Abstractions and Directives for Adapting Wavefront Algorithms to Future Architectures

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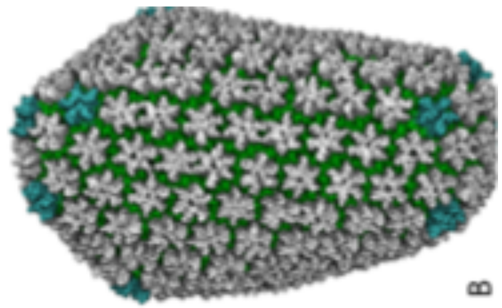
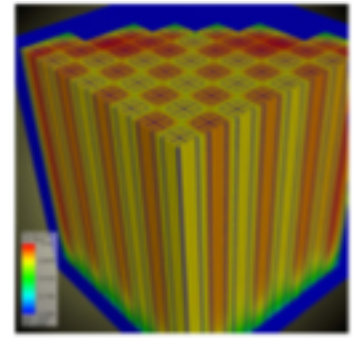
Motivation

- Parallel programming is software's future
  - Acceleration
- State-of-the-art abstractions handle simple parallel patterns well
- Complex patterns are hard!

Our Contributions

- An abstract representation for wavefront algorithms
- A performance portable proof-of-concept of this abstraction using directives: OpenACC
  - Evaluation on multiple state-of-the-art platforms
- A description of the limitations of existing high-level programming models

Several ways to accelerate

Applications

Libraries

Programming Languages

Directives

Drop in acceleration

Maximum Flexibility

Used for easier acceleration

Directive-Based Programming Models

- OpenMP (current version 4.5)
  - Multi-platform shared multiprocessing API
  - Since 2013, supporting device offloading
- OpenACC (current version 2.6)
  - Directive-based model for heterogeneous computing

OpenMP OpenACC
More Science, Less Programming

Serial Example

```
for (int i = 0; i < N; i++) {
        c[i] = a[i] + b[i];
}
```

OpenACC Example

```
#pragma acc parallel loop independent
for (int i = 0; i < N; i++) {
        c[i] = a[i] + b[i];
}
```

CUDA Example

Host Code

```
cudaError_t cudaStatus;

// Choose which GPU to run on, change this on a multi-GPU system.
cudaStatus = cudaSetDevice(0);

// Allocate GPU buffers for three vectors (two input, one output)
cudaStatus = cudaMalloc((void**)&dev_c, N* sizeof(int));
cudaStatus = cudaMalloc((void**)&dev_a, N* sizeof(int));
cudaStatus = cudaMalloc((void**)&dev_b, N* sizeof(int));

// Copy input vectors from host memory to GPU buffers.
cudaStatus = cudaMemcpy(dev_a, a, N* sizeof(int), cudaMemcpyHostToDevice);
cudaStatus = cudaMemcpy(dev_b, b, N* sizeof(int), cudaMemcpyHostToDevice);

// Launch a kernel on the GPU with one thread for each element.
addKernel<<<N/BLOCK_SIZE, BLOCK_SIZE>>>(dev_c, dev_a, dev_b);

// cudaThreadSynchronize waits for the kernel to finish, and returns
// any errors encountered during the launch.
cudaStatus = cudaThreadSynchronize();

// Copy output vector from GPU buffer to host memory.
cudaStatus = cudaMemcpy(c, dev_c, N* sizeof(int), cudaMemcpyDeviceToHost);

cudaFree(dev_c);
cudaFree(dev_a);
cudaFree(dev_b);

return cudaStatus;
```

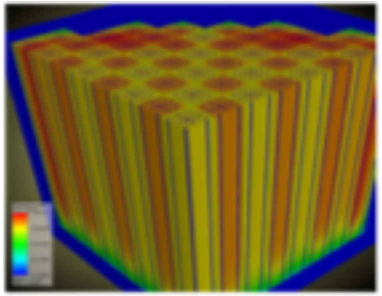
Kernel

```
__global__ void addKernel(int *c, const int *a, const int *b)
{
   int i = threadIdx.x + blockIdx.x * blockDim.x;
   c[i] = a[i] + b[i];
}
```

Pattern-Based Approach in Parallel Computing

- Several parallel patterns
  - Existing high-level languages provide abstractions for many simple patterns
- However there are complex patterns often found in scientific applications that are a challenge to be represented with software abstractions
  - Require manual code rewrite
- Need additional features/extensions!
  - How do we approach this? (Our paper's contribution)

Application Motivation: Minisweep

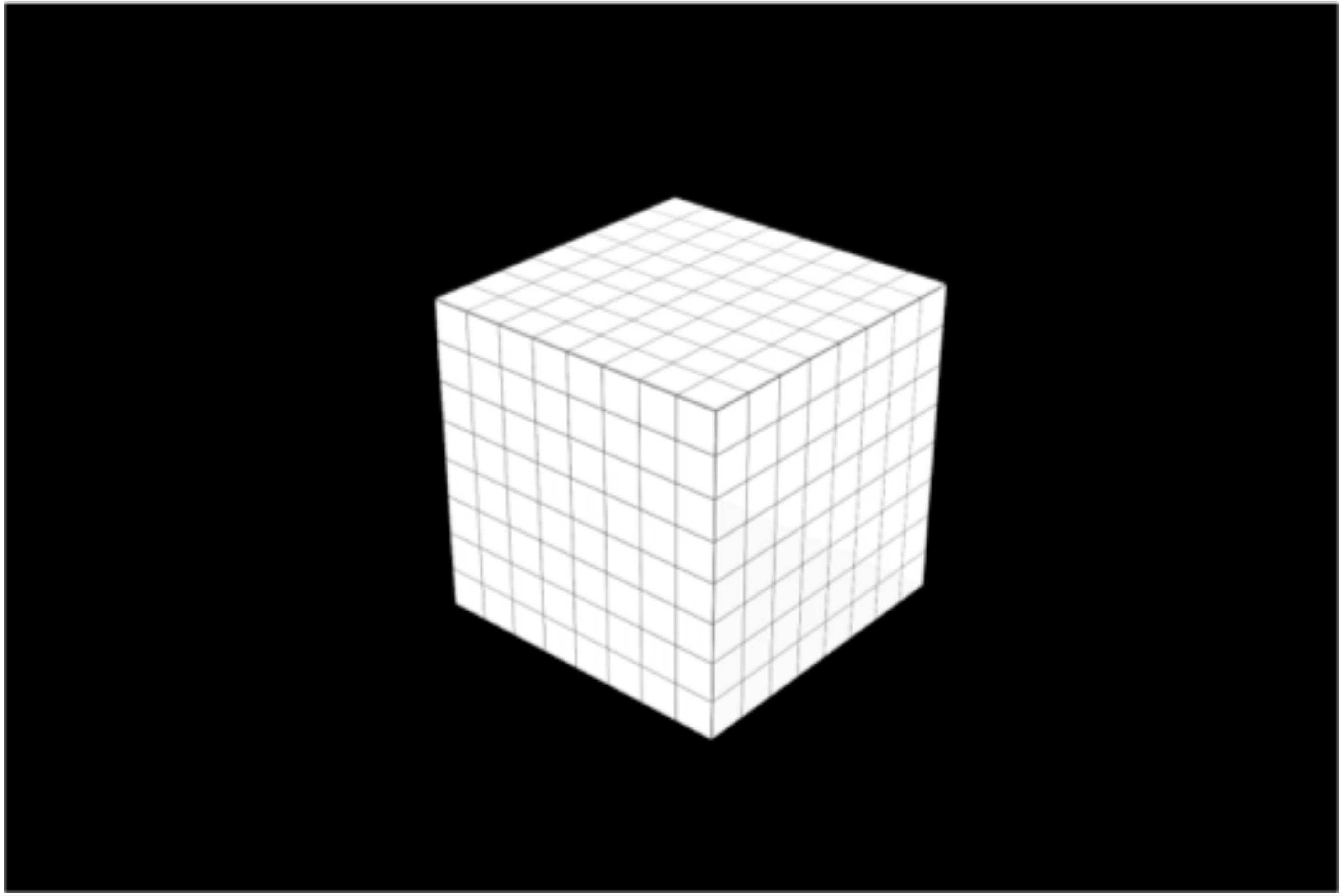


- A miniapp modeling wavefront sweep component of Denovo Radiation transport code from ORNL
  - Minisweep, a miniapp, represents 80-90% of Denovo
- Denovo - part of DOE INCITE project, is used to model fusion reactor – CASL, ITER
- Run many times with different parameters
- The faster it runs, the more configurations we can explore
- Poses a six dimensional problem
- 3D in space, 2D in angular particle direction and 1D in particle energy

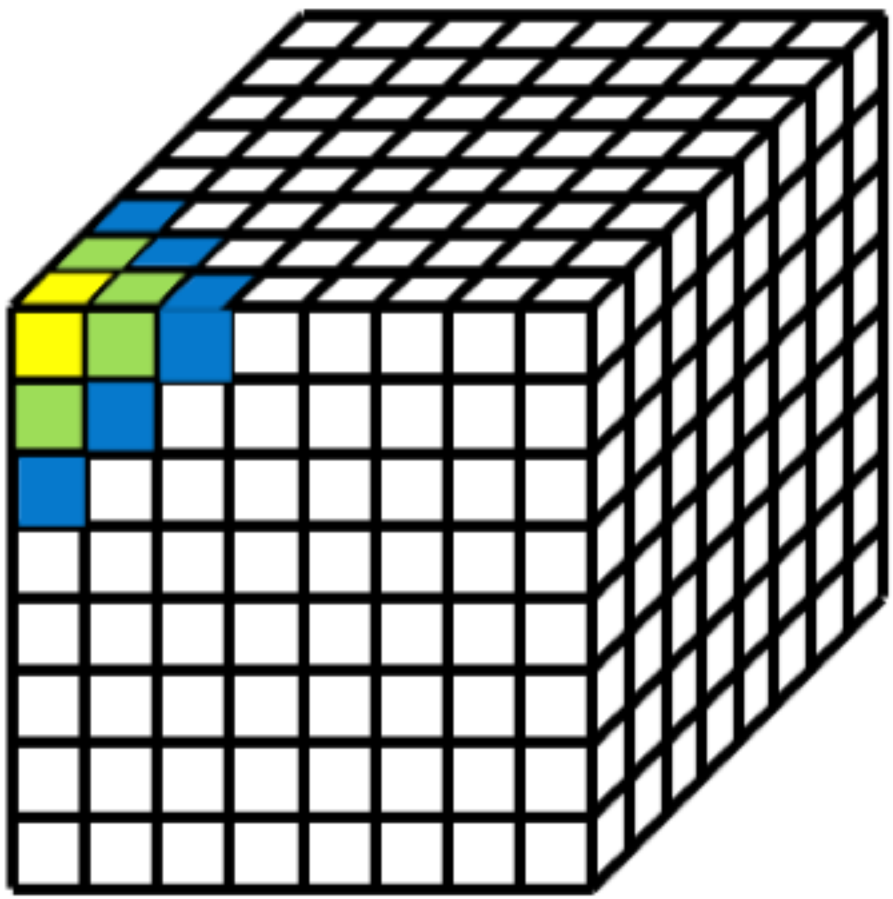
Minisweep code status

- Github: https://github.com/wdj/minisweep
- Early application readiness on ORNL Titan
- Being used for #1 TOP500 -> Summit acceptance testing
- Has been ported to Beacon and Titan (ORNL machines) using OpenMP and CUDA

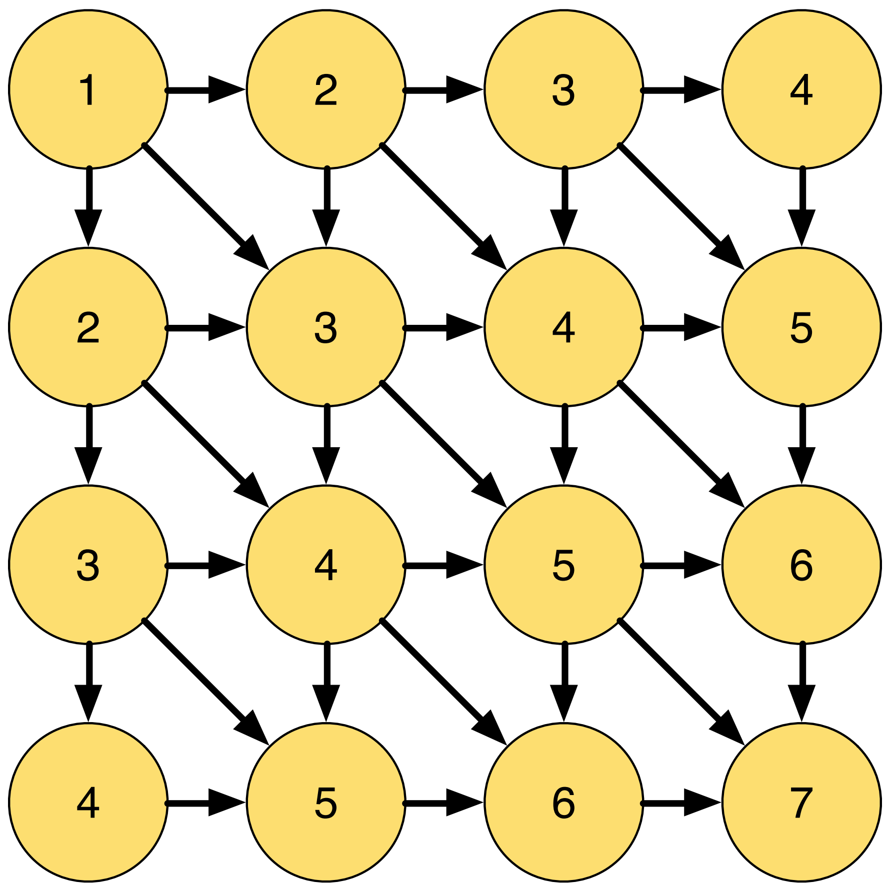
Minisweep: The Basics



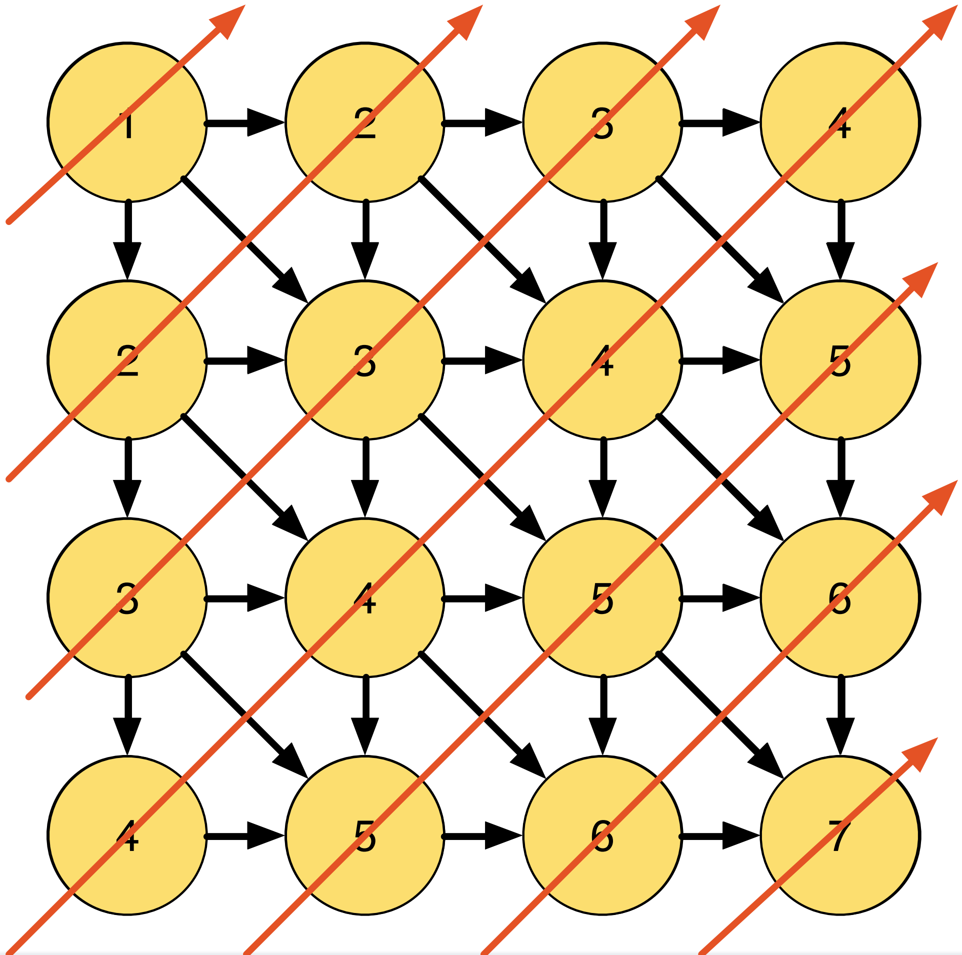
Parallelizing Sweep Algorithm



Complex Parallel Pattern Identified: Wavefront



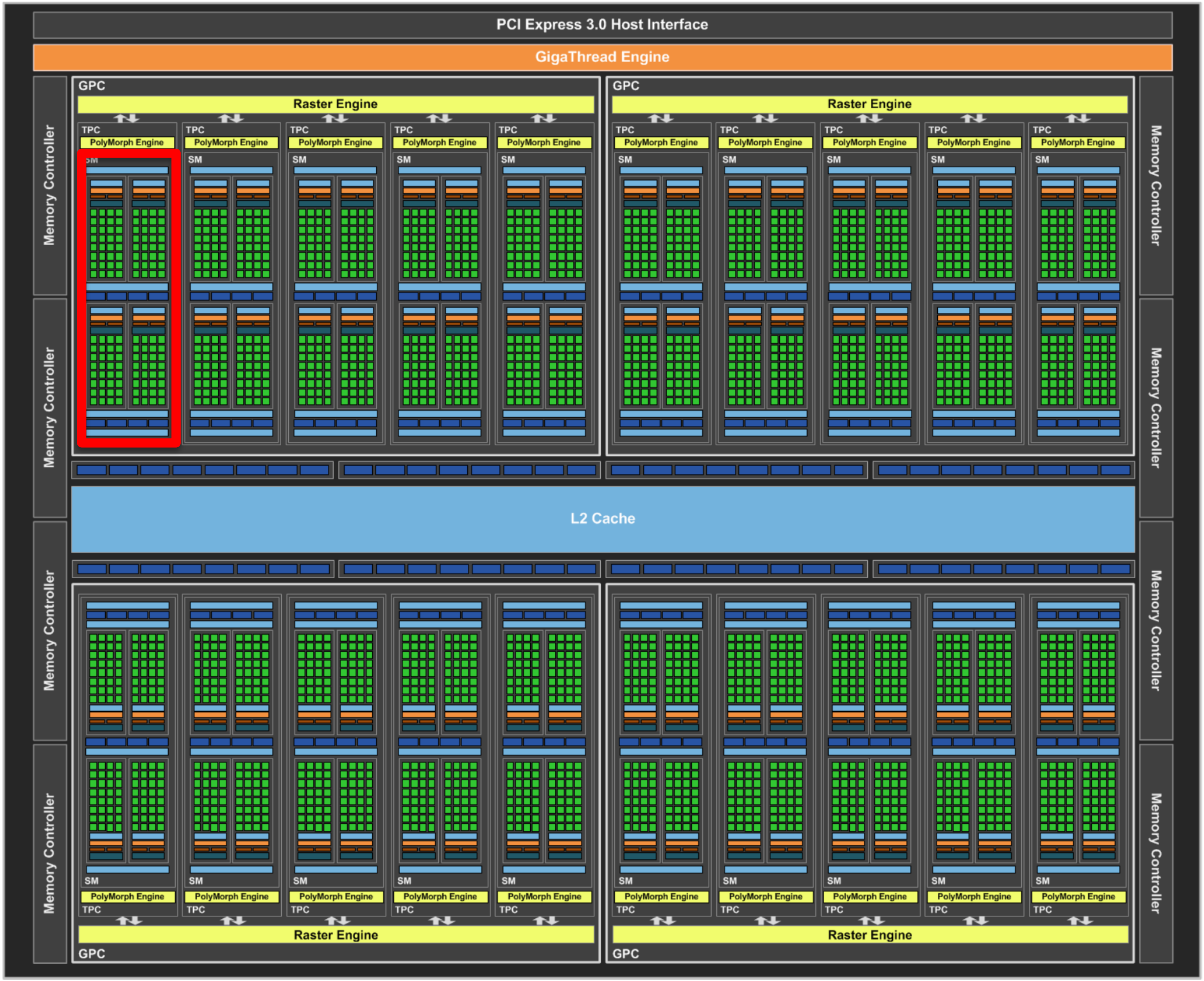
Complex Parallel Pattern Identified: Wavefront



Overview of Sweep Algorithm

- 5 nested loops
  - X, Y, Z dimensions, Energy Groups, Angles
  - OpenACC/PGI only offers 2 levels of parallelism: gang and vector (worker clause not working properly)
  - Upstream data dependency

PCI Express 3.0 Host Interface
GigaThread Engine
GPC
Raster Engine
TPC
PolyMorph Engine
SM
Memory Controller
L2 Cache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Parallelizing Sweep Algorithm: KBA

- Koch-Baker-Alcouffe (KBA)
- Algorithm developed in 1992 at Los Alamos
- Parallel sweep algorithm that overcomes some of the dependencies using a wavefront.

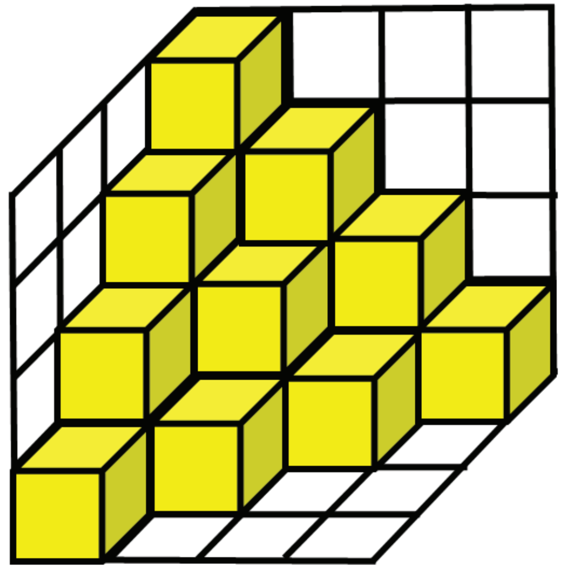


Image credit: High Performance Radiation Transport Simulations: Preparing for TITAN
C. Baker, G. Davidson, T. M. Evans, S. Hamilton, J. Jarrell and W. Joubert, ORNL, USA

Expressing Wavefront via Software Abstractions – A Challenge

- Existing solutions involve manual rewrites, or compiler-based loop transformations
  - Michael Wolfe. 1986. Loop skewing: the wavefront method revisited. *Int. J. Parallel Program.* 15, 4 (October 1986), 279-293. DOI=http://dx.doi.org/10.1007/BF01407876
  - Polyhedral frameworks, only support affine loops, ChiLL and Pluto
- No solution in high-level languages like OpenMP/OpenACC; no software abstractions

Our Contribution: Create Software Abstractions for Wavefront pattern

- Analyzing flow of data and computation in wavefront codes
- Memory and threading challenges
- Wavefront loop transformation algorithm

Abstract Parallelism Model

```
for( iz=izbeg; iz!=izend; iz+=izinc )
for( iy=iybeg; iy!=iyend; iy+=iyinc )
for( ix=ixbeg; ix!=ixend; ix+=ixinc )   { // space

  for( ie=0; ie<dim_ne; ie++ ) { // energy
    for( ia=0; ia<dim_na; ia++ ) {  // angles
      // in-gridcell computation
    }
  }
}
```

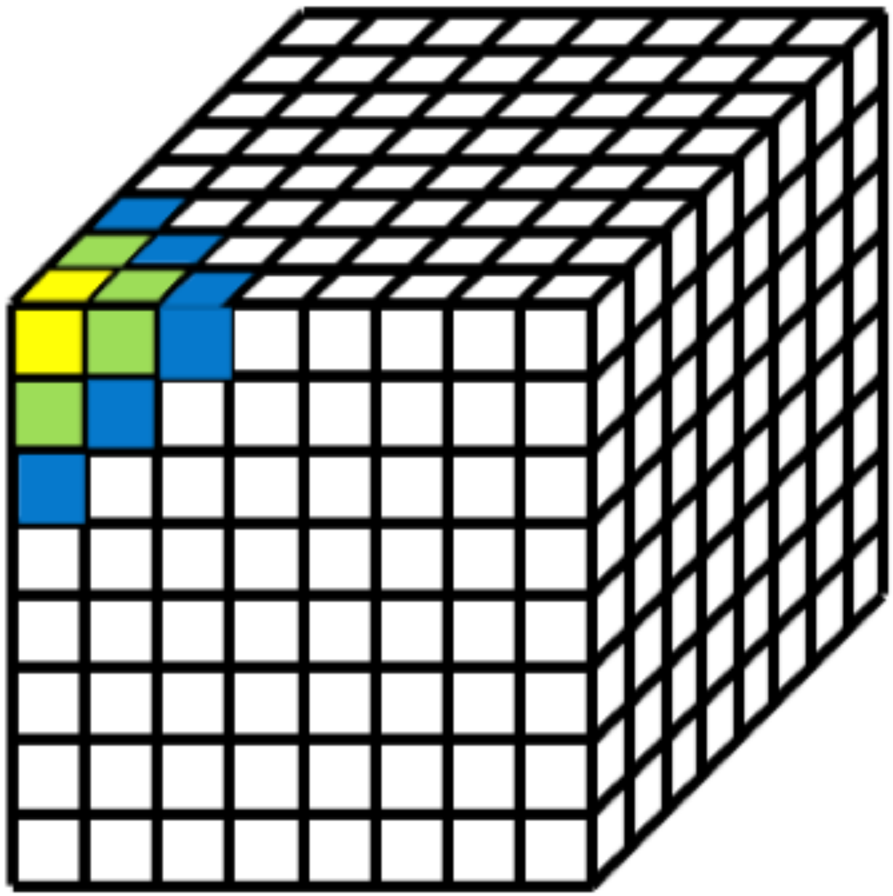
Abstract Parallelism Model

- Spatial decomposition = outer layer (KBA)
  - No existing abstraction for this
- In-gridcell computations = inner layer
  - Application specific
- Upstream data dependencies
  - Slight variation between wavefront applications

Data Model

- Storing all previous wavefronts is unnecessary
  - How many neighbors and prior wavefronts are accessed?
- Face arrays make indexing easy
  - Smaller data footprint
- Limiting memory to the size of the largest wavefront is optimal, but not practical

Parallelizing Sweep Algorithm: KBA



Programming Model Limitations

- No abstraction for wavefront loop transformation
  - Manual loop restructuring
- Limited layers of parallelism
  - 2 isn't enough (worker is broken)
  - Asynchronous execution?

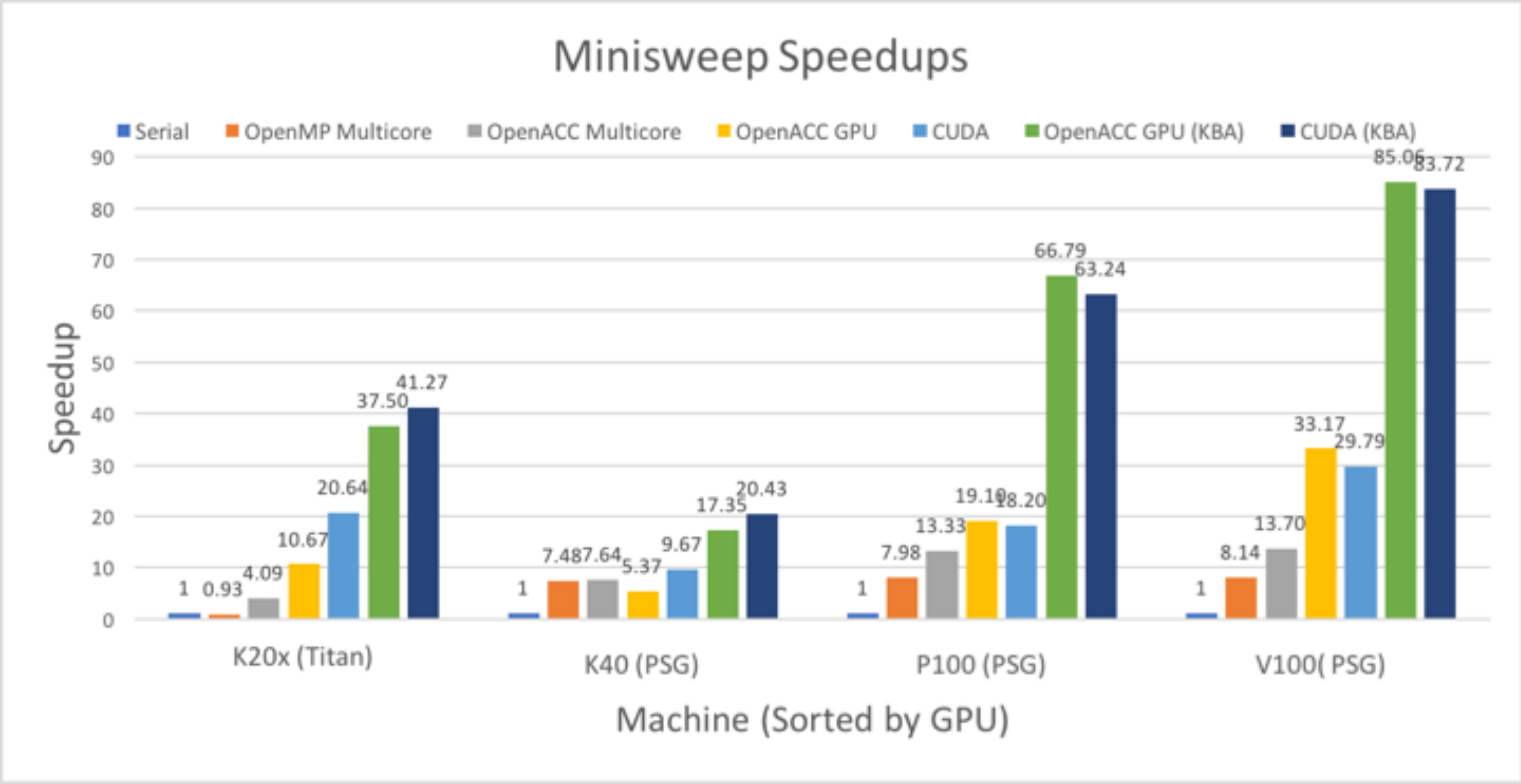
Experimental Setup

- NVIDIA PSG Cluster
  - CPU: Intel Xeon E5-2698 v3 (16-core) and Xeon E5-2690 v2 (10-core)
  - GPU: NVIDIA Tesla P100, Tesla V100, and Tesla K40 (4 GPUs per node)
- ORNL Titan
  - CPU: AMD Opteron 6274 (16-core)
  - GPU: NVIDIA Tesla K20x
- ORNL SummitDev
  - CPU: IBM Power8 (10-core)
  - GPU: NVIDIA Tesla P100
- PGI OpenACC Compiler 17.10
- OpenMP – GCC 6.2.0
  - Issues running OpenMP minisweep code on Titan but works OK on PSG.

Input Parameters

- Scientifically
  - X/Y/Z dimensions = 64
  - # Energy Groups = 64
  - # Angles = 32
- Goal is to explore larger spatial dimensions

Machine	CPU	GPU
NVIDIA PSG (V100)	Intel Xeon E5-2698 v3 (16 cores)	NVIDIA Tesla V100 (16GB HBM2)
NVIDIA PSG (P100)	Intel Xeon E5-2698 v3 (16 cores)	NVIDIA Tesla P100 (16GB HBM2)
NVIDIA PSG (K40)	Intel Xeon E5-2690 v2 (10 cores)	NVIDIA Tesla K40 (12GB GDDR5)
ORNL Titan	AMD Opteron 6274 (16 cores)	NVIDIA Tesla K20X (6GB GDDR5)



Contributions

- An abstract representation of wavefront algorithms
- A performance portable proof-of-concept of this abstraction using OpenACC
  - Evaluation on multiple state-of-the-art platforms
- A description of the limitations of existing high-level programming models

Next Steps

- Asynchronous execution
- MPI - multi-node/multi-GPU
- Develop a generalization/extension to existing high-level programming models
  - Prototype

Preliminary Results/Ongoing Work

- MPI + OpenACC
  - 1 node x 1 P100 GPU = 66.79x speedup
  - 4 nodes x 4 P100 GPUs/node = 565.81x speedup
  - 4 nodes x 4 V100 GPUs/node = 624.88x speedup
- Distributing the workload lets us examine larger spatial dimensions
  - Future: Use blocking to allow for this on a single GPU

Takeaway(s)

- Using directives is not magical! Compilers are already doing a lot for us! ☺
- Code benefits from incremental improvement – so let's not give up! ☺
- *Profiling and Re-profiling is highly critical*
- Look for any serial code refactoring, if need be
  - Make the code parallel and accelerator-friendly
- Watch out for compiler bugs and *report them*
  - The programmer is not 'always' wrong
- Watch out for *novel language extensions and propose to the committee* - User feedback
  - Did you completely change the loop structure? Did you notice a parallel pattern for which we don't have a high-level directive yet?

Contributions

- An abstract representation of wavefront algorithms
- A performance portable proof-of-concept of this abstraction using directives, OpenACC
  - Evaluation on multiple state-of-the-art platforms
- A description of the limitations of existing high-level programming models
- Contact: rsearles@udel.edu
- Github: https://github.com/rsearles35/minisweep

Additional Material

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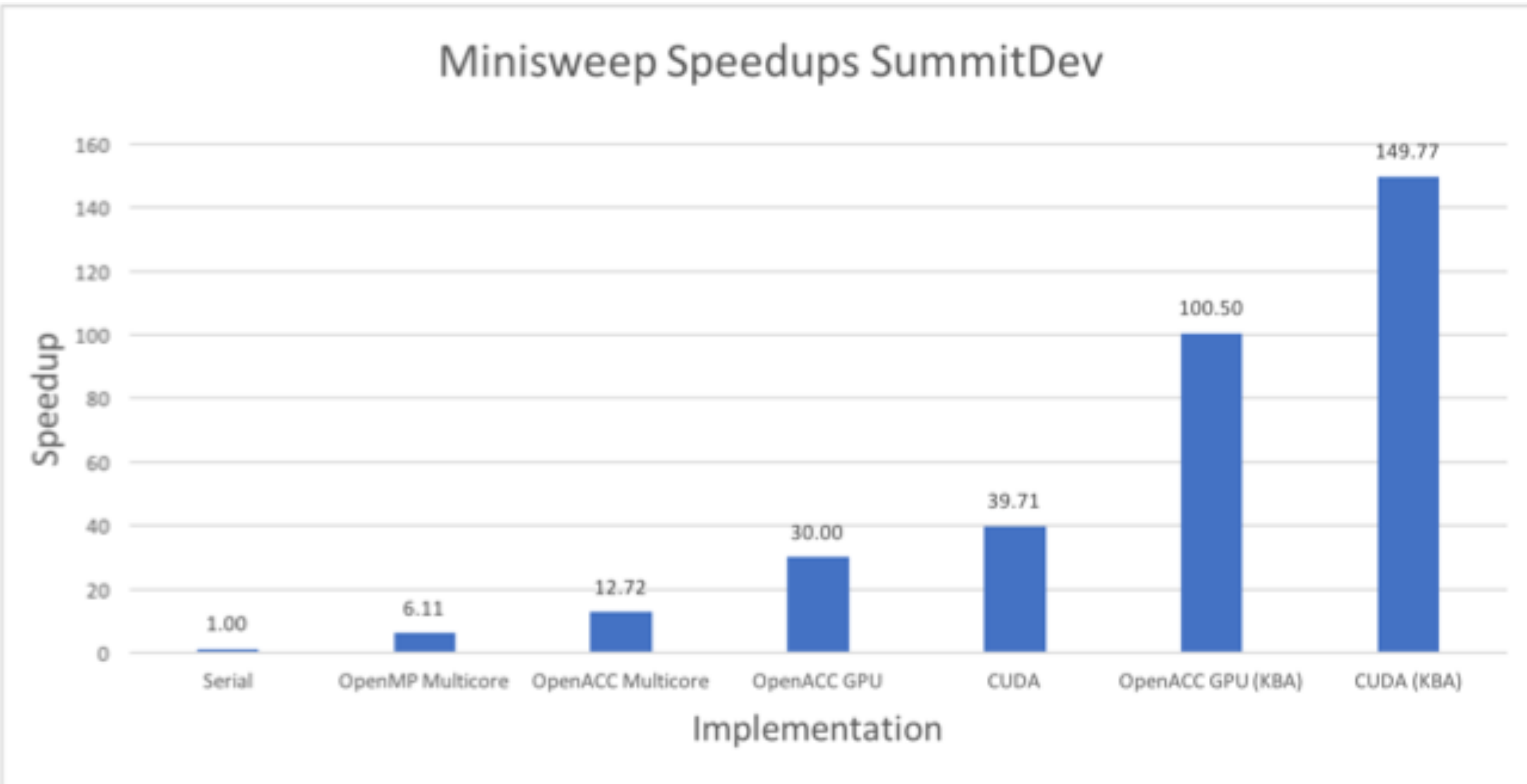
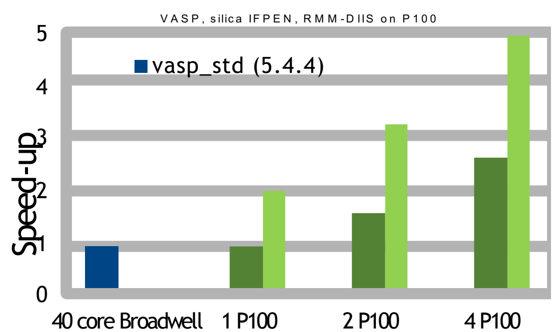


OPENACC GROWING MOMENTUM

Wide Adoption Across Key HPC Codes

ANSYS Fluent, Gaussian, VASP



* OpenACC port covers more VASP routines than CUDA, OpenACC port planned top down, with complete analysis of the call tree, OpenACC port leverages improvements in latest VASP Fortran source base

3 of Top 5 HPC Applications Use OpenACC

GTC
XGC
ACME
FLASH
LSDalton

CAAR Codes Use OpenACC

<u>Key Codes Globally</u>

COSMO, IFS(ESCAPE), NICAM, ICON, MPAS

<u>Gordon Bell Finalist</u>

CAM-SE on Sunway Taihulight

OpenACC Dominates in Climate & Weather

OpenACC

- Minisweep, a miniapp, represents 80-90% of Denovo S_n code
- Denovo S_n (discrete ordinate), part of DOE INCITE project, is used to model fusion reactor – CASL, ITER
- **Impact:** By running Minisweep faster, experiments with more configurations can be performed directly impacting the determination of accuracy of radiation shielding
- Poses a six dimensional problem
- 3D in space, 2D in angular particle direction and 1D in particle energy