Imperial College London

Delivering and generalising domain-specific program optimisations

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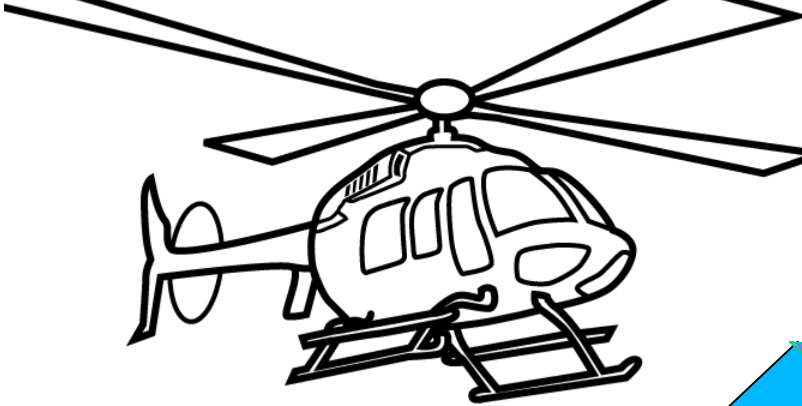
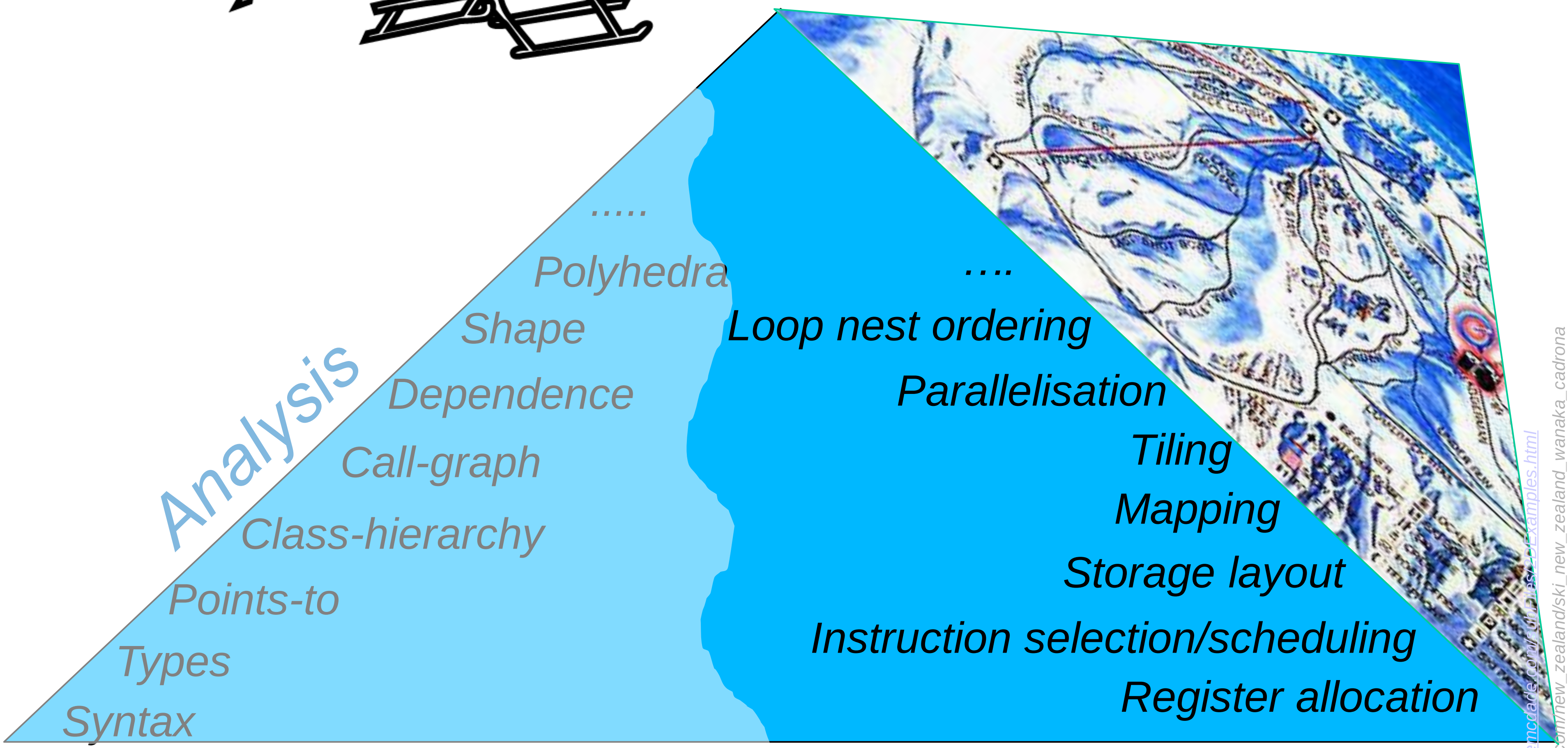
Carlo Bertolli (IBM Research), Ram Ramanujam (Louisiana State University)
Doru Thom Popovici, Franz Franchetti (CMU), Karl Wilkinson (Capetown), Chris–Kriton Skylaris (Southampton)



Compilation is like skiing



- Analysis is not always the interesting part....
- It's more fun the higher you start!

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

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

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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?

What we are doing….

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

Technologies

- *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*

Contexts

- *Finite difference*
- *Finite-volume*
- *Finite-element*
- *Real-time 3D scene understanding*
- *Adaptive-mesh CFD*
- *Unsteady CFD - higher-order flux-reconstruction*
- *Ab-initio computational chemistry (ONETEP)*

Projects

- ***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*

Applications

- *Aeroengine turbo-machinery*
- *Weather and climate*
- *Domestic robotics, augmented reality*
- *Tidal turbines*
- *Formula-1, UAVs*
- *Solar energy, drug design*

This talk

- What compilers can do
- What stops the compiler from doing what it can do
- What you might hope the compiler might do

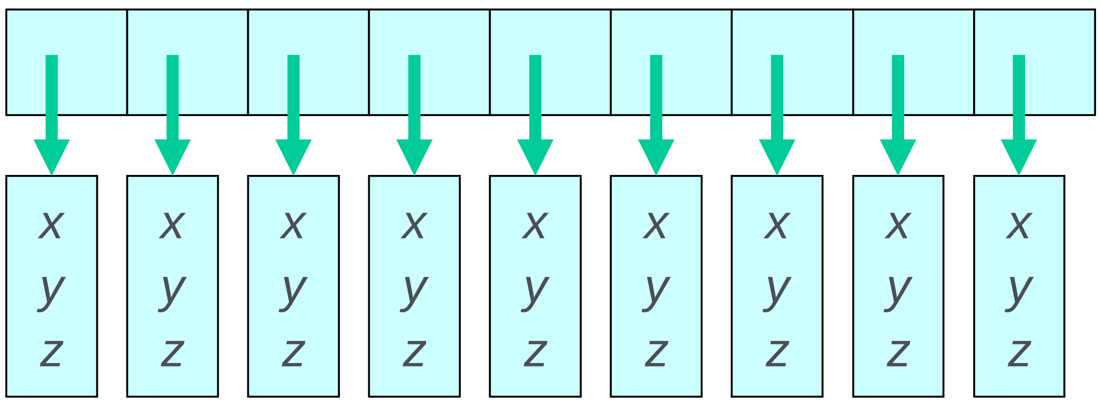
- Domain-specific optimisations
- Getting the abstraction right
- Delivering

Easy parallelism

Example:

```
for (i=0; i<N; ++i) {
  points[i]->x += 1;
}
```

- Can the iterations of this loop be executed in parallel?



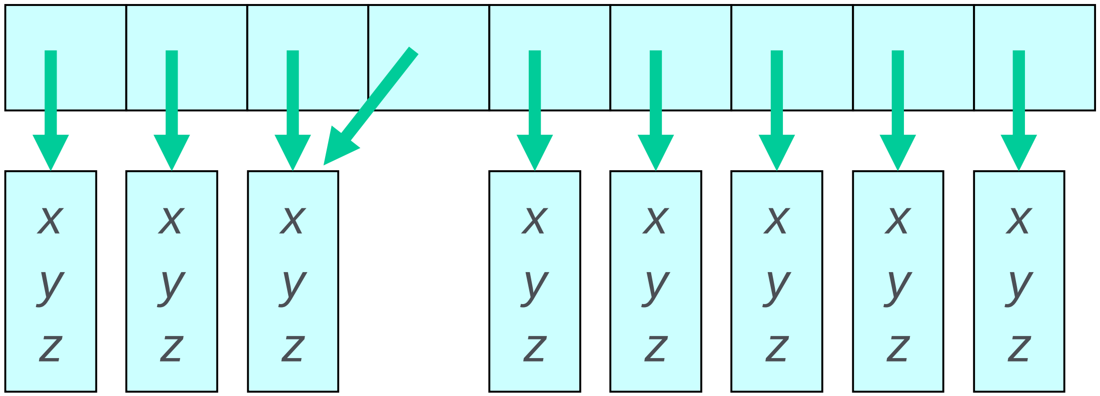
- No problem: each iteration is independent

Easy parallelism

Example:

```
for (i=0; i<N; ++i) {
  points[i]->x += 1;
}
```

- Can the iterations of this loop be executed in parallel?



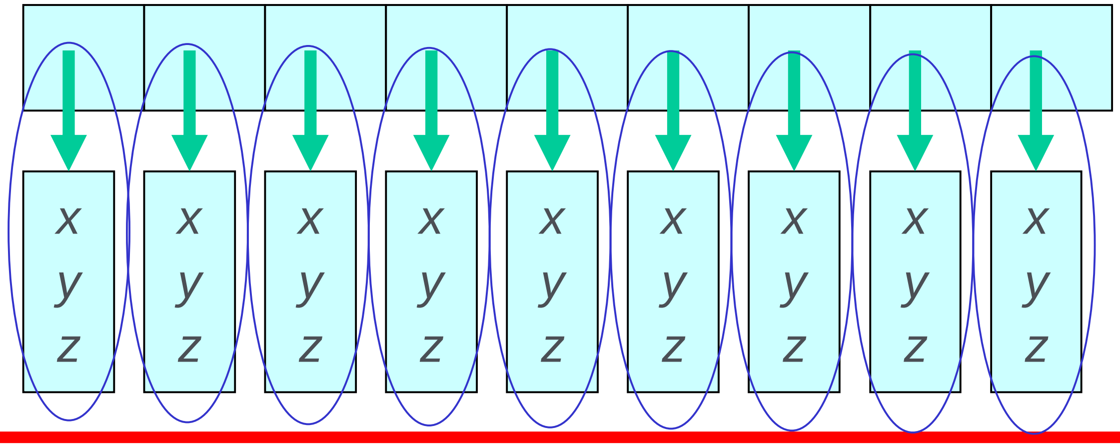
- Oh no: not all the iterations are independent!
  - You want to re-use piece of code in different contexts
  - Whether it's parallel depends on context!

Easy parallelism

Example:

```
for (i=0; i<N; ++i) {
  points[i]->x += 1;
}
```

- Can the iterations of this loop be executed in parallel?



Sergio Almeida's 1998 PhD thesis:

"Balloon types" ensure that each cell is reached only by its owner pointer – see also ownership in Rust

Points-to analysis

2006 PhD thesis work of David Pearce,
(based on Andersen'94)

```
int *f(int *p) {
  return p;
}
int g() {
  int x,y,*p,*q,**r,**s;
  s=&p;
  if(...) p=&x;
  else p=&y;
  r=s;
  q=f(*r);
}
```

(1) $f_* \supseteq f_p$

(2) $g_s \supseteq \{g_p\}$

(3) $g_p \supseteq \{g_x\}$

(4) $g_p \supseteq \{g_y\}$

(5) $g_r \supseteq g_s$

(6) $f_p \supseteq *g_r$

(7) $g_q \supseteq f_*$

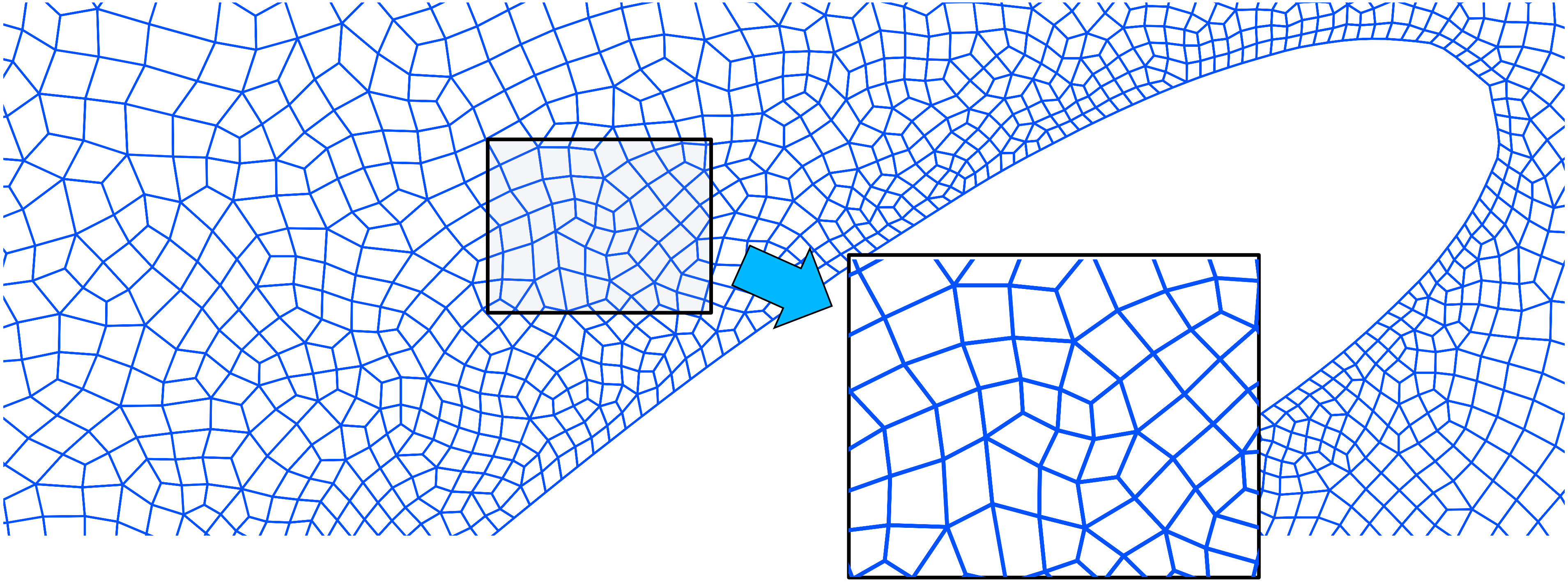
Variable s of function g might point to variable p of function g

R might point to anything s might point to

f's p might point to anything r might point to

q might point to anything f returns

- Goal: for each pointer variable (p,q,r,s), find the set of objects it might point to at runtime



- Unstructured meshes require pointers/indirection because adjacency lists have to be represented explicitly
- A controlled form of pointers (actually a general graph)

- **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

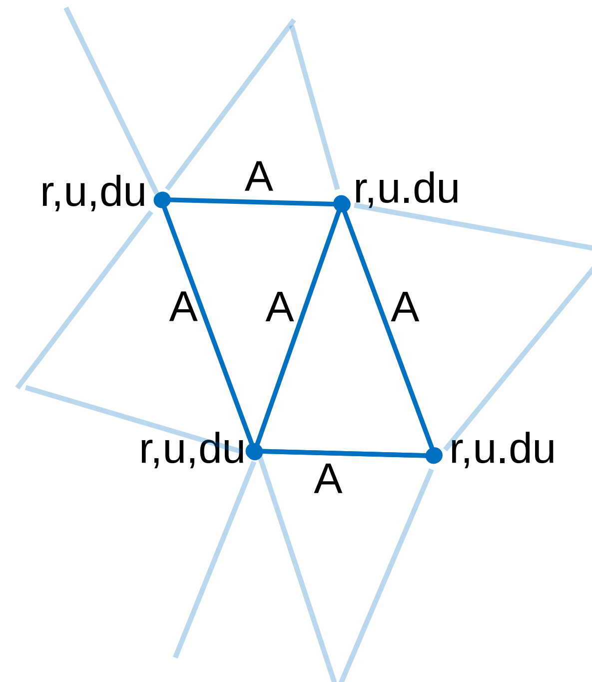
- Generates highly-optimised CUDA, OpenMP and MPI code

```
# declare sets, maps, and datasets
nodes = op2.Set(nnode)
edges = op2.Set(nedge)

ppedge = op2.Map(edges, nodes, 2, pp)

p_A = op2.Dat(edges, data=A)
p_r = op2.Dat(nodes, data=r)
p_u = op2.Dat(nodes, data=u)
p_du = op2.Dat(nodes, data=du)

# global variables and constants declarations
alpha = op2.Const(1, data=1.0, np.float32)
beta = op2.Global(1, data=1.0, np.float32)
```

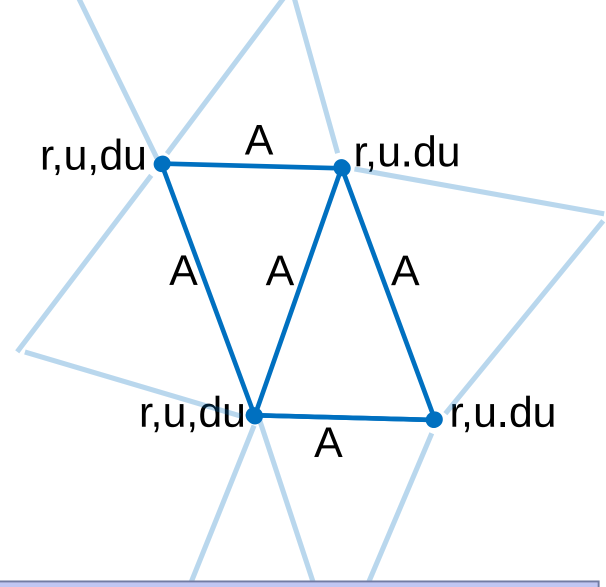


https://github.com/OP2/PyOP2/blob/master/demo/jacobi.py

Example – Jacobi solver

PyOP2: "decoupled access-execute"

- Parallel loops, over sets (nodes, edges etc)
- Access descriptors specify how to pass data to and from the C kernel
- The kernel operates only on local data




```
for iter in xrange(0, NITER):
    u_sum = op2.Global(1, data=0.0, np.float32)
    u_max = op2.Global(1, data=0.0, np.float32)
    op2.par_loop(res, edges,
                 p_A(op2.READ),
                 p_u(op2.READ, ppedge[1]),
                 p_du(op2.INC, ppedge[0]),
                 beta(op2.READ))

    op2.par_loop(update, nodes,
                 p_r(op2.READ),
                 p_du(op2.RW),
                 p_u(op2.INC),
                 u_sum(op2.INC),
                 u_max(op2.MAX))
```

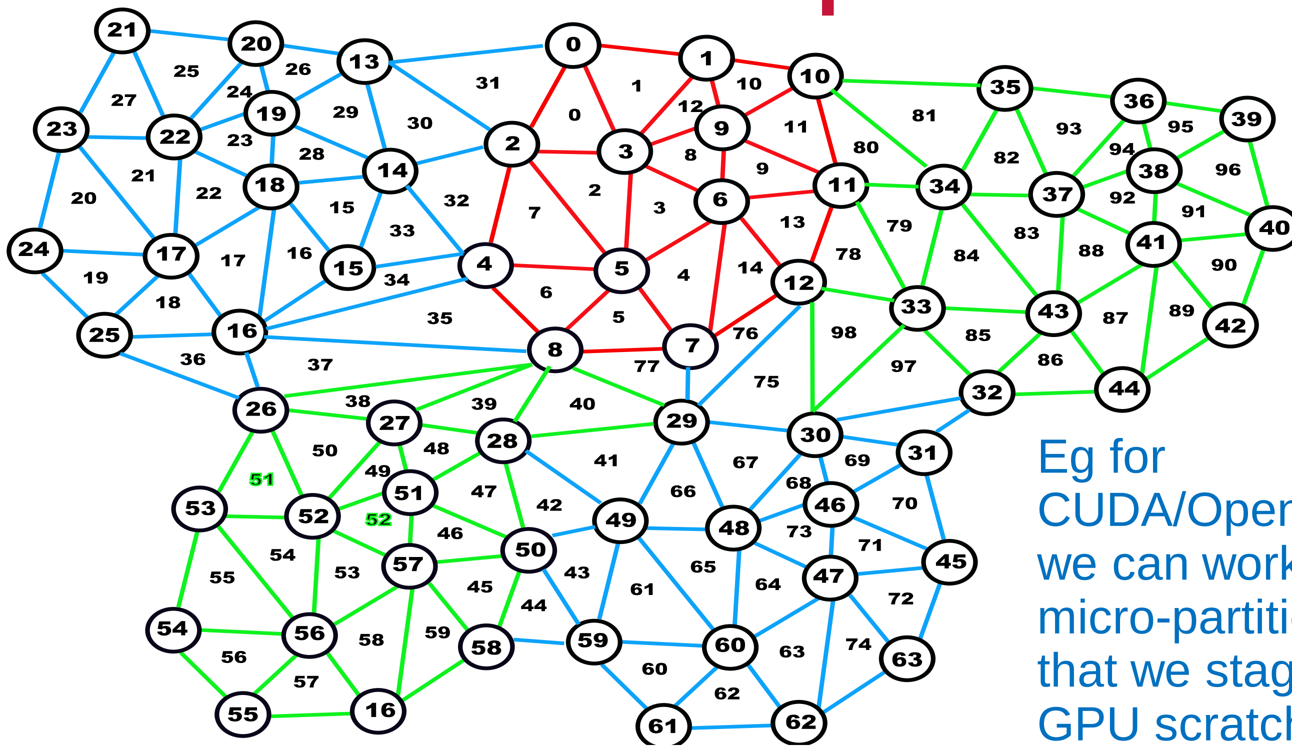
Access descriptors specify how to feed the kernel from the mesh

```
void res(float *A, float *u, float *du,
         const float *beta) {
  *du += (*beta) * (*A) * (*u);
}
```

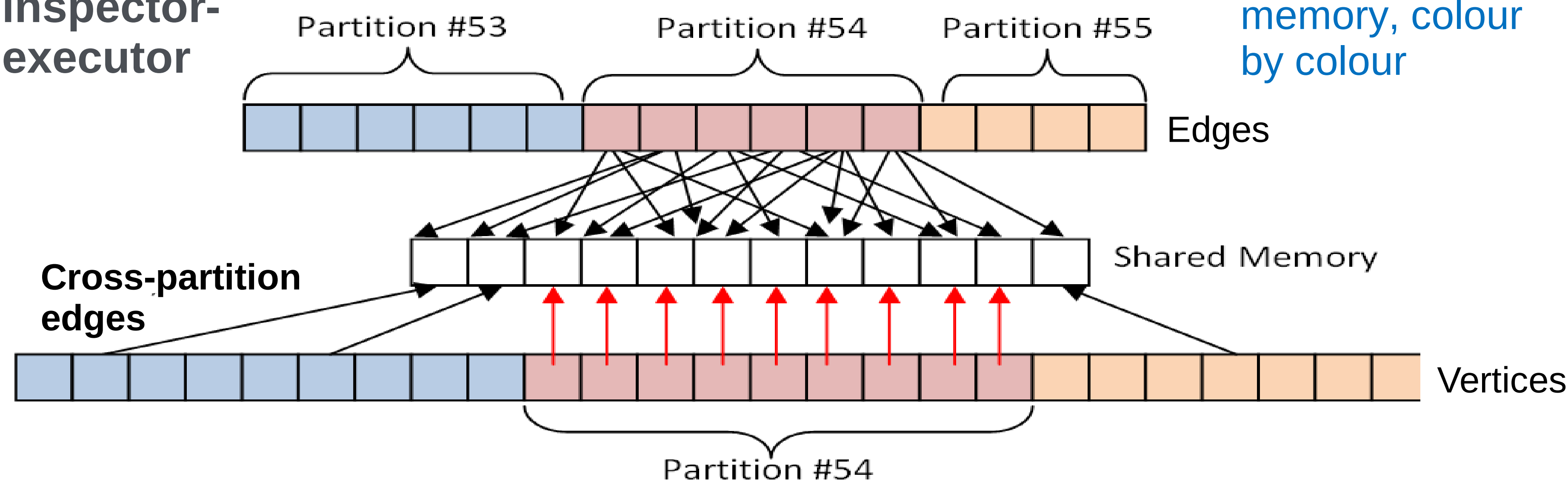
```
void update(float *r, float *du, float *u, float
       *u_sum, float *u_max) {
  *u += *du + alpha * (*r);
  *du = 0.0f;
  *u_sum += (*u) * (*u);
  *u_max = *u_max > *u ? *u_max : *u;
}
```

Code generation for indirect loops in OP2

- Supports diverse code generation schemes
- For MPI, OpenMP, GPU, and in prototype form for FPGA
- Key idea: **inspector-executor**

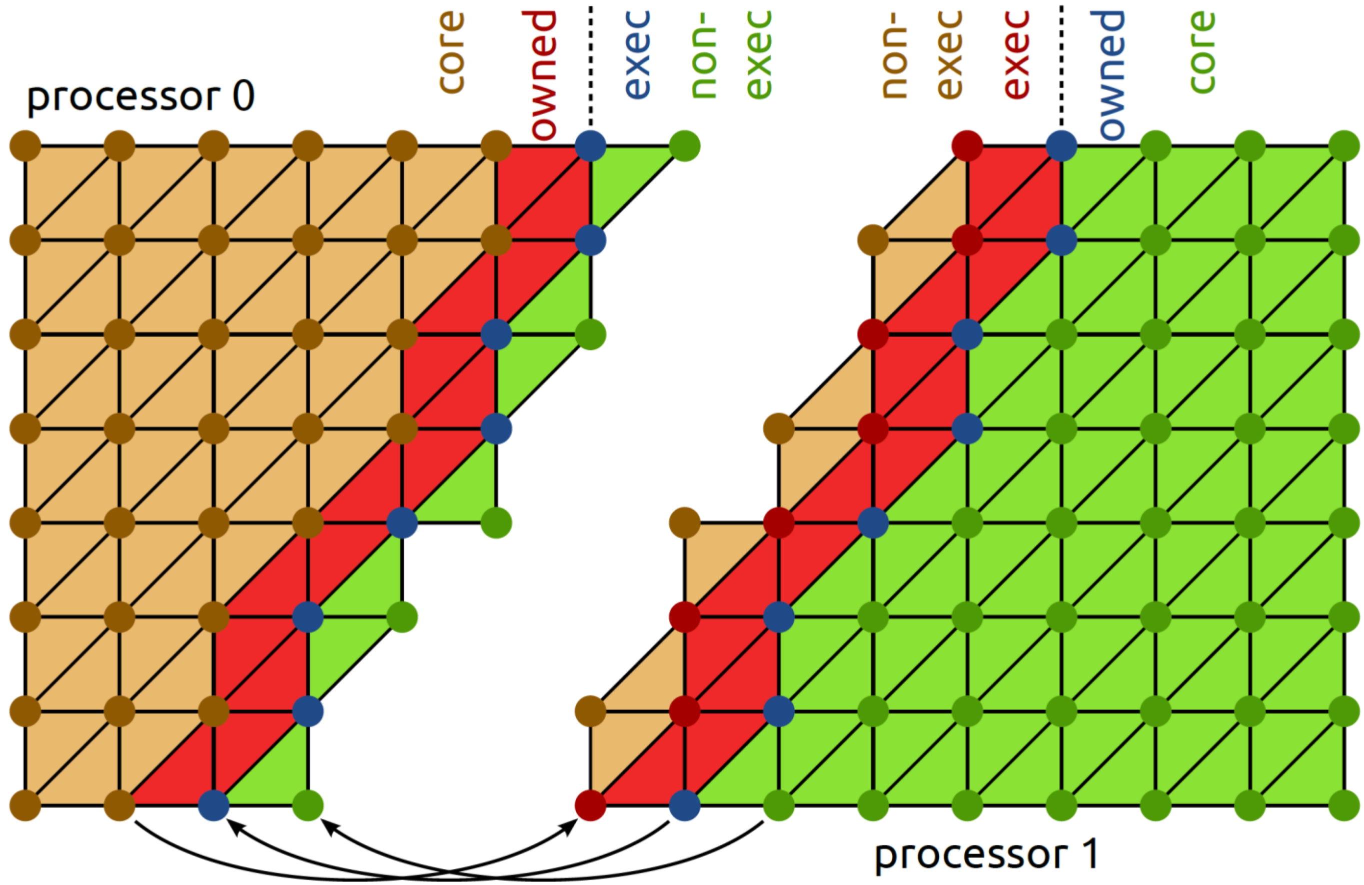


Eg for CUDA/OpenCL we can work with micro-partitions that we stage into GPU scratchpad memory, colour by colour



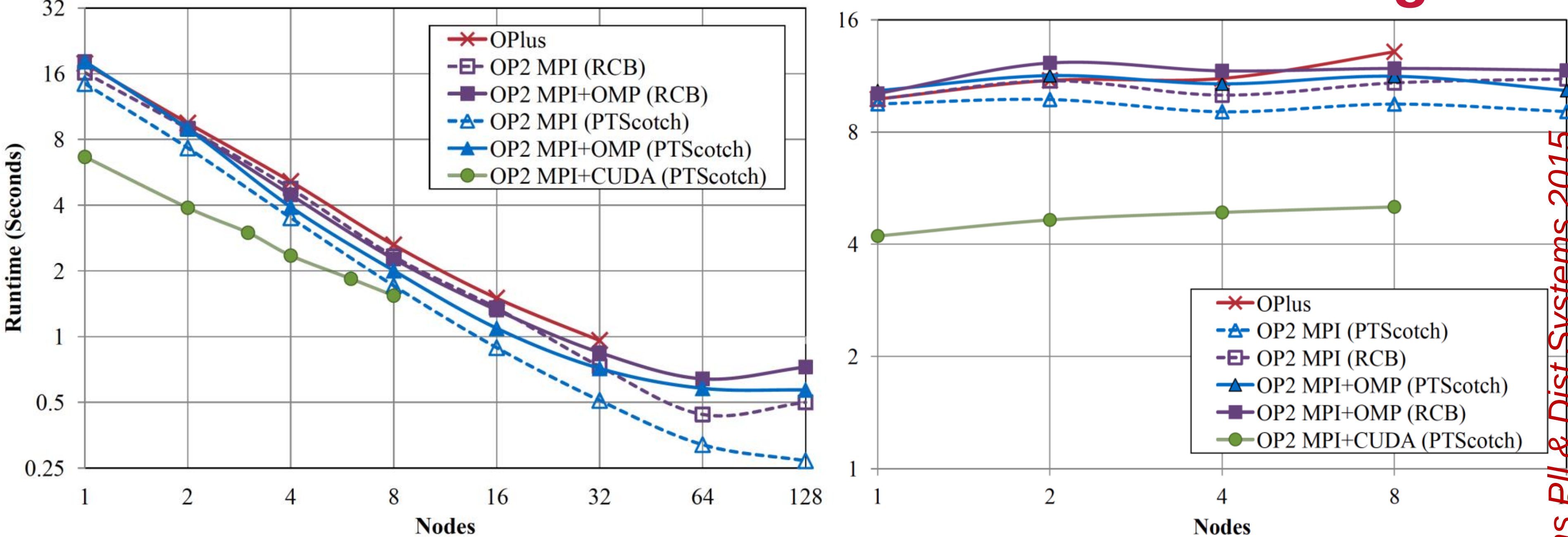
Code generation for indirect loops in PyOP2

- For MPI we precompute partitions & haloes
- Derived from PyOP2 access descriptors, implemented using PetSC DMPlex
- At partition boundaries, the entities (vertices, edges, cells) form layered halo region



- **Core:** entities owned which can be processed without accessing halo data.
- **Owned:** entities owned which access halo data when processed
- **Exec halo:** off-processor entities which are redundantly executed over because
- they touch owned entities
- **Non-exec halo:** off-processor entities which are not processed, but read when computing the exec halo

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***

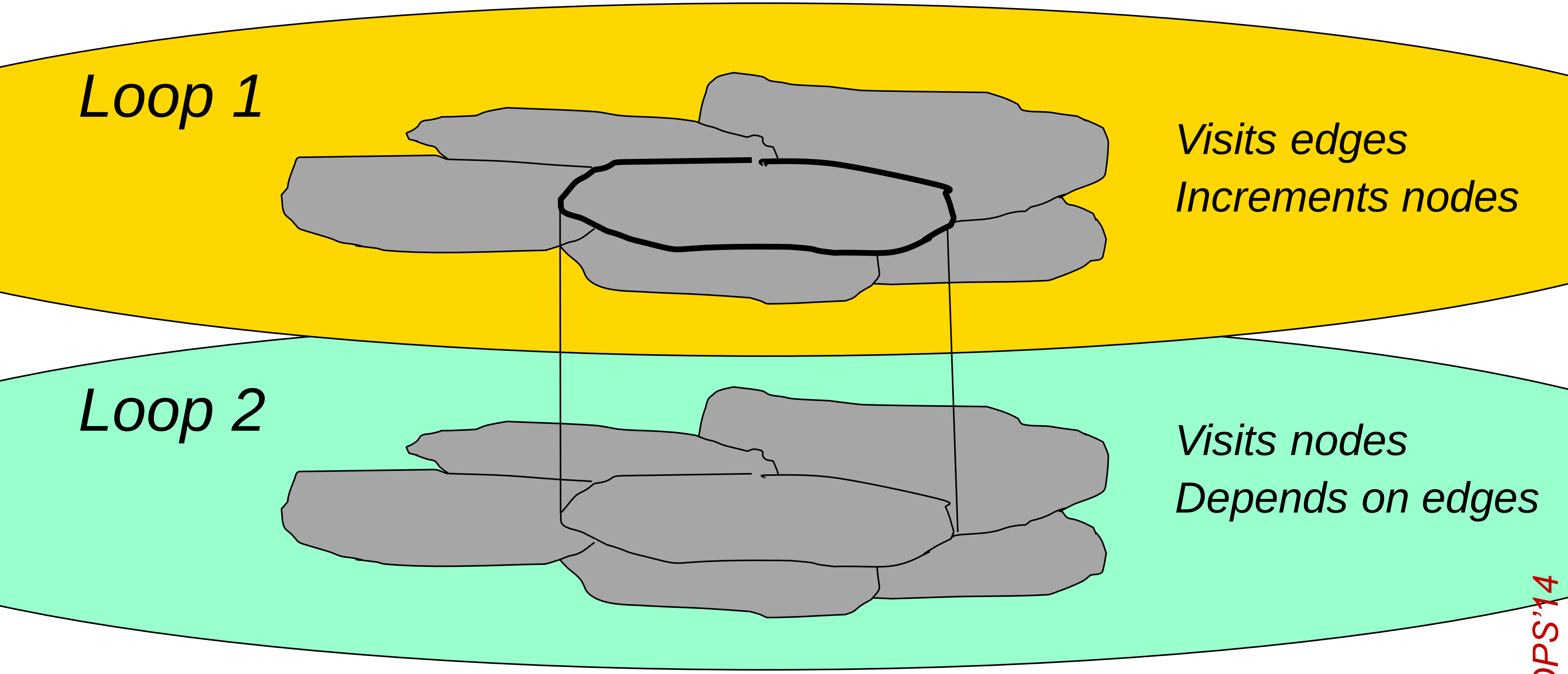
(joint work with Mike Giles, Istvan Reguly, Gihan Mudalige at Oxford)

- ***"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

Sparse split tiling on an unstructured mesh, for locality



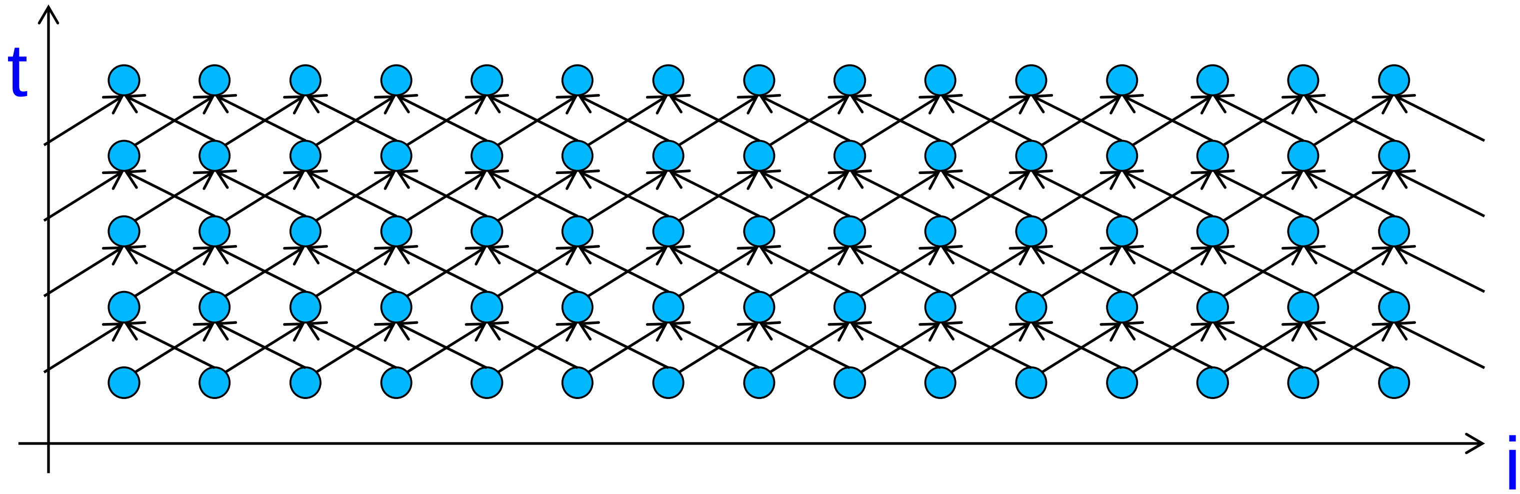
- How can we fuse two loops, when there is a “halo” dependence?
- I.e. load a block of mesh and do the iterations of loop 1, then the iterations of loop 2, before moving to the next block
- If we could, we could dramatically improve the memory access behaviour!

Strout, Luporini et al, IPDPS’14

Tiling a *structured* mesh for locality

- To understand sparse split tiling, we need to first understand *split* tiling
- Consider a 1D stencil loop, iterated a number of times

```
for (t=0; t<N; ++t)
  for (i=1; i<M-1; ++i)
    U[t+1][i] = U[t][i-1] + U[t][i+1]
```

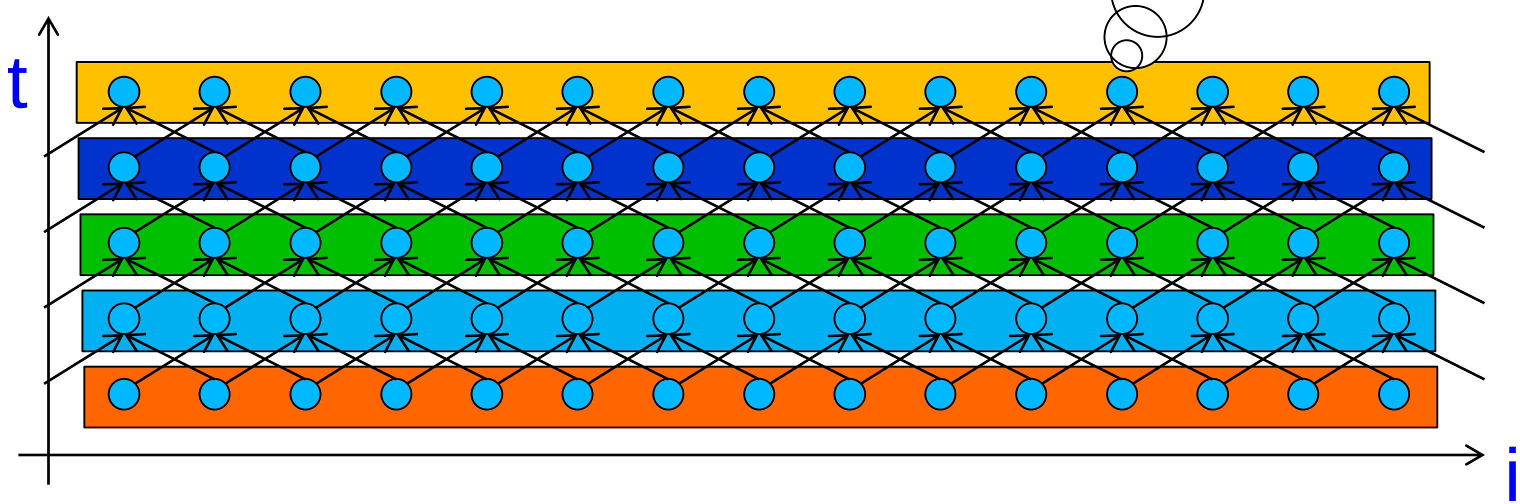


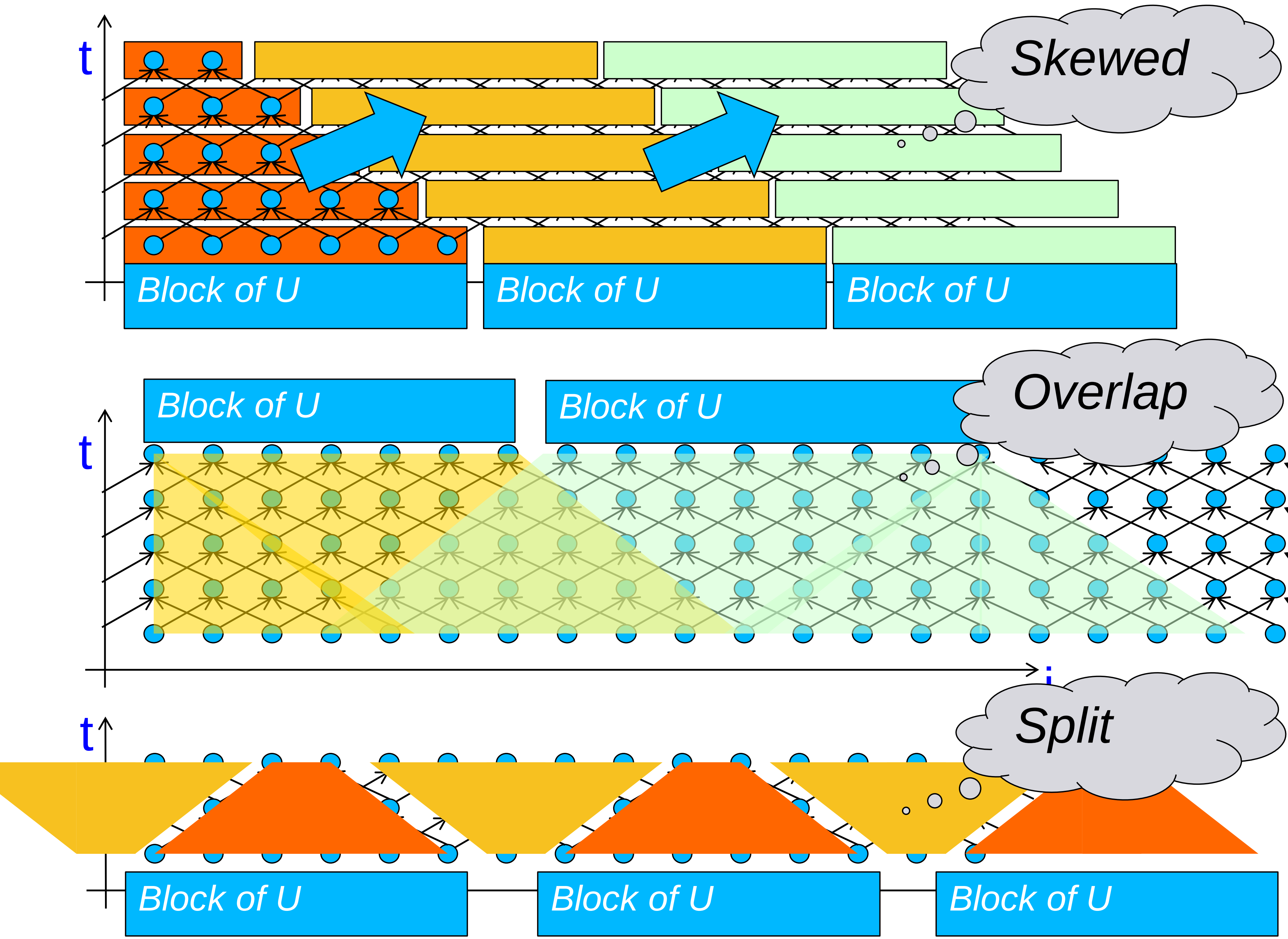
Tiling a *structured* mesh for locality

- To understand sparse split tiling, we need to first understand *split* tiling
- Consider a 1D stencil loop … number of times

```
for (t=0; t<N; ++t)
  for (i=1; i<M-1; ++i)
    U[t+1][i] = U[t][i-1] + U[t
```

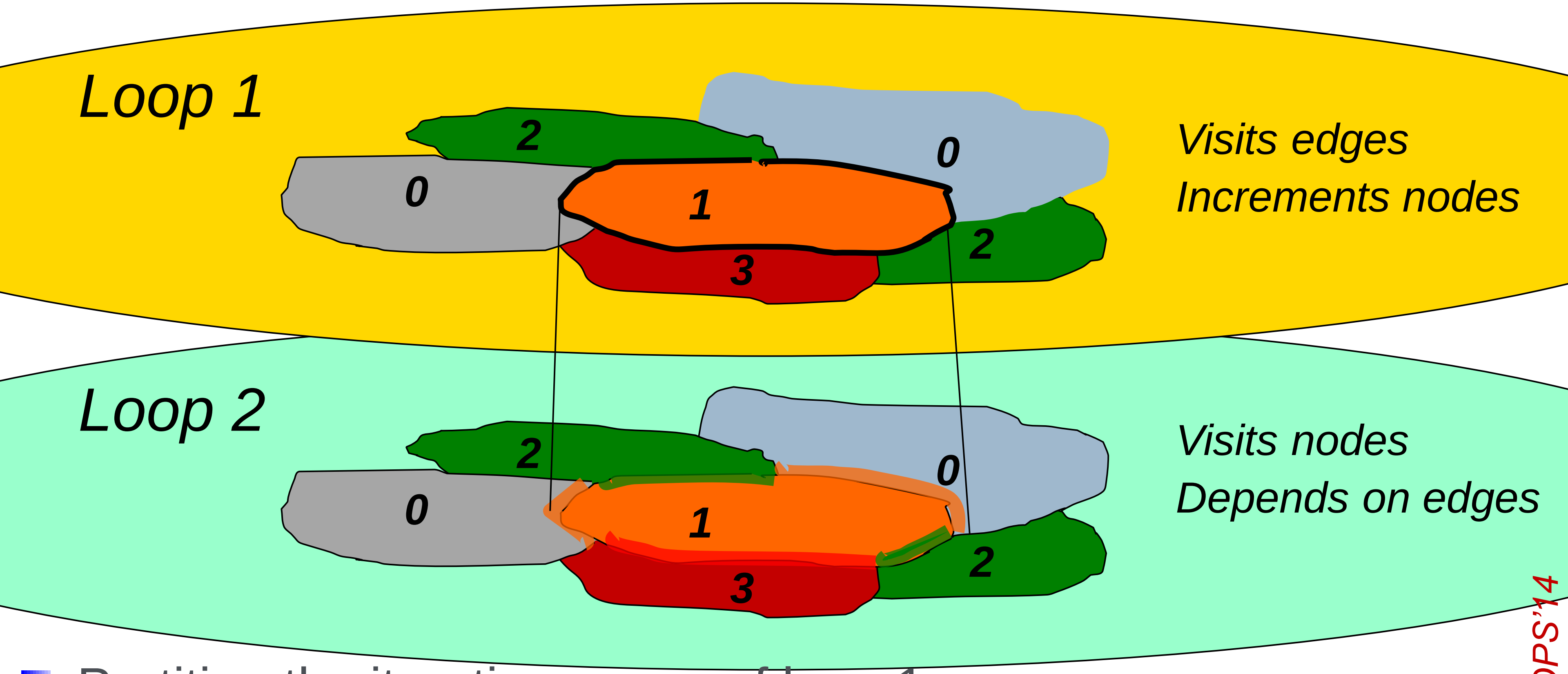
Lots of parallelism – but lots of *data movement*





t
Skewed
Block of U
Block of U
Block of U
t
Overlap
Block of U
Block of U
i
t
Split
Block of U
Block of U
Block of U

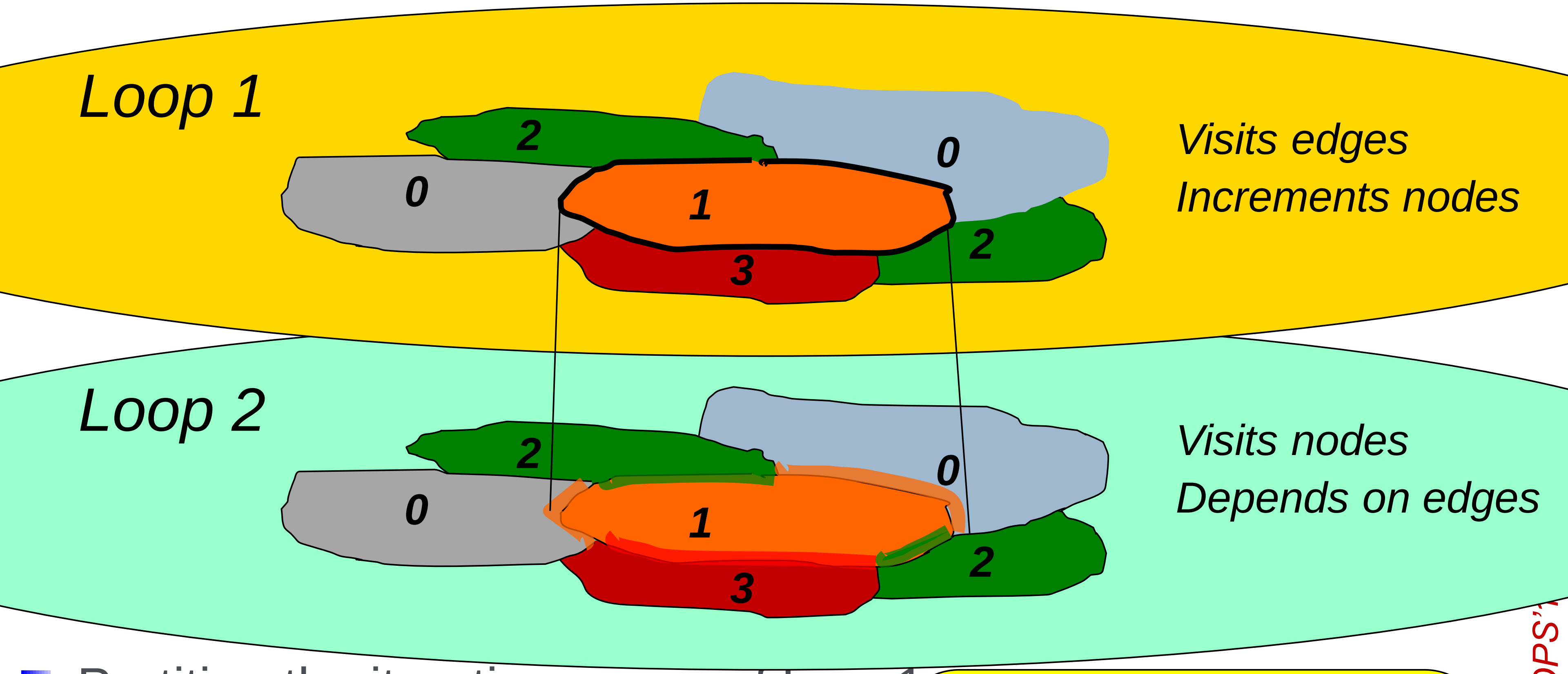
Sparse split tiling



- Partition the iteration space of loop 1
- Colour the partitions, execute the colours in order
- 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

Sparse split tiling



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- Colour the partitions
- Project the tiles, using the knowledg
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- Thus, the tile coloured #1 grows wh
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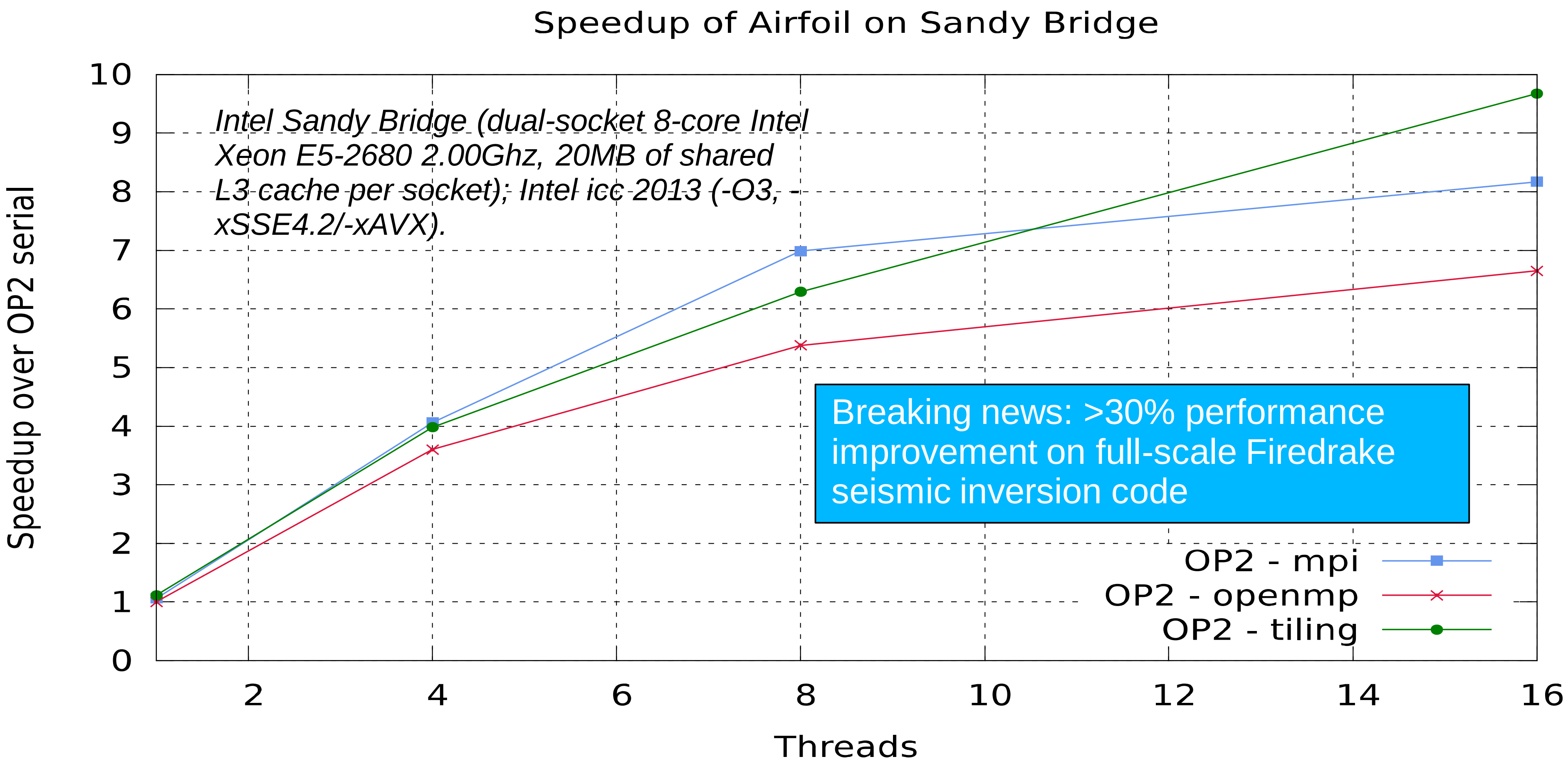
Inspector-executor: derive tasks and task graph from the mesh, ***at runtime***

Strout, Luporini et al, IPDPS'1

OP2 loop fusion in practice

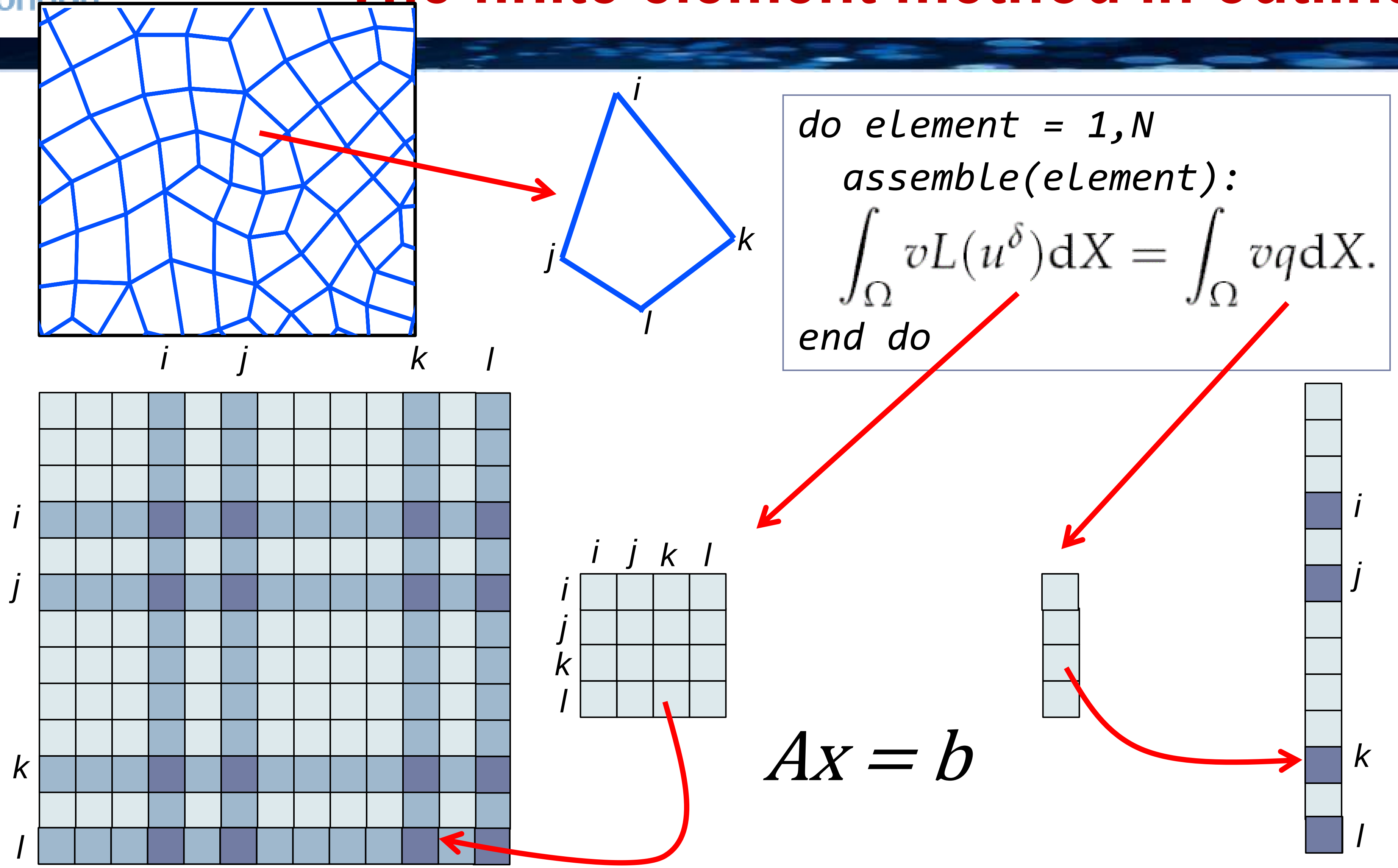


- *Mesh size = 1.5M edges*
- *# Loop chain = 6 loops*
- *No inspector/plans overhead*
- *Airfoil test problem*
- *Unstructured-mesh finite-volume*

- **Where did the domain-specific advantage come from?**
  - OP2's access descriptors provide precise dependence iteration-to-iteration information
    - Could easily be delivered in a lambda-based parallel loop framework
  - 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
Luporini PhD thesis, forthcoming

The finite element method in outline




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

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

```
end do
```

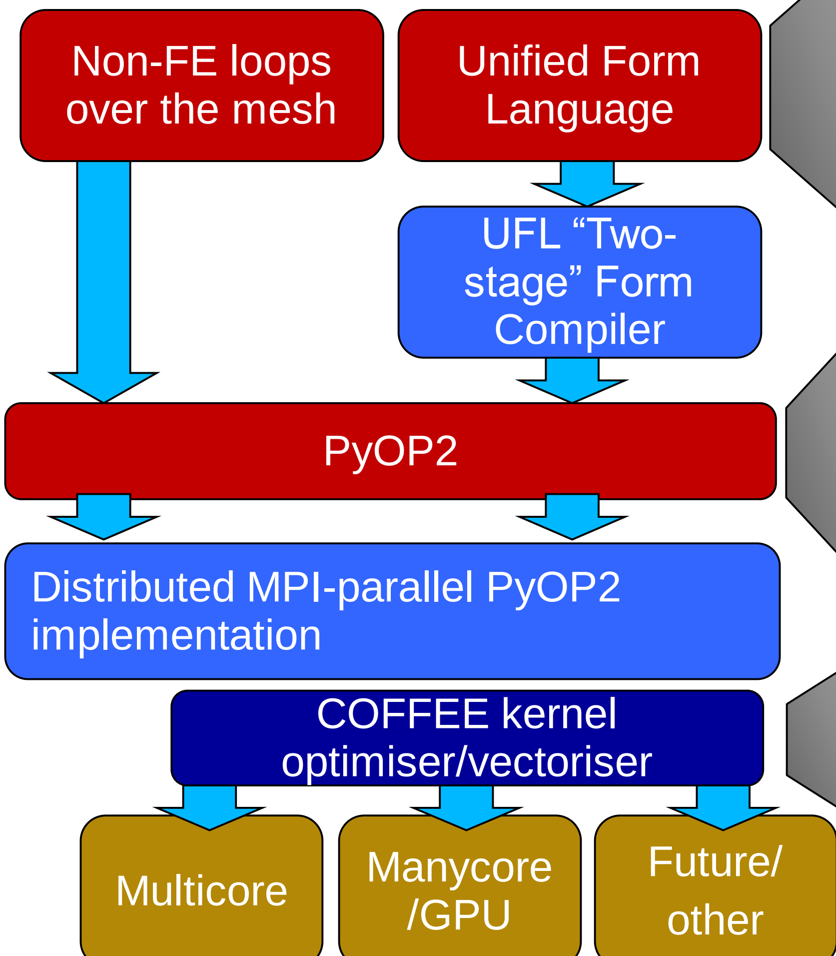
- Key data structures: Mesh, dense local assembly matrices, sparse global system matrix, and RHS vector

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:
  - *PyOP2*
  - *Loops over the mesh*
  - *Key is orchestration of data movement*
- Solver:
  - Interfaces to standard solvers, such as PetSc

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 using runtime code generation



- 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

- Domain-specific loop optimizer
- For finite-element assembly and similar loop nests
- Vectorisation and flop-minimisation

Rathgeber, Ham, Mitchell et al, ACM TOMS 2016

- **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

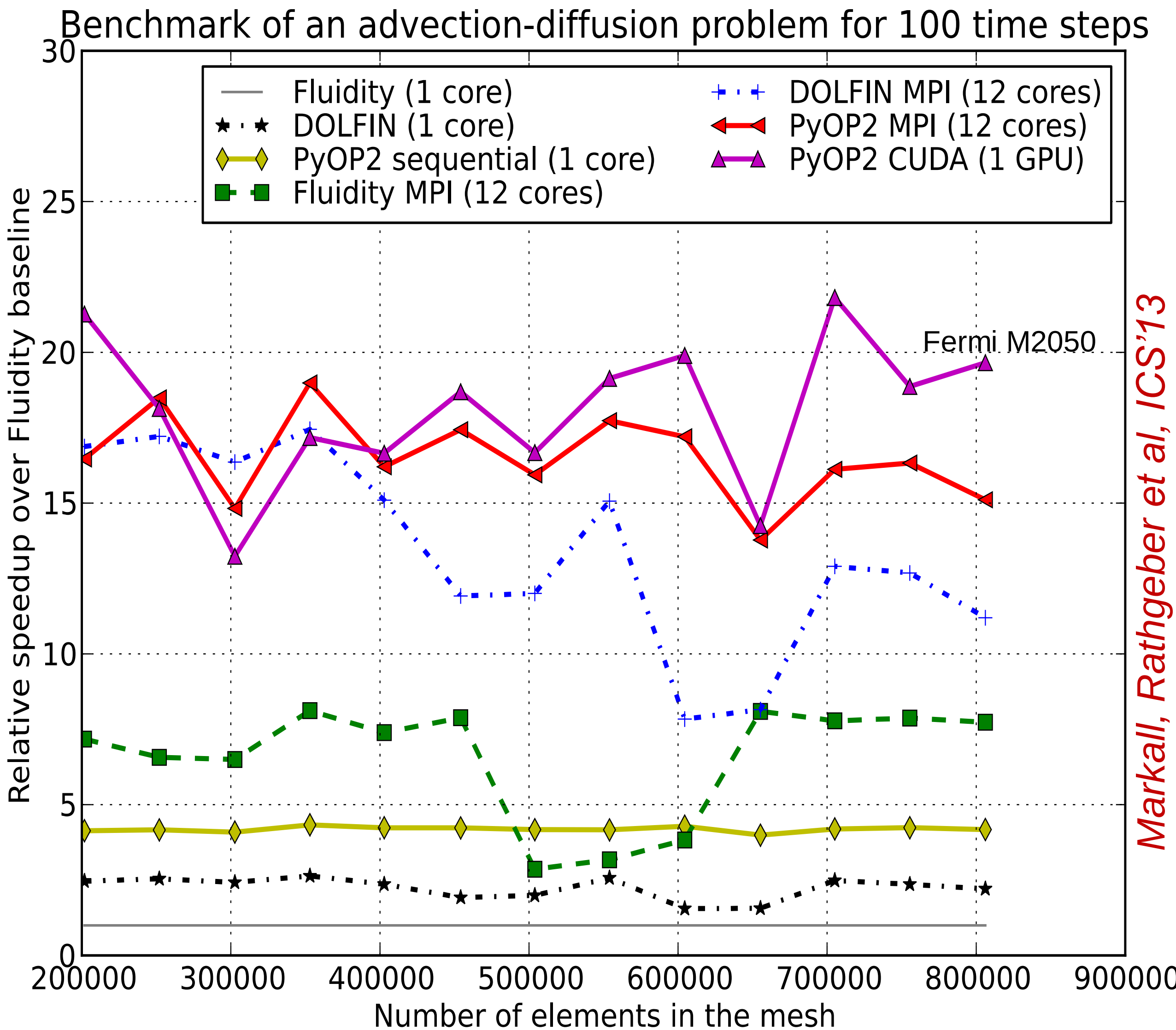
adv = (q*t+dt*dot(grad(q),u)*t)*dx      # Advection RHS
diff = action(M+0.5*d,t)                # Diffusion RHS

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

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 and up to date evaluation



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

- **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

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
- 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

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  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

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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

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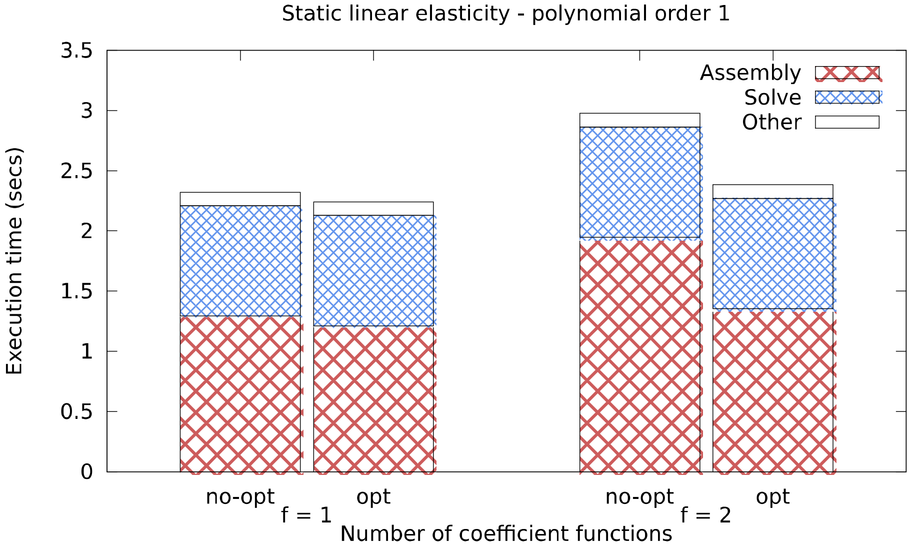
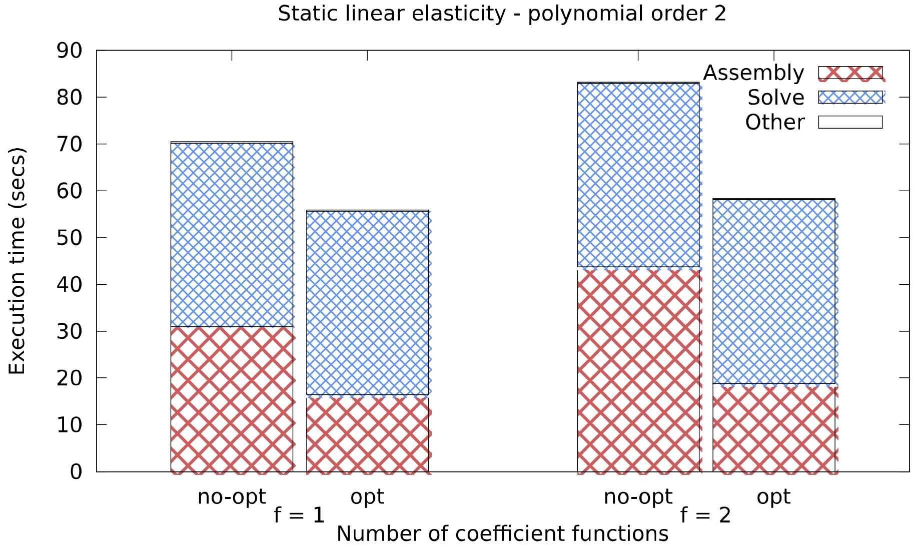
COFFEE: Performance impact





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- 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
    - **For the linear operators arising in finite-element assembly we can show that it's possible to *minimise* the inner-loop flop count**

Luporini, Ham, Kelly: An algorithm for the optimization of finite element integration loops, in revision

Conclusions (but wait…)

- Pointers lead to the compiler making conservative decisions
  - Idea: capture the key data structures at a higher level of abstraction
    - Let the tools "own the data" – and control its distribution
    - "inspector-executor" – take time to derive a schedule from the specific mesh at runtime
- Your compiler doesn't know things that you know
  - That you will iterate over the mesh *many* times without changing it
  - That the graph is easily-partitionable and colourable
- Your compiler won't do optimisations that *we* know are good for your code
  - Policy vs mechanism – good for *your* code might not be good *in general*
- Runtime code generation is liberating
  - **We do not try to do static analysis on client code**
  - **We encourage client code to use powerful abstractions**

Challenge 1/3: Domain-specific optimisations

- 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 (or instead to use a matrix-free or local-assembly scheme)

  - **How can we engage with the application specialists to expose and automate domain-specific optimisations?**

Challenge: 2/3: PyOP2 layer

- The key idea in OP2/PyOP2 is ***access descriptors***
- OP2's access descriptors are ***declarative specifications*** of how each loop iteration is connected to the abstract mesh
- The kernels do not access the mesh
- The implementation is responsible for connecting the kernel to the data
- The implementation is free to select layout, stage data, schedule loops
  - We can map from data to iterations

- **What *would* a programming abstraction for data locality look like?**

Challenge: 3/3: Firedrake layer

- Dramatically raised level of abstraction
- But we still can match or exceed hand-coded, in-production code
- Costs of abstraction are eliminated by dynamic generation of code specialised to context
- Domain-specific optimisations can yield big speedups over the best available general-purpose compilers

- **The real payoff lies in supporting the users in navigating freely to the best way to model their problem**

- **How can the *barriers to adoption* of DSLs be overcome?**

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- AMD, Codeplay, Maxeler Technologies

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