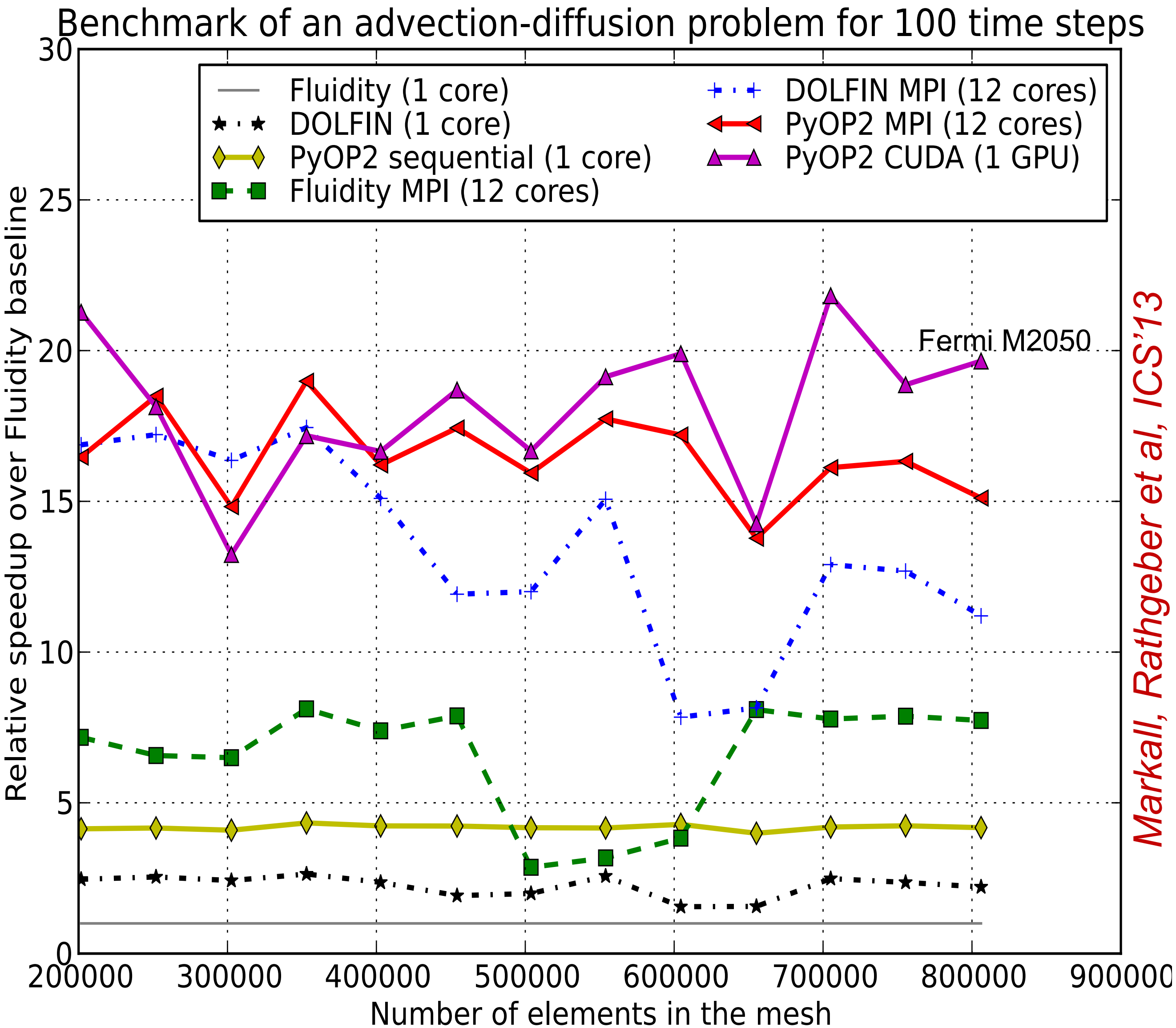
solve(M == adv, t)                        # Solve advection
solve(D == diff, t)                       # Solve diffusion
```

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

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

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:

$$
\begin{tikzcd}
\boxed{\text{discrete forward equations}} \arrow[r, "\text{implement model by hand}"] & \boxed{\text{forward code}} \arrow[d, "\text{algorithmic differentiation}"'] \\
 & \boxed{\text{adjoint code}}
\end{tikzcd}
$$

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

$$
\begin{tikzcd}
\boxed{\text{discrete forward equations}} \arrow[r, "\text{FEniCS/Firedrake}"] \arrow[d, "\text{libadjoint}"'] & \boxed{\text{forward code}} \\
\boxed{\text{discrete adjoint equations}} \arrow[r, "\text{FEniCS/Firedrake}"] & \boxed{\text{adjoint code}}
\end{tikzcd}
$$

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

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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

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Kernels are often a lot more complicated

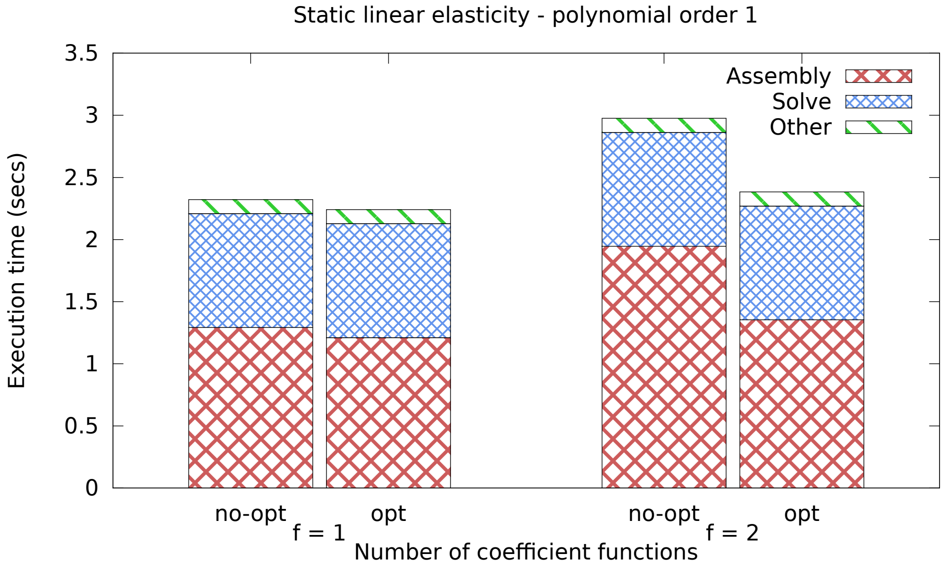
```
void burgers(double A[12][12], double **coords, double **w) {
  // K, det = Compute Jacobian (coords)

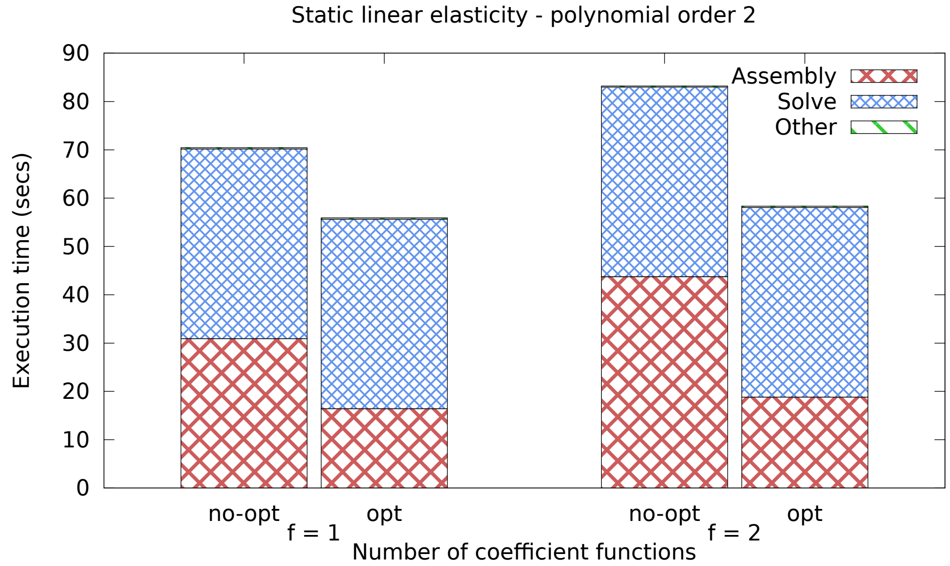
  static const double W[5] = {...}
  static const double X1_D001[5][12] = {{...}}
  static const double X2_D001[5][12] = {{...}}
  //11 other basis functions definitions.
  ...
  for (int i = 0; i<5; i++) {
    double F0 = 0.0;
    //10 other declarations (F1, F2,...)
    ...
    for (int r = 0; r<12; 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





Luporini, Varbenescu et al, AC TACO/HiPEAC 2015

- 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

- **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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- AMD, Codeplay, Maxeler Technologies

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

PyOP2 is on github

op2.github.io/PyOP2/

PyOP2 0.10.0 documentation »

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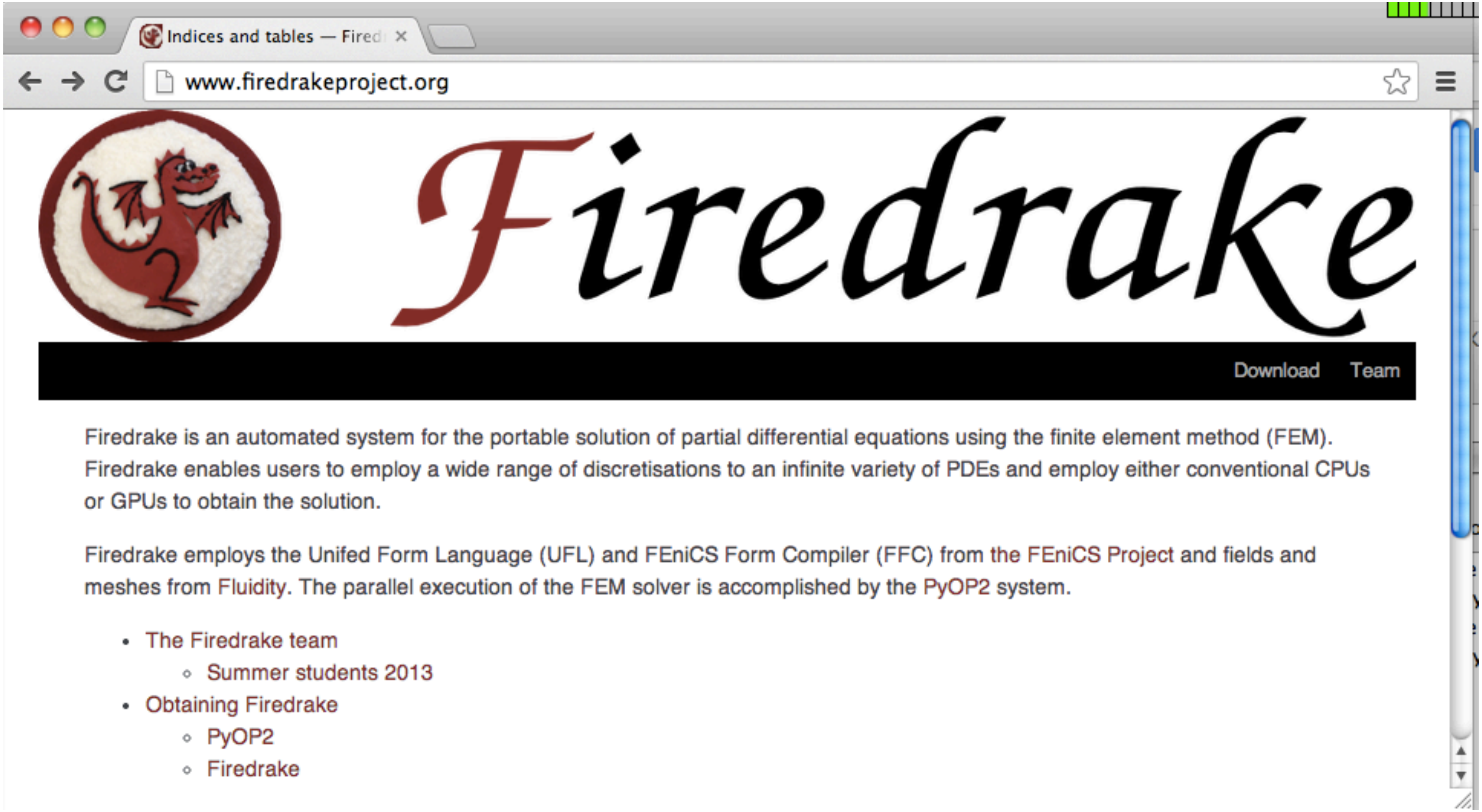

The FEniCS project... The book

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)