The OPS Domain Specific Abstraction for Multi-Block Structured Grid Computations

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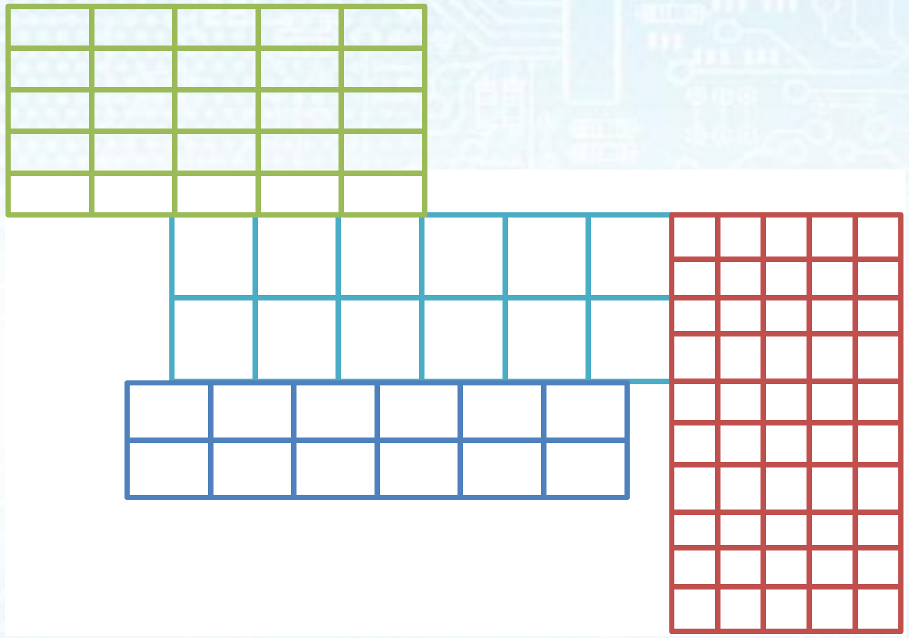
Introduction

- Importance of Domain Specific approaches in HPC
  - Performance, Maintenance, Future Proofing
  - But then again, you already know this…
- Originally from CFD: the OP2 domain specific active library for unstructured meshes
  - Active Library
  - Rolls-Royce Hydra, VOLNA tsunami simulation
  - C, Fortran + a reluctance for maintaining compilers

Multi-Block Structured Grids

- Structured grids are popular due to their implicit connectivity
- Commonly used in CFD with finite difference and finite volume algorithms
- Realistic codes tend to use many blocks, different resolutions
  - Cloverleaf: Nuclear/Defence
  - ROTORSIM @ Bristol: helicopter rotors - sliding planes
  - SBLI @ Southampton: compressible Navier-Stokes



Designing an abstraction

Challenge: design an abstraction that:

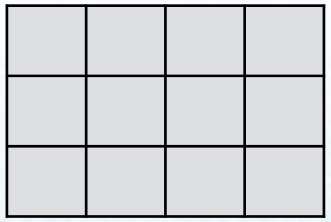
- Covers a wide range of applications
- Intuitive to use
- Abstracts away parallelisation and data movement
- Still specific enough so that we can make aggressive platform-specific optimisations

The OPS Abstraction

- **Blocks**
  - A dimensionality, no size
  - Serves to group datasets together

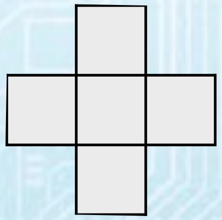
ops_block = ops_decl_block(dim, name);

- **Datasets on blocks**
  - With a given arity, type, size, optionally stride



ops_dat = ops_decl_dat(block, arity, size, halo, …, name);

- **Stencils**
  - Number of points, with relative coordinate offsets, optionally strides

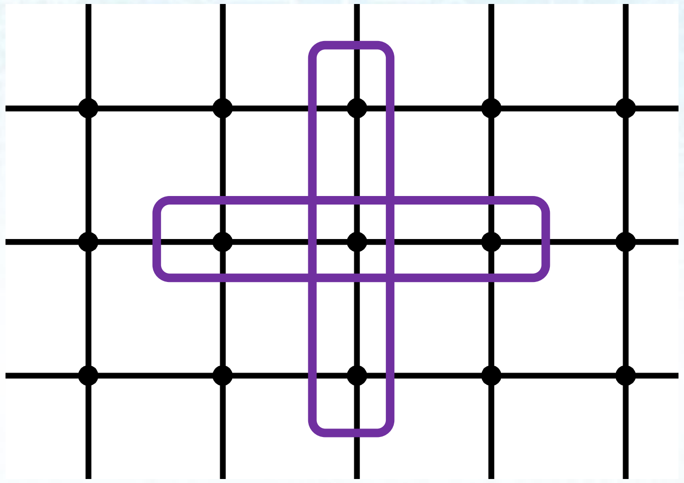


ops_stencil = ops_decl_stencil(dim, npoints, points, name);

Computations

- The description of computations follows the Access-Execute abstraction

- Loop over a given block, accessing a number of datasets with given stencils and type of access, executing a kernel function on each one



  - Principal assumption: order of iteration through the grid doesn't affect the results

User kernel

```
void calc(double *a, const double *b) {
  a[OPS_ACC0(0,0)] = b[OPS_ACC1(0,0)] + b[OPS_ACC1(0,1)] +
                     b[OPS_ACC1(1,0)];
}
...
```

Iteration range

```
int range[4] = {12,50,12,50};
ops_par_loop(calc, block, 2, range,
```

Arguments

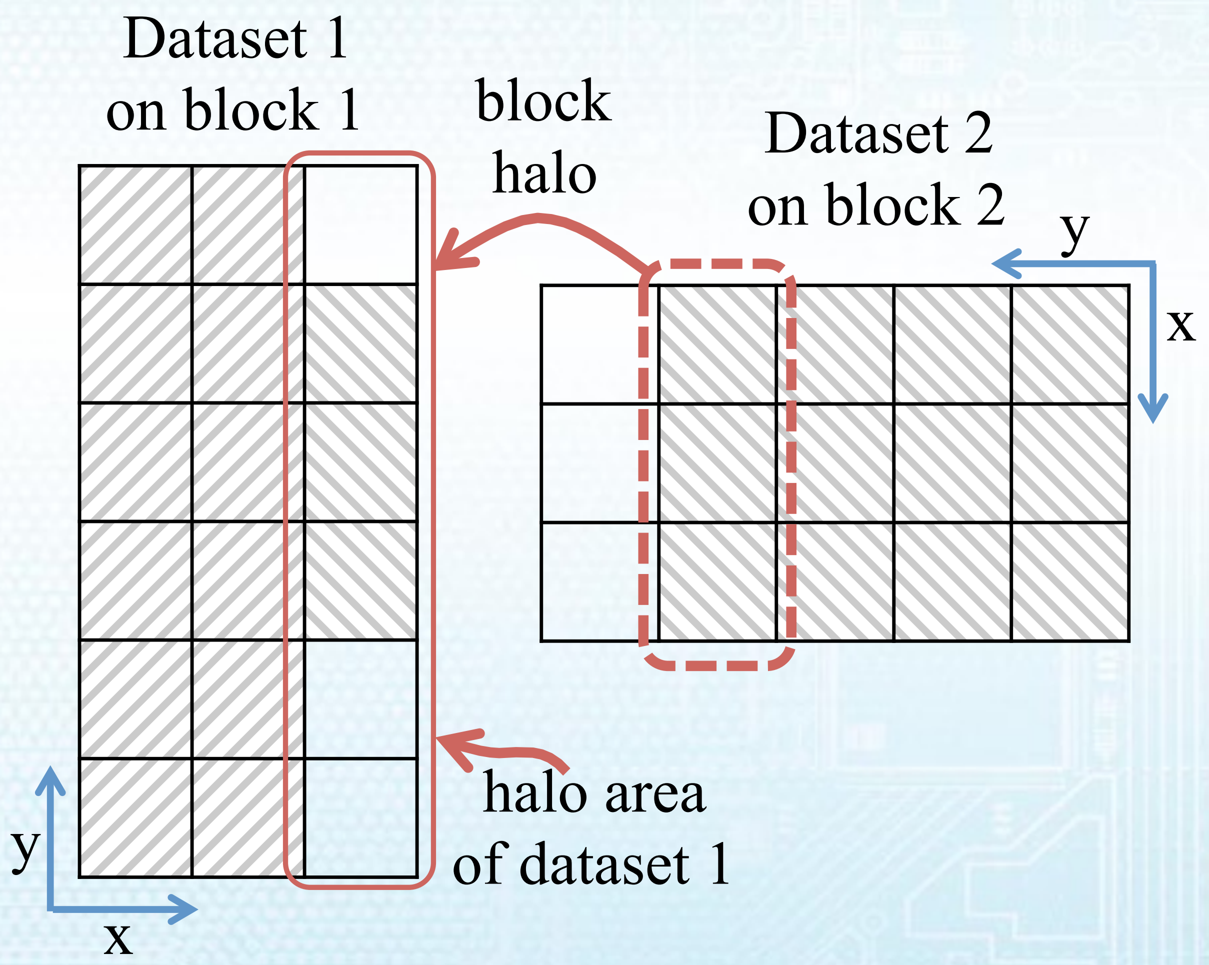
```
             ops_arg_dat(a,S2D_0,"double",OPS_WRITE),
             ops_arg_dat(b,S2D_1,"double",OPS_READ));
```

Computations

- This definition decouples the **specification** of computations from their parallel **implementation**
  - No assumption about data layout or movement
  - Parallelism is implicit
  - Easy to understand, maintain
  - Enough information to organise execution & apply optimisations

The OPS Abstraction

- Multi-Block API
  - User specified halo
  - Exchange manually triggered
- In development
  - Multigrid API
  - Sliding planes
- Future
  - AMR, Multi-material



What the abstraction lets us do

- The library “owns” all the data
  - Access to it only through API calls
- Description of computations implicitly contain parallelism
- We can organise execution: parallelism & data movement
  - Code generation
  - Back-end

Code generation

- We parse the OPS API calls
  - Contain all the information
- Generate parallel implementations for
  - Sequential, OpenMP, OpenACC
  - CUDA, OpenCL
  - Callbacks to backend

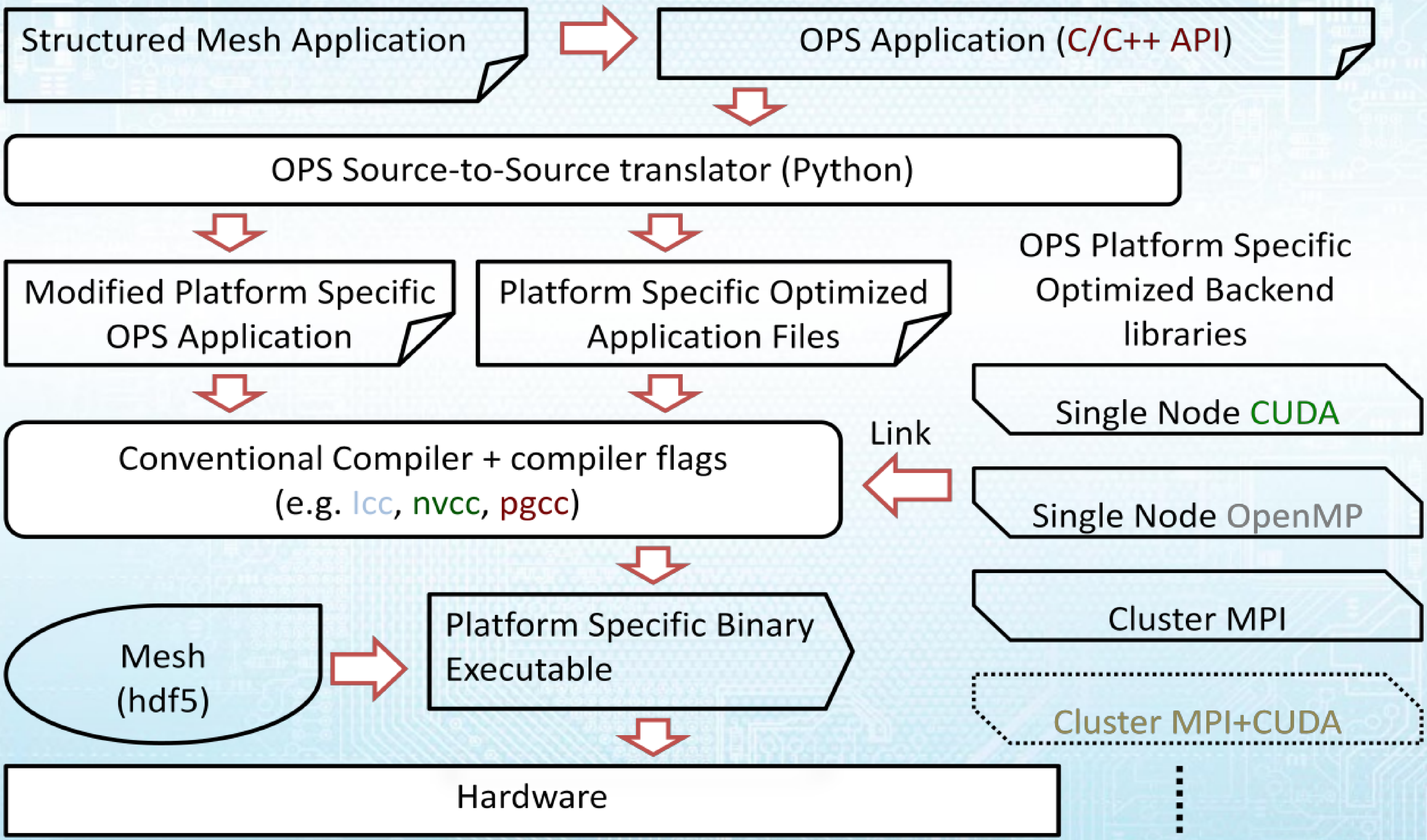
```
#define OPS_ACC0(j,i) j*xdim0+i
#define OPS_ACC1(j,i) j*xdim1+i

//user kernel
void calc(double *a, const double *b) {...}

void ops_par_loop_calc(int ndim, int range,
                       ops_arg arg0, ops_arg arg1){
//set up pointers and strides
double *p_a0 = (double*)ops_base_ptr(range, arg0);
double *p_a1 = (double*)ops_base_ptr(range, arg1);
xim0 = arg0.dat->size[0]; xim1 = arg1.dat->size[0];
//do the computation
for(int j = 0; j < range[3]-range[2]; j++) {
  for(int i = 0; i < range[1]-range[0]; i++) {
    calc(&p_a0[j*xdim0+i],&p_a1[j*xdim1+i]);
  }
}
```

Code generation

OpenMP	CUDA & OpenCL	OpenACC
↓	↓	↓
Explicit assignment of a block of rows to each thread	1 grid point per thread	Nested loop with OpenACC pragmas (kernels/loop)
NUMA issues!	Use of non-coherent cache Runtime compilation	Currently links to CUDA backend, and uses `deviceptr()`

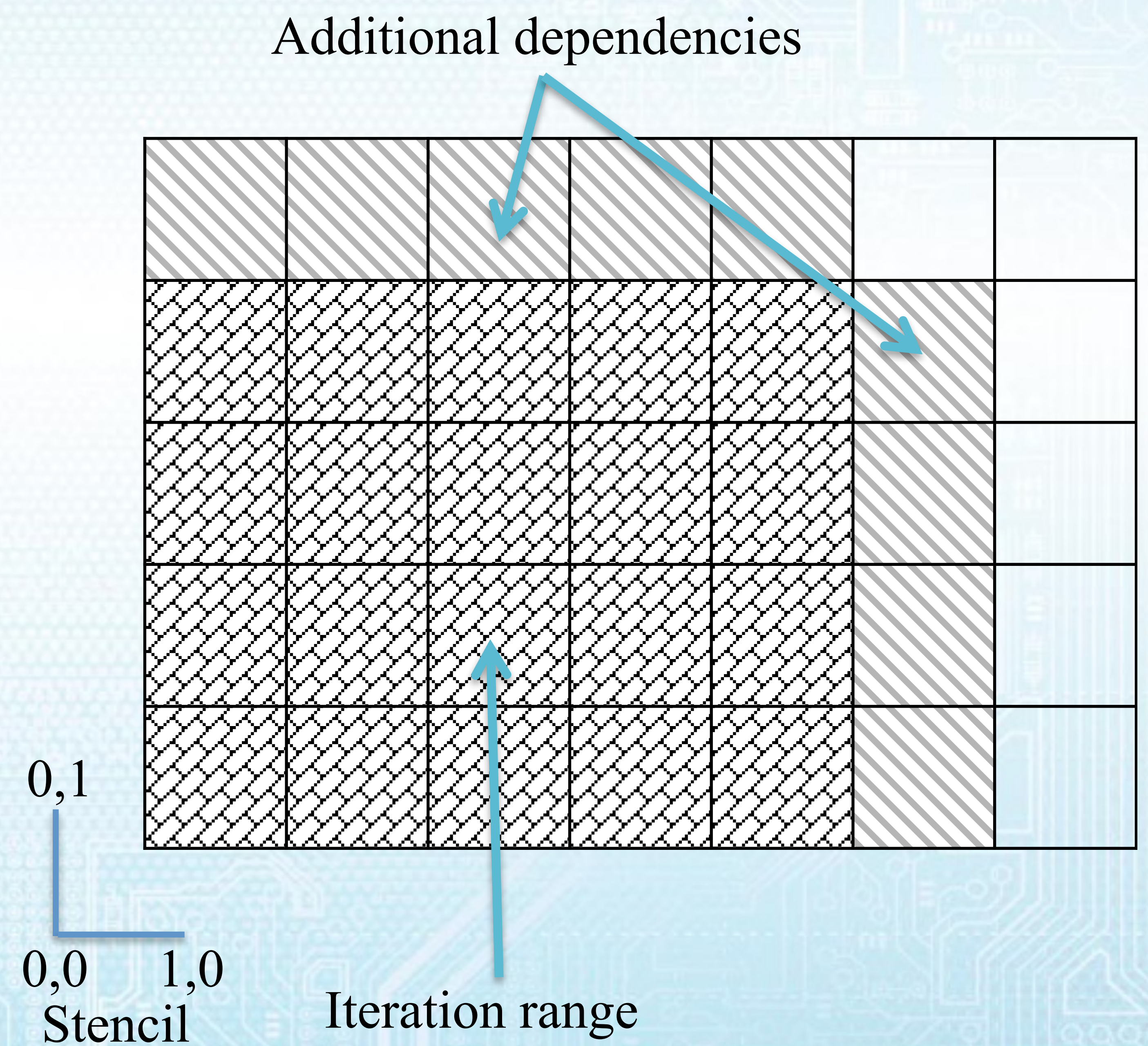
- Checking consistency with declared stencils
- Adding `const`, `restrict`, and other keywords
- Deploying optimisations

Build process



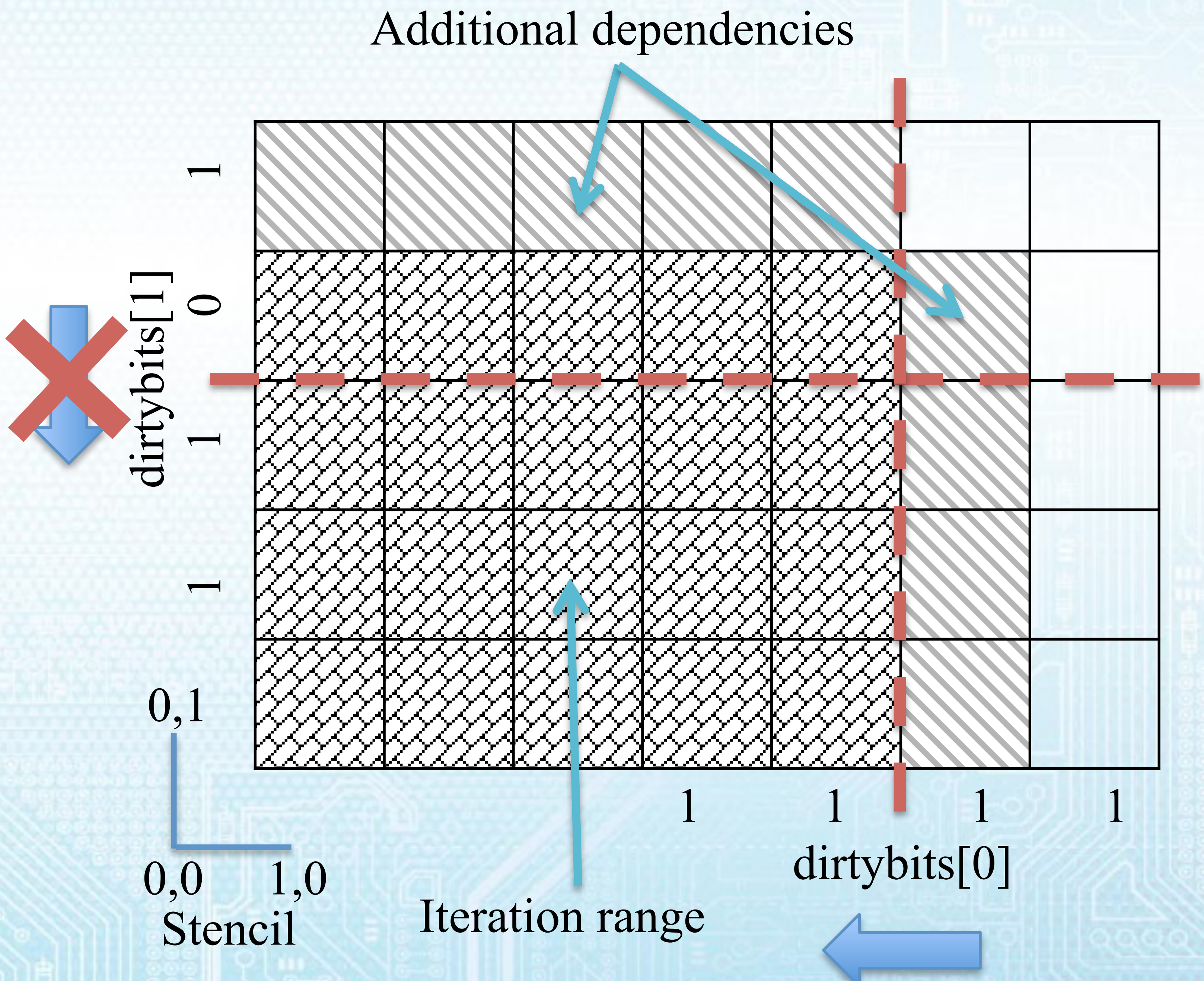
Backend logic

- We know:
  - iteration range
  - what data is accessed, how
  - stencils



Distributed Memory

- How much halo for each dataset
- What exactly is modified
- On-demand messaging with aggregation
- Dirtybits to keep track of changes



Checkpointing

- On the granularity of parallel loops
  - We know exactly what data is accessed and how
- We know when data leaves the realm of OPS
  - Need to save anything that leaves
- No need to save data that is going to be overwritten
- Fast-forward: re-start and just not do any of the computations

Checkpointing

- Only a few datasets touched in any loop
- Checkpointing regions
- Decide what needs to be save over a number of loops
- Save to local & neighbouring SSD

	Dataset 1	Dataset 2	Dataset 3	Dataset 4
Loop 1	R	W	?	?
Loop 2		R	W	
Loop 3			R	W

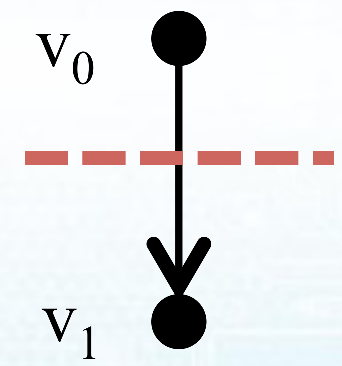
Lazy execution

- OPS API expresses everything involved with computations
- We know when data leaves OPS (e.g. reduction)
- Loop chaining abstraction
  - We can carry out operations, optimisations that span several loops
  - Queue up a number of kernels, trigger execution when e.g. a reduction is encountered
- Implemented, works well - so what can we do with it?

MPI messaging

Default messaging strategy:

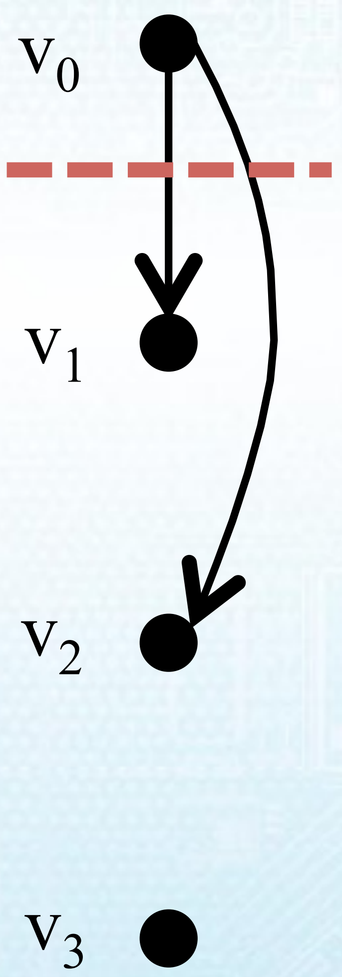
- On-demand
- Given loops v_0 and v_1
- Satisfy all dependencies before executing v_1



MPI messaging I.

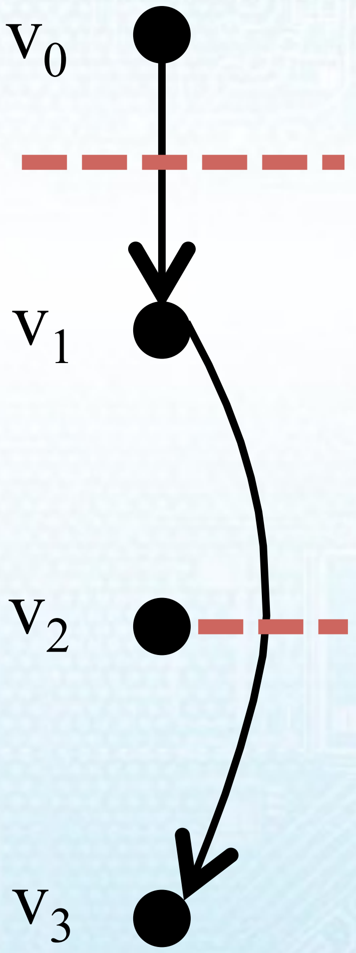
Strategy 1:

- Given dependencies between v_0->v_1 and v_0-> v_2
- Combine messages to hide latency



MPI messaging II.

- Strategy 2
- Given dependency v_1 -> v_3 but none to v_2
- Hide latency of message



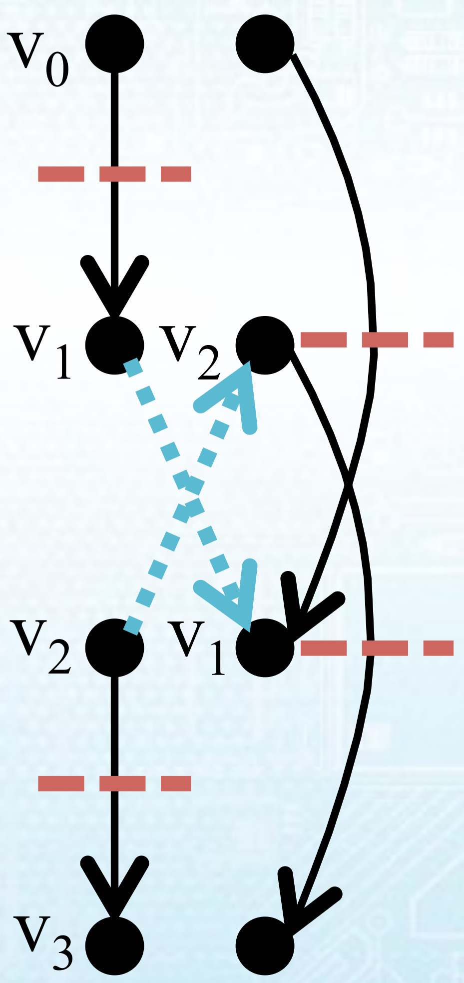
MPI messaging III.

- Strategy 3

- Given dependencies between v_0 -> v_1 and v_2 -> v_3 but not v_1 -> v_2

MPI messaging III.

- Strategy 3
- Given dependencies between v_0 -> v_1 and v_2 -> v_3 but not v_1 -> v_2
- Exchange loops v_1 and v_2, and hide latency of messages

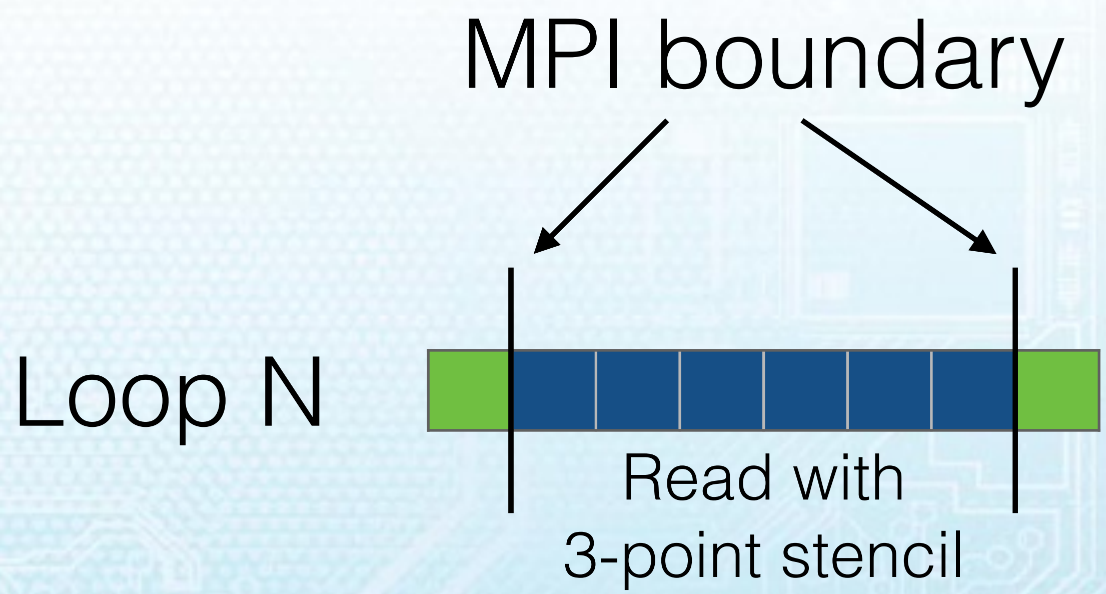


MPI Communication avoidance

Given a sequence of loops

- Iterate backwards through a loop chain and determine dependencies

- Exchange wider halo at the beginning of the chain



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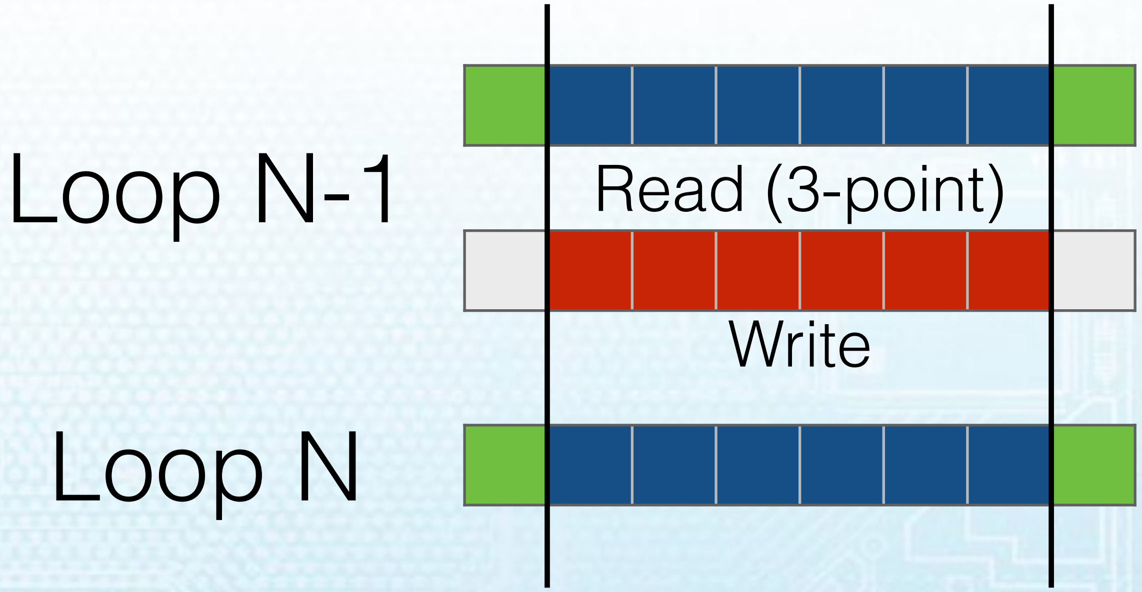

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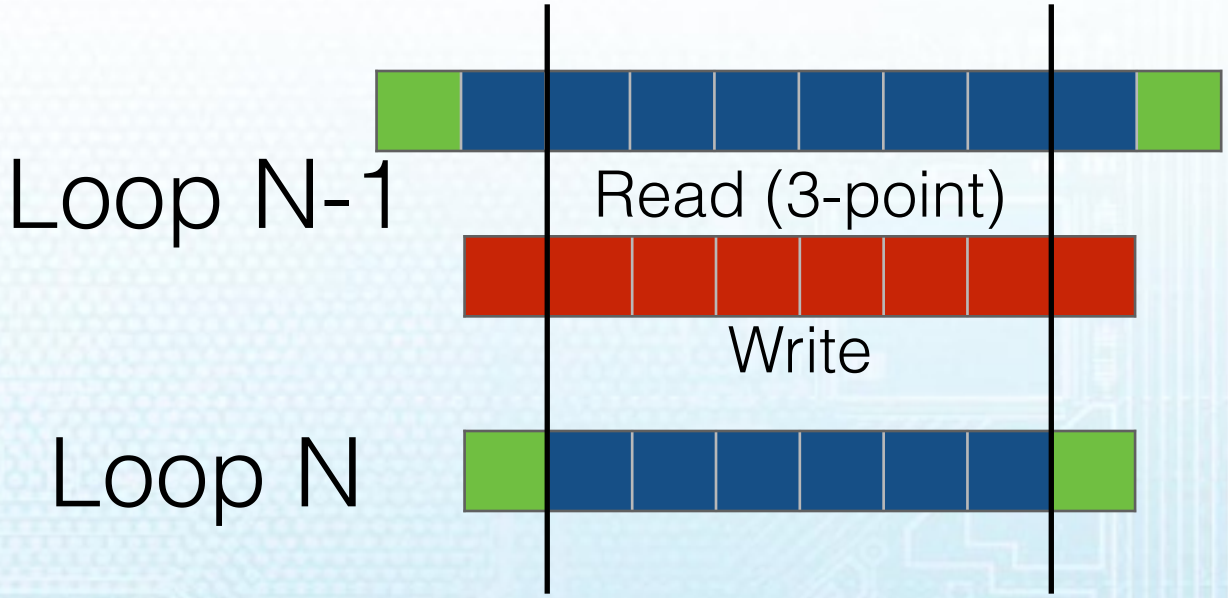

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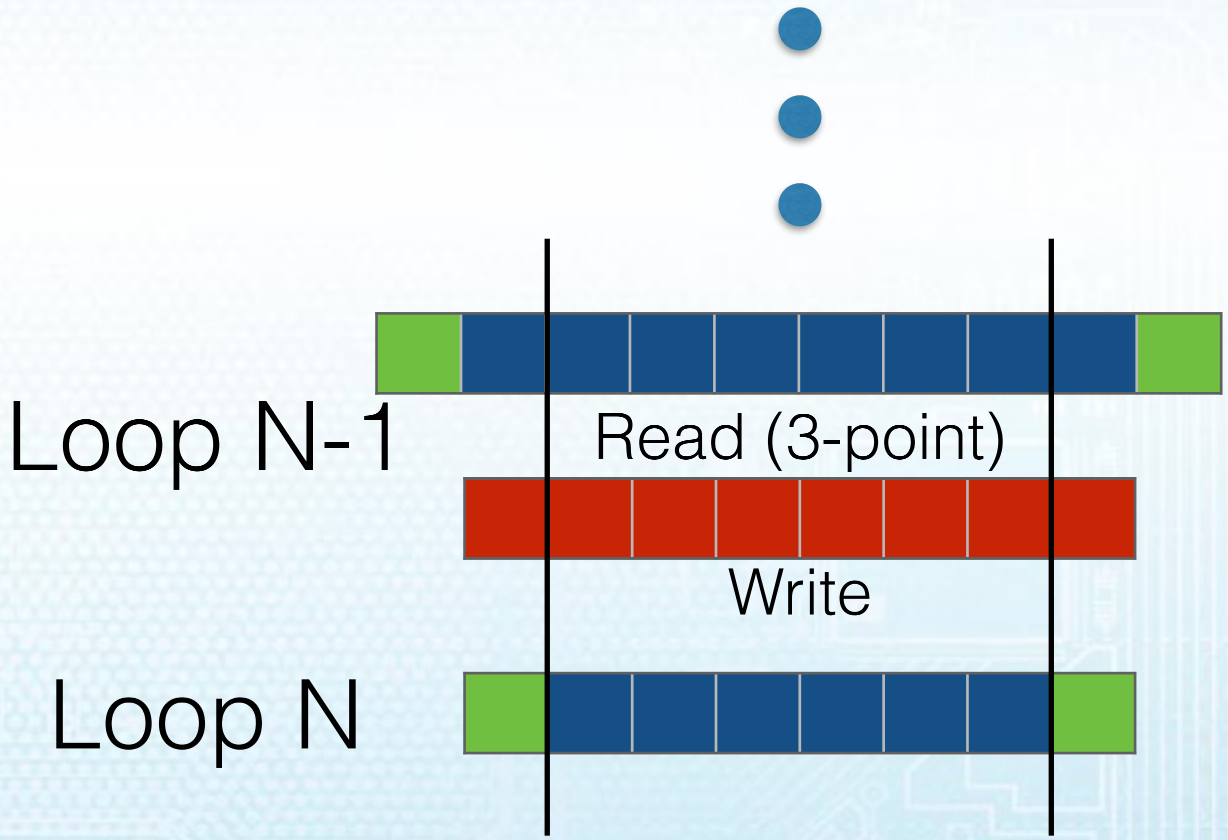
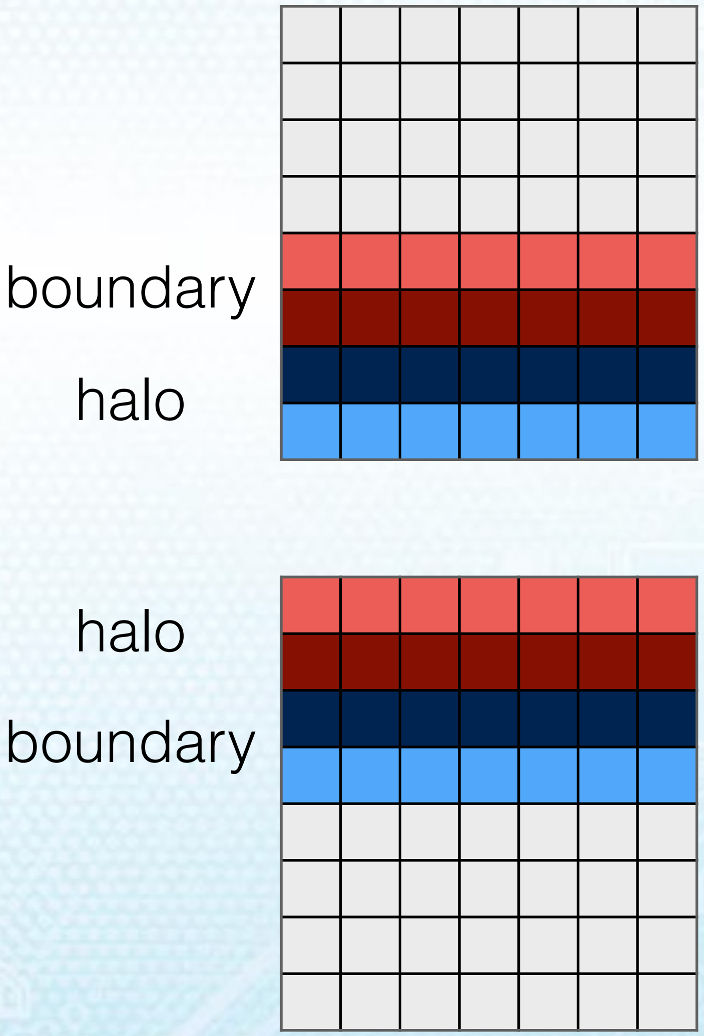


MPI Communication avoidance

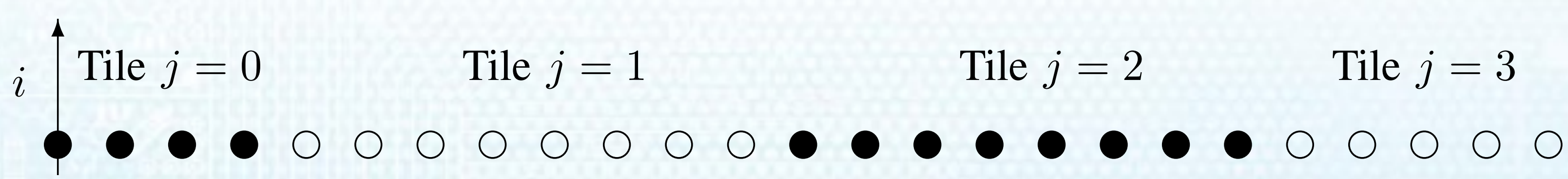
- Extend halo region
- Redundant computations
- Fewer communications points
    - Larger messages
    - Fewer datasets need exchange in the end



Cache blocking

- Similar idea to communication-avoiding algorithm, except not over MPI and not with redundant compute
- Cache blocking, tiling; lot of work out there on polyhedral compilers

3-point stencil



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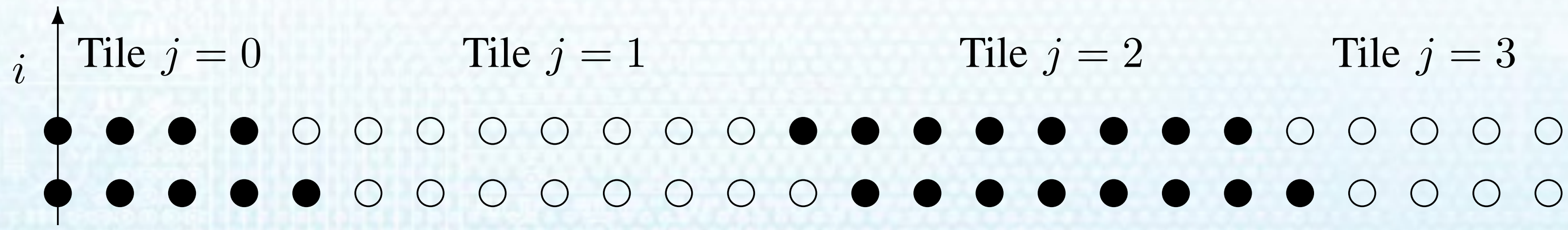

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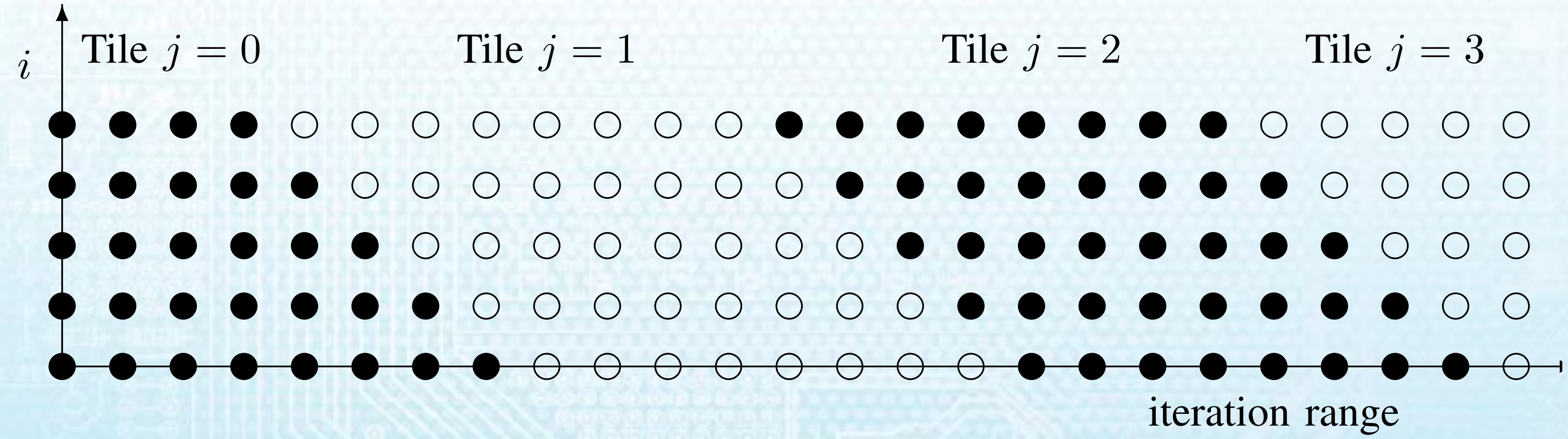
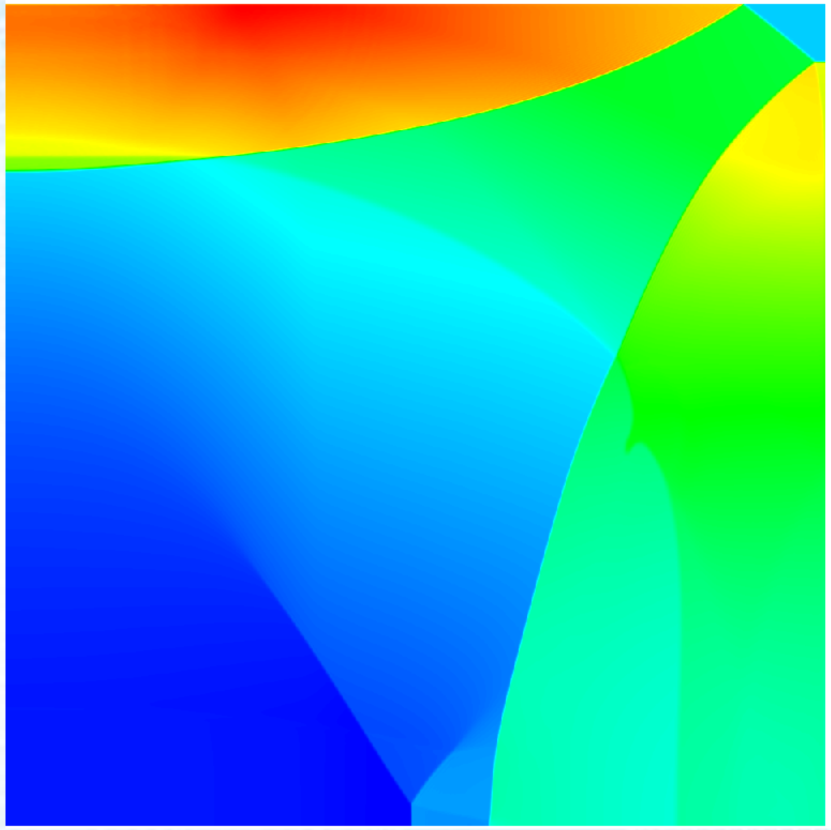


CloverLeaf



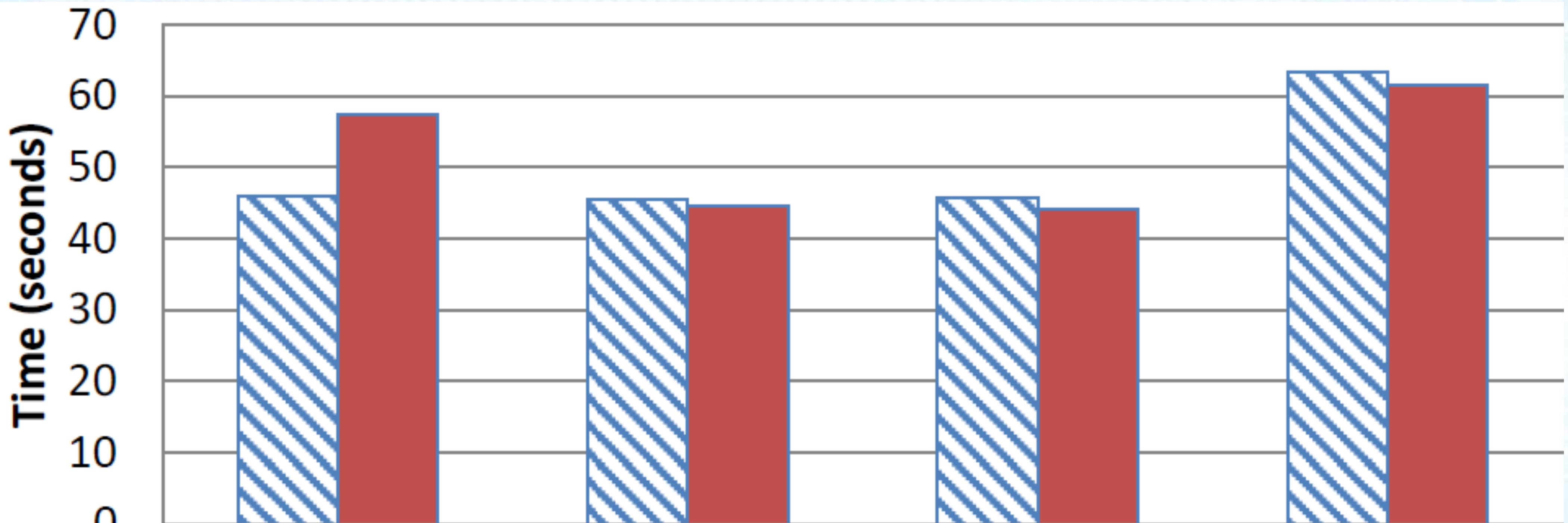
- Mini app in the Mantevo suite
- 2D/3D Structured hydrodynamics
- Explicit compressible Euler
- ~6k LoC
- Existing parallelizations (OpenMP, MPI, OpenACC, CUDA, OpenCL)
- Porting effort & performance?
  - Re-engineering, readability, tools, debugging
  - Is it worth the effort - maintainability, performance?

Porting CloverLeaf

- Initial 2D version
  - Fortran to C, 85 loops
  - Took about 1-2 months to port (including development of OPS)
  - Debugging
- 3D version 5 days
- No more difficult than porting to e.g. CUDA, but you get one codebase

Performance - CPU

3840*3840 mesh, 87 iterations

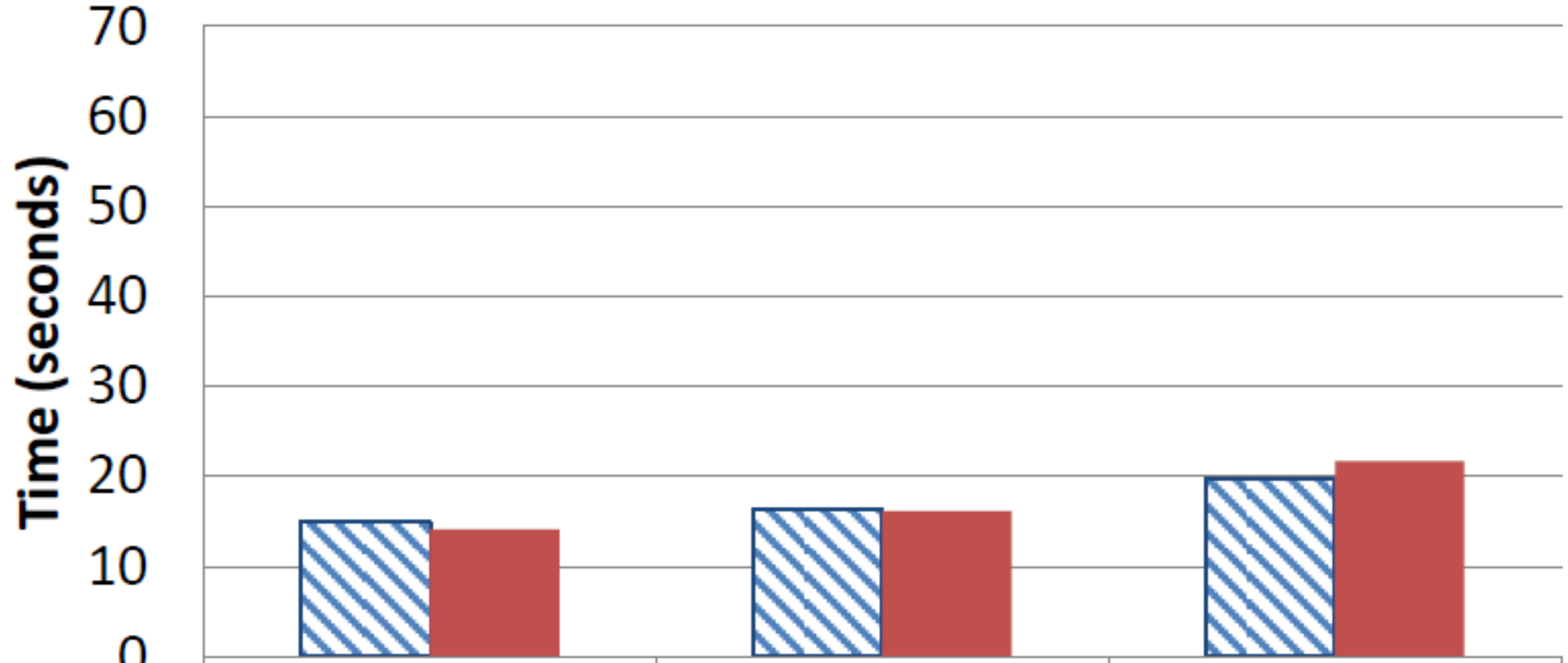


	32 OMP	32 MPI	2OMPx16MPI	OpenCL
OPS	45.92	45.55	45.82	63.35
Original	57.39	44.60	44.22	61.54

Xeon E5-2680 @ 2.7 GHz
Intel 14.0, Intel MPI

Performance - GPU

3840*3840 mesh, 87 iterations

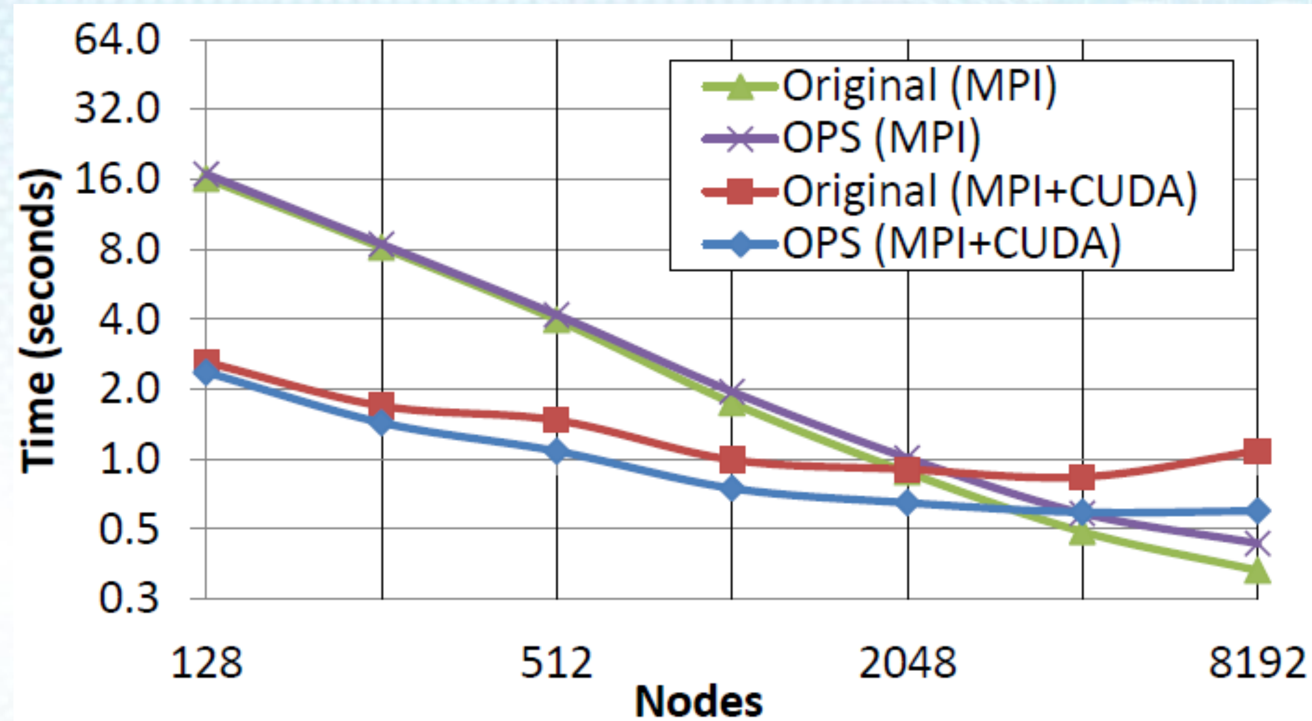


	CUDA	OpenCL	OpenACC
OPS	15.01	16.27	19.82
Original	14.14	16.19	21.67

NVIDIA K20c, CUDA 6.0, PGI 14.2

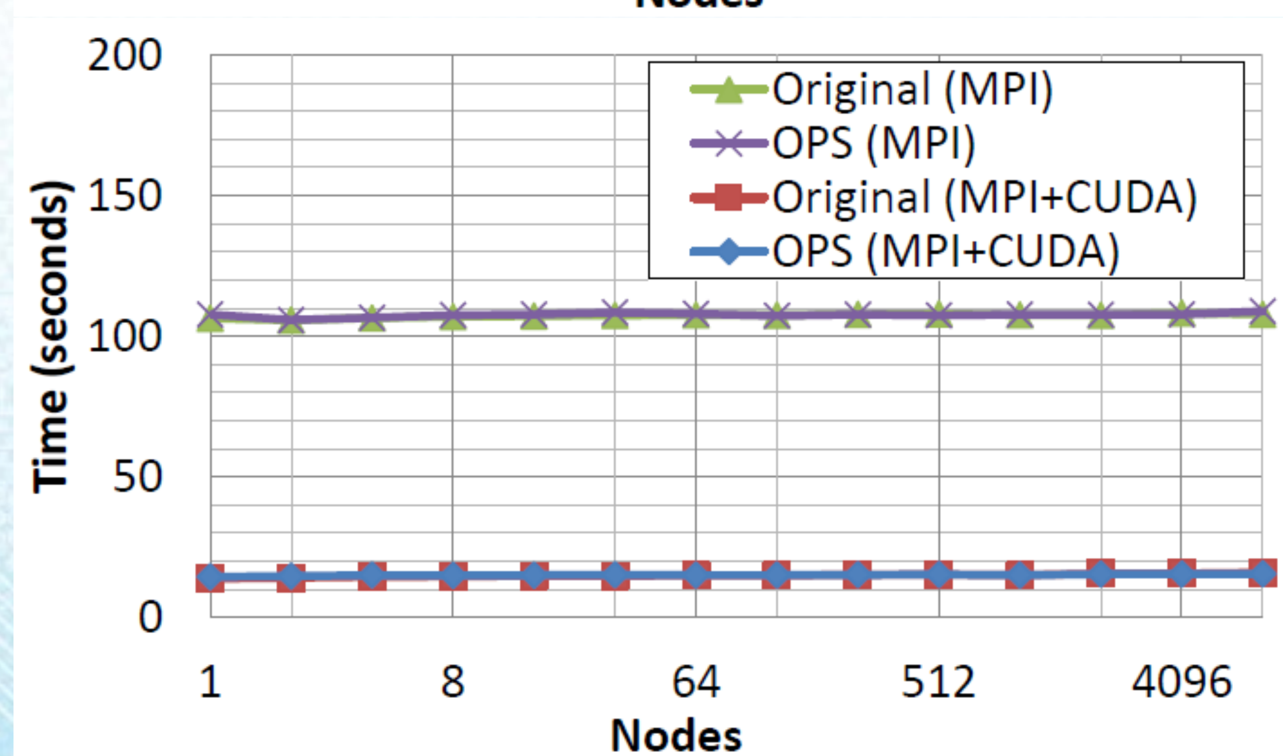
Performance - Scaling

STRONG SCALING
15360 x 15360 MESH
(87 ITERATIONS)



Titan, Cray XK7

WEAK SCALING
3840 x 3840
MESH PER NODE
(87 ITERATIONS)



Conclusions

- An abstraction for multi-block structured codes
- Covers a sufficiently wide range of applications
- Viability of the Active Library approach
  - Performance, Productivity, Maintainability
- Advanced optimisations relying on the access-execute and loop chaining abstractions

Thank you! istvan.reguly@oerc.ox.ac.uk