OP2: an open-source library for unstructured grid applications

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IMA, University of Minnesota, Jan 10-14, 2011

Outline

- opportunity, challenges, context
- user perspective (i.e. application developer)
  - API
  - build process
- implementation issues
  - hierarchical parallelism on GPUs
  - data dependency
  - code generation
- current status
- lessons learned so far

New heterogeneous hardware

For 10 years, 1995-2005, HPC was relatively simple:

- large clusters, with each node having 2 scalar CPUs
- MPI programming with FORTRAN / C / C++

Now things have become much more complicated:

- multi-core CPUs – up to 12 cores / 24 threads per CPU and each core also has an incrasingly large vector unit
- GPUs have up to 512 cores
- hybrid CPU/GPU SoC chips emerging
- best programming approach unclear:
  - MPI + OpenMP, or MPI + ArBB for CPUs
  - CUDA for GPUs (and CPUs?)
  - OpenCL?

Software Challenges

- HPC application developers want the benefits of the latest hardware but are very worried about the software development costs, and the level of expertise required
- status quo is not an option – running 24 MPI processes on a single CPU would give very poor performance, plus we need to exploit the vector units
- For GPUs, I'm happy with CUDA, but like MPI it's too low-level for many people
- For CPUs, MPI + OpenMP may be a good starting point, and PGI/CRAY are proposing OpenMP extensions which would support GPUs and vector units
- However, hardware is likely to change rapidly in next few years, and developers can not afford to keep changing their software implementation

Software Abstraction

To address these challenges, need to move to a suitable level of abstraction:

- separate the user's specification of the application from the details of the parallel implementation
- aim to achieve application level longevity with the top-level specification not changing for perhaps 10 years
- aim to achieve near-optimal performance through re-targetting the back-end implementation to different hardware and low-level software platforms

Context

Unstructured grid methods are one of Phil Colella's seven dwarfs (*Parallel Computing: A View from Berkeley*)

- dense linear algebra
- sparse linear algebra
- spectral methods
- N-body methods
- structured grids
- unstructured grids
- Monte Carlo

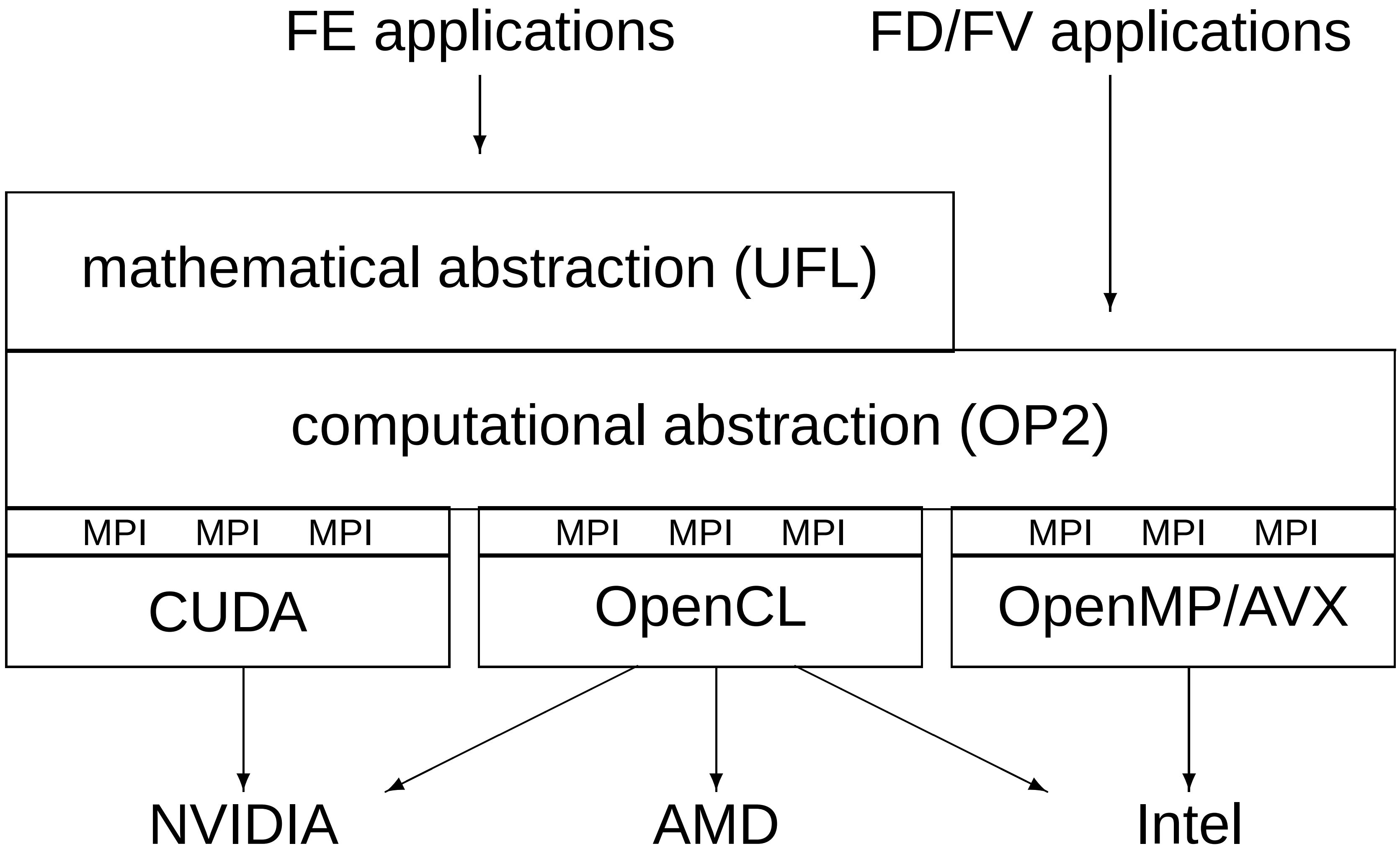
Extensive GPU work for the other dwarfs, except perhaps for direct sparse linear algebra.

Other work

- an increasing number of “one-off” applications, particularly for unstructured grid CFD
- project at George Mason University on auto-porting of FEFLO CFD code to CUDA, using code parsing and generation
- Liszt project at Stanford
  - similar goals to ours
  - funded as part of PSAAP (Predictive Science Academic Alliance Program)
  - defines a domain-specific language using Scala software from ETH Zurich

Context

Part of a larger project led by Paul Kelly at Imperial College



History

OPlus (Oxford Parallel Library for Unstructured Solvers)

- developed for Rolls-Royce 10 years ago
- MPI-based library for HYDRA CFD code on clusters with up to 200 nodes

OP2:

- open source project
- keeps OPlus abstraction, but slightly modifies API
- an “active library” approach with code transformation to generate CUDA, OpenCL and OpenMP/AVX code for GPUs and CPUs

OP2 Abstraction

- sets (e.g. nodes, edges, faces)
- datasets (e.g. flow variables)
- mappings (e.g. from edges to nodes)
- parallel loops
  - operate over all members of one set
  - datasets have at most one level of indirection
  - user specifies how data is used
    (e.g. read-only, write-only, increment)

OP2 Restrictions

- set elements can be processed in any order, doesn’t affect result to machine precision
  - explicit time-marching, or multigrid with an explicit smoother is OK
  - Gauss-Seidel or ILU preconditioning in not
- static sets and mappings (no dynamic grid adaptation)

OP2 API

```
op_init(int argc, char **argv)

op_decl_set(int size, op_set *set, char *name)

op_decl_map(op_set from, op_set to, int dim,
            int *imap, op_map *map, char *name)

op_decl_const(int dim, char *type,
            T *dat, char *name)

op_decl_dat(op_set set, int dim, char *type,
            T *dat, op_dat *data, char *name)

op_exit()
```

OP2 API

Example of parallel loop syntax for a sparse matrix-vector product:

```
op_par_loop_3(res,"res", edges,
   A, -1,OP_ID, 1,"float",OP_READ,
   u,  0,pedge2,1,"float",OP_READ,
   du, 0,pedge1,1,"float",OP_INC);
```

This is equivalent to the C code:

```
for (e=0; e<nedges; e++)
   du[pedge1[e]] += A[e] * u[pedge2[e]];
```

where each “edge” corresponds to a non-zero element in the matrix A, and `pedge1` and `pedge2` give the corresponding row and column indices.

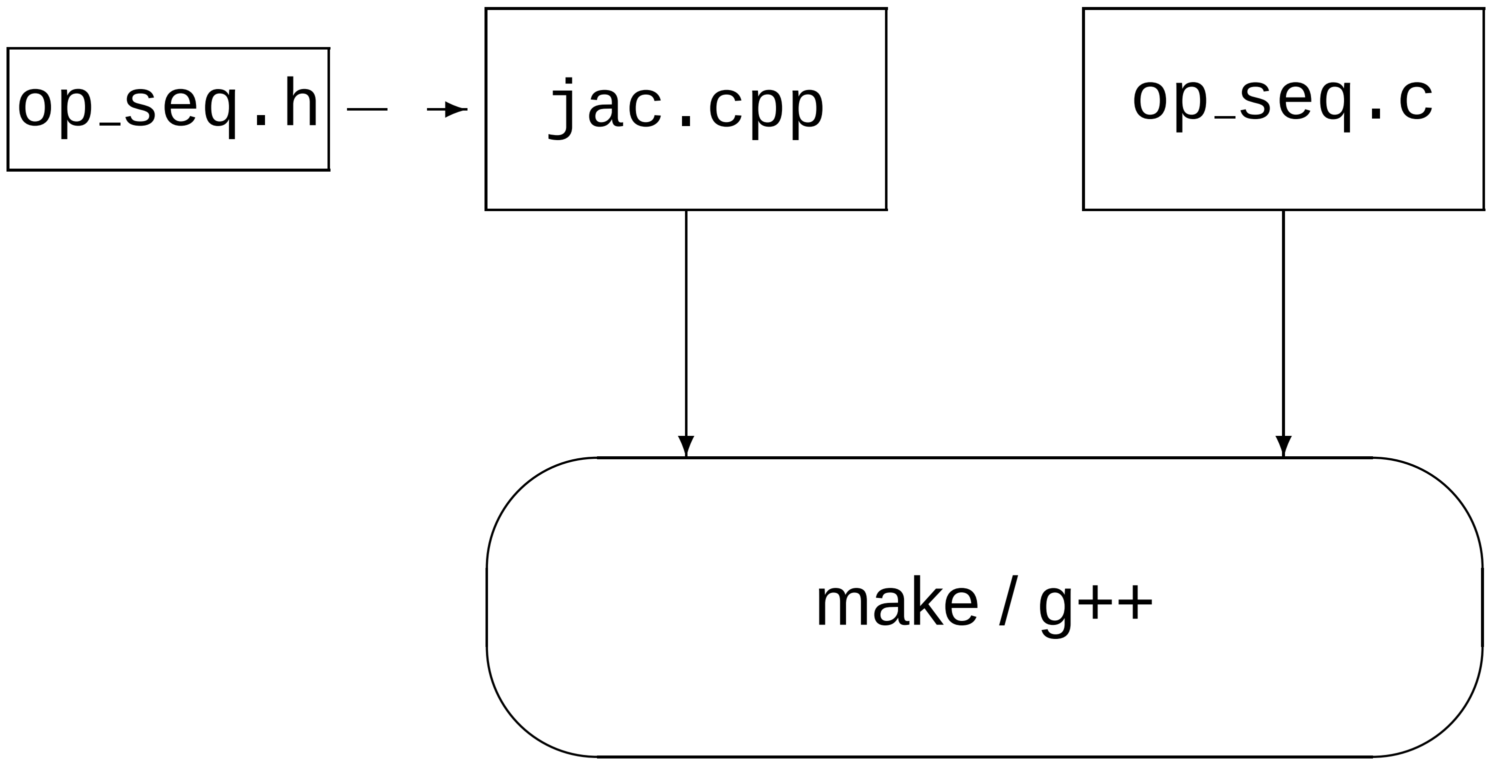
User build processes

Using the same source code, the user can build different executables for different target platforms:

- sequential single-thread CPU execution
  - purely for program development and debugging
  - very poor performance
- CUDA / OpenCL for single GPU
- OpenMP/AVX for multicore CPU systems
- MPI plus any of the above for clusters

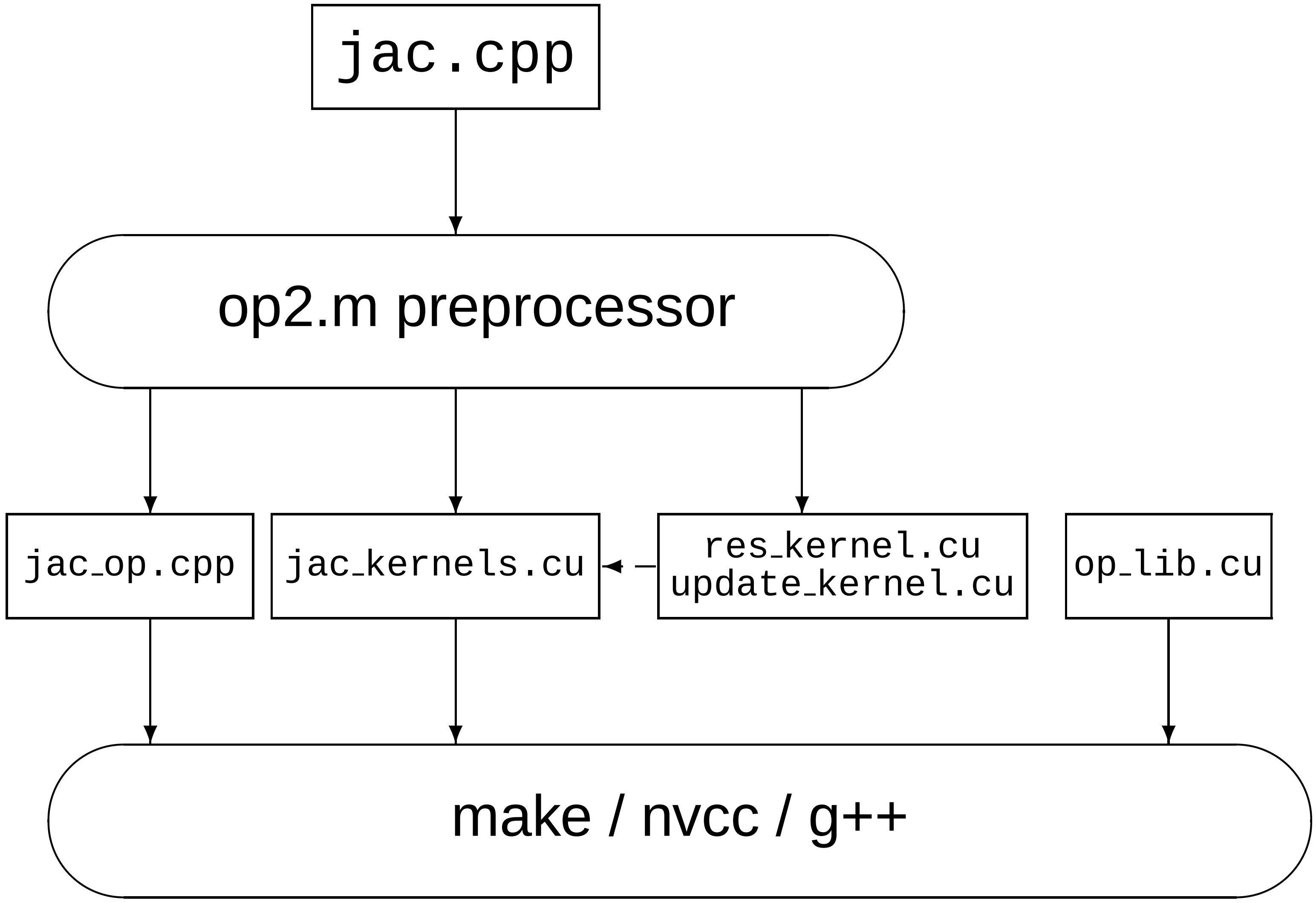
Sequential build process

Traditional build process, linking to a conventional library in which many of the routines do little but error-checking:



CUDA build process

Preprocessor parses user code and generates new code:



GPU Parallelisation

Could have up to 10^6 threads in 3 levels of parallelism:

- MPI distributed-memory parallelism (1-100)
  - one MPI process for each GPU
  - all sets partitioned across MPI processes, so each MPI process only holds its data (and halo)
- block parallelism (50-1000)
  - on each GPU, data is broken into mini-partitions, worked on separately and in parallel by different functional units in the GPU
- thread parallelism (32-128)
  - each mini-partition is worked on by a block of threads in parallel

GPU Parallelisation

The 14 units in an NVIDIA C2050/70 GPU each have

- 32 cores
- 48kB of shared memory and 16kB of L1 cache (or vice versa)

Mini-partitions are sized so that all of the indirect data can be held in shared memory and re-used as needed

- reduces data transfer from/to main graphics memory
- very similar to maximising cache hits on a CPU to minimise data transfer from/to main system memory
- implementation requires re-numbering from global indices to local indices – tedious but not difficult

GPU Parallelisation

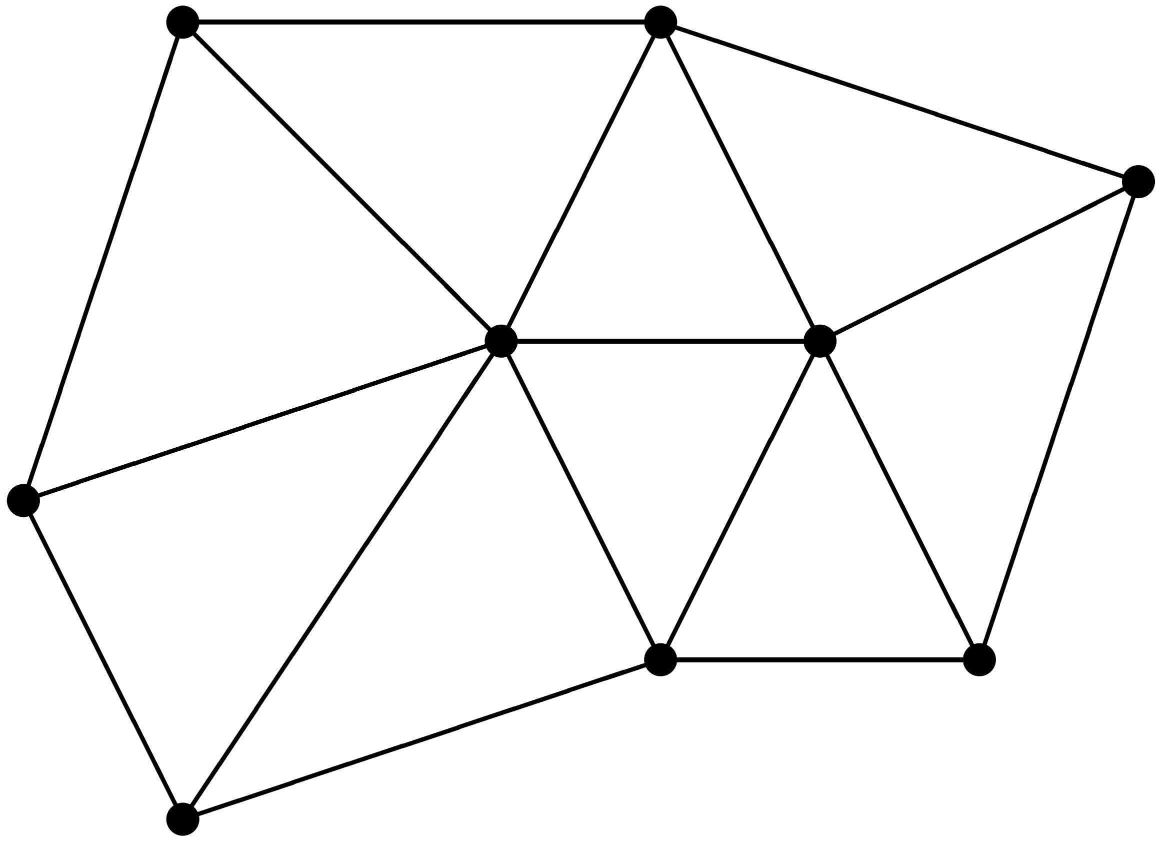
One important difference from MPI parallelisation

- when using one GPU, all data is held in graphics memory in between each parallel loop
- each loop can use a different set of mini-partitions
- current implementation constructs an “execution plan” the first time the loop is encountered
- auto-tuning will be used in the future to optimise the plan, either statically based on profiling data, or dynamically based on run-time timing

Data dependencies

Key technical issue is data dependency when incrementing indirectly-referenced arrays.

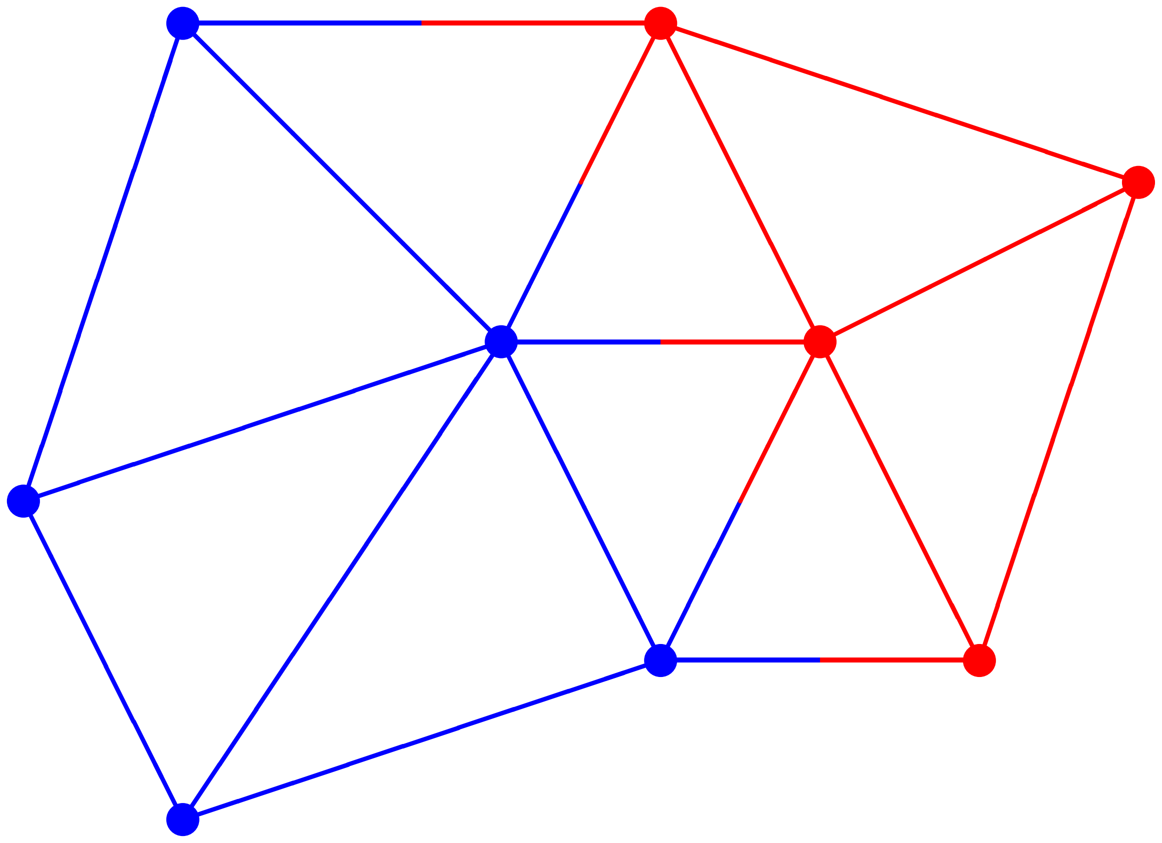
e.g. potential problem when two edges update same node



Data dependencies

Method 1: “owner” of nodal data does edge computation

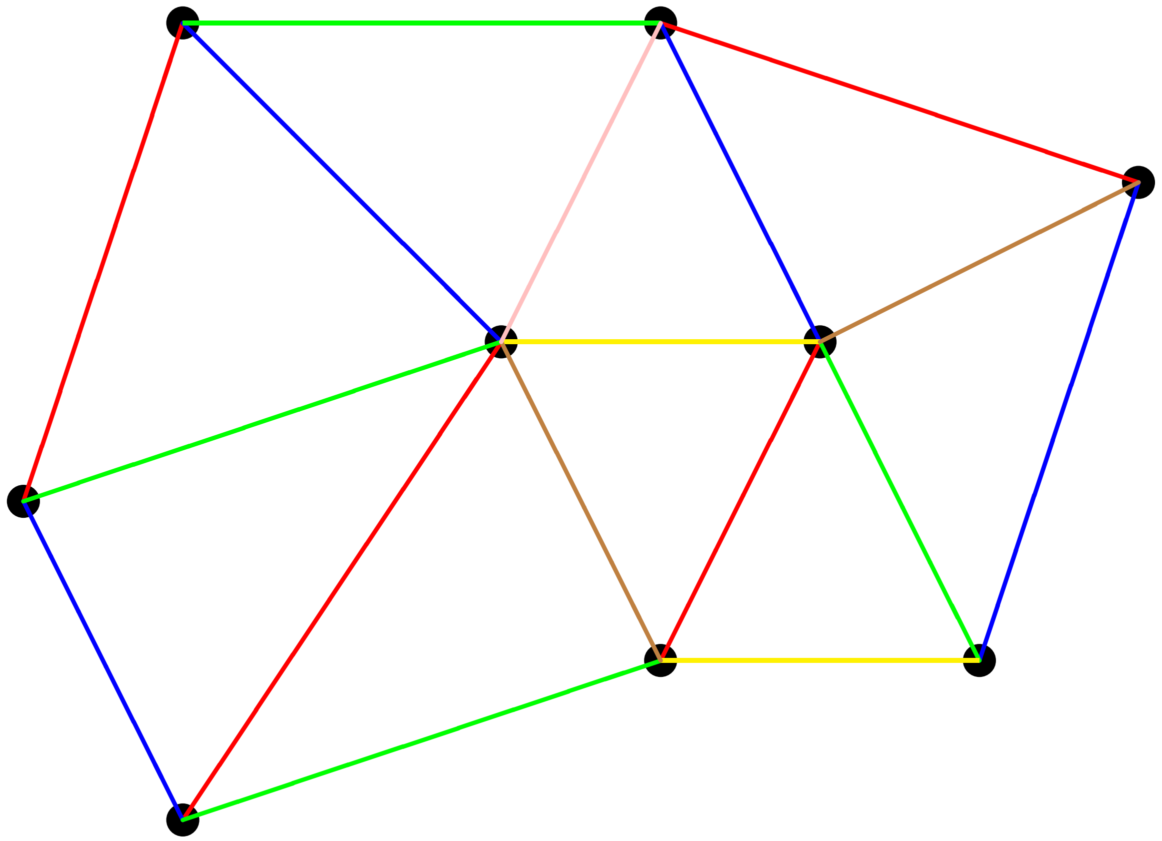
- drawback is redundant computation when the two nodes have different “owners”



Data dependencies

Method 2: “color” edges so no two edges of the same color update the same node

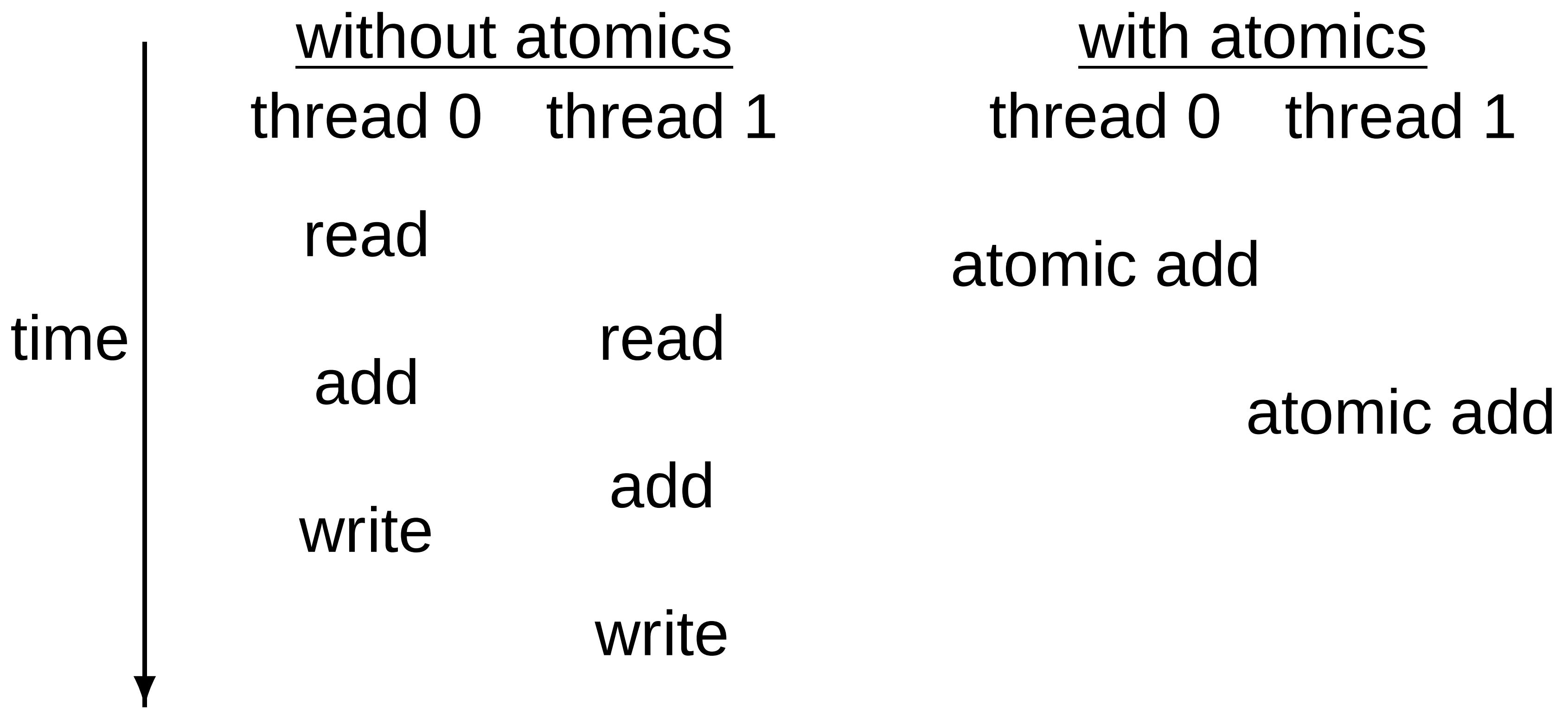
- parallel execution for each color, then synchronize
- possible loss of data reuse and some parallelism



Data dependencies

Method 3: use “atomic” add which combines read/add/write into a single operation

- avoids the problem but needs hardware support
- drawback is slow hardware implementation



Data dependencies

Which is best for each level?

- MPI level: method 1
  - each MPI process does calculation needed to update its data
  - partitions are large, so relatively little redundant computation
- GPU level: method 2
  - plenty of blocks of each color so still good parallelism
  - data reuse within each block, not between blocks
- block level: method 2
  - indirect data in local shared memory, so get reuse
  - individual threads are colored to avoid conflict when incrementign shared memory

Current status

Initial prototype, with code parser/generator written in MATLAB, can generate:

- CUDA code for a single GPU
- OpenMP code for multiple CPUs

The parallel loop API requires redundant information:

- simplifies MATLAB program generation – just need to parse loop arguments, not entire code
- numeric values for dataset dimensions enable compiler optimisation of CUDA code
- “programming is easy; it’s debugging which is difficult” – not time-consuming to specify redundant information provided consistency is checked automatically

Airfoil test code

- 2D Euler equations, cell-centred finite volume method with scalar dissipation (miminal compute per memory reference – should consider switching to more compute-intensive “characteristic” smoothing more representative of real applications)
- roughly 1.5M edges, 0.75M cells
- 5 parallel loops:
  - `save_soln` (direct over cells)
  - `adt_calc` (indirect over cells)
  - `res_calc` (indirect over edges)
  - `bres_calc` (indirect over boundary edges)
  - `update` (direct over cells with RMS reduction)

Airfoil test code

Current performance relative to a single CPU thread:

- 35$\times$ speedup on a single GPU
- 7$\times$ speedup for 2 quad-core CPUs

OpenMP performance seems bandwidth-limited – loops use in excess of 20GB/s bandwidth from main memory.

CUDA performance also seems bandwidth-limited:

count	time	GB/s	GB/s	kernel name
1000	0.2137	107.8126		save_soln
2000	1.3248	61.0920	63.1218	adt_calc
2000	5.6105	32.5672	53.4745	res_calc
2000	0.1029	4.8996	18.4947	bres_calc
2000	0.8849	110.6465		update

Airfoil test code

Library is instrumented to give lots of diagnostic info:

```
new execution plan #1 for kernel res_calc
number of blocks          = 11240
number of block colors    = 4
maximum block size        = 128
average thread colors     = 4.00
shared memory required    = 3.72 KB
average data reuse        = 3.20
data transfer (used)      = 87.13 MB
data transfer (total)     = 143.06 MB
```

- factor 2-4 data reuse in indirect access, but up to 40% of cache lines not used on average
- best performance achieved 8 thread blocks, each with 128 threads, running at same time in each SM (streaming multiprocessor)

Lessons learned so far

1) Code generation works, and it’s not too difficult!

- in the past I’ve been scared of code generation since I have no computer science background
- key is the routine arguments have all of the information required, so no need to parse the entire user code
- now helping a maths student develop a code generator for stochastic simulations in computational biology
  - a generic solver is inefficient – a “hand-coded” specialised implementation for one specific model is much faster
  - code generator takes in model specification and tries to produce “hand-coded” custom implementation

Lessons learned so far

2) The thing which is now causing me most difficulty / concern is the limited number of registers per thread

- limited to about 50 32-bit registers per thread
- above this the data is spilled to L1 cache, but only 16kB of this so when using 256 threads only an extra 16 32-bit variables
- above this the data is spilled to L2 cache, which is 384kB but shared between all of the units in the GPU, so only an extra 48 32-bit variables
- the compiler can maybe be improved, but also there are tricks an expert programmer can use
- points to the benefits of an expert framework which does this for novice programmers

Lessons learned so far

3) Auto-tuning is going to be important

- there are various places in the CUDA code where I have a choice of parameter values (e.g. number of threads, number of blocks, size of mini-partitions, use of L1 cache, 16kB/48kB split between L1 cache and shared memory)
- there are also places where I have a choice of implementation strategy (e.g. thread coloring or atomic updates?)
- what I would like is a generic auto-tuning framework which will optimise these choices for me, given a reasonably small set of possible values
- as a first step, a undergraduate CS student is working with me on a 3rd year project on this

Lessons learned so far

4) Unstructured grids lead to lots of integer pointer arithmetic

- “free” on CPUs due to integer pipelines
- costs almost as much as floating point operations on GPU, at least in single precision
- reduces maximum benefits from GPUs?

5) Open source development leads to great collaboration

- others test code and find bugs – even better, they figure out how to fix them
- will share code development in the future
- everything is available on project webpage: `http://people.maths.ox.ac.uk/gilesm/op2/`

Conclusions

- have created a high-level framework for parallel execution of algorithms on unstructured grids
- looks encouraging for providing ease-of-use, high performance, and longevity through new back-ends
- next step is addition of MPI layer for cluster computing
- key challenge then is to build user community

Acknowledgements

- Paul Kelly, Graham Markall (Imperial College)
- Tobias Brandvik, Graham Pullan (Cambridge)
- Nick Hills (Surrey) and Paul Crumpton
- Leigh Lapworth, Yoon Ho, David Radford (Rolls-Royce)
  Jamil Appa, Pierre Moinier (BAE Systems)
- Tom Bradley, Jon Cohen and others (NVIDIA)
- EPSRC, NVIDIA and Rolls-Royce for financial support
- Oxford Supercomputing Centre