LULESH and OpenACC:
To Exascale and Beyond!!!

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1. Introduction and Motivations

2. OpenACC

3. Challenges

4. Methodologies and Results

5. Conclusions

Exascale Architectures

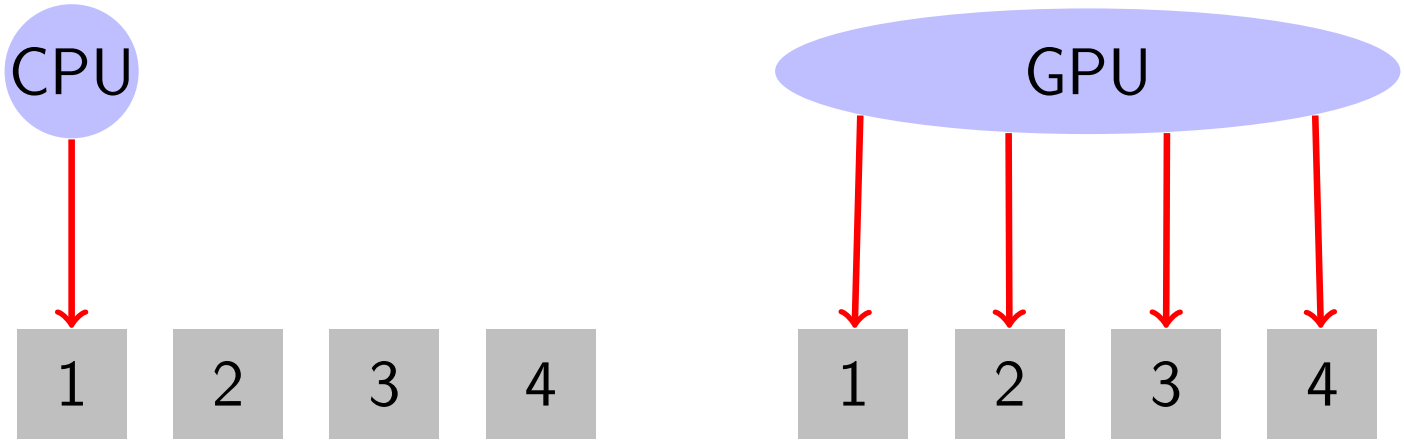
Heterogeneity

- Supercomputers will no longer have simple, homogeneous nodes with many CPU cores
- GPUs and other accelerators are dominating the horsepower of new systems

	Sequoia	**Titan**	**Tianhe-2**
PFLOPS	17.17	17.59	33.86
Architecture	BG/Q	AMD CPU + NVIDIA GPU	Intel CPU + MIC
Nodes/Cores	98.30K / 1.57M	18.68K / 0.56M	16.00K / 3.12M
Power	7.89MW	8.20MW	17.80MW

GPU Overview

- GPUs are massively parallel accelerators designed for graphics processing
- Very good at *stream processing*
  - Scan over a large list of data, doing identical math on each index
- The CPU and GPU do not share memory
  - The programmer must maintain copies on both



Proxy Applications

Motivation

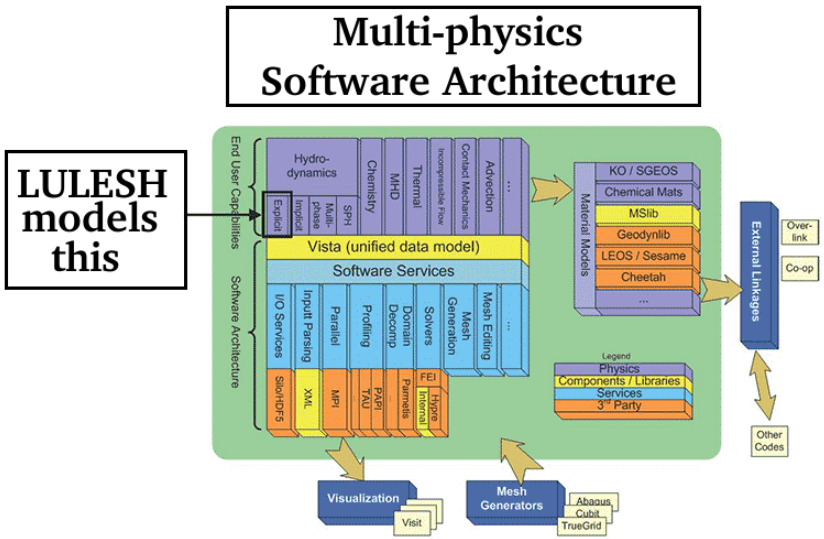
- Rewriting a large simulation code is a major investment
- Instead, extract a small but representative portion
- Can be modified and also released for public use
  - Great for hardware co-design!

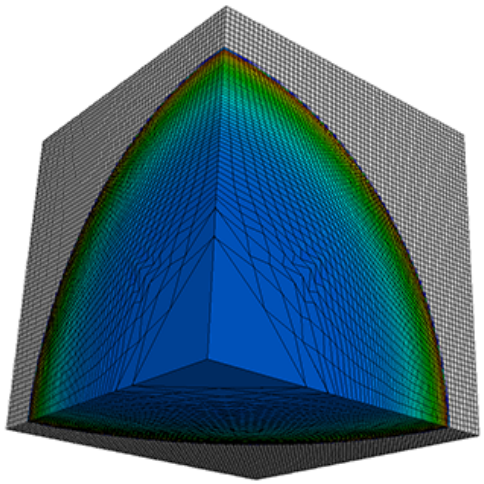
Proxy Apps

- AMG2013
- **LULESH**
- MCB
- UMT

LULESH Overview

- Data layout, memory access patterns, and computation are very similar to a typical multi-physics code's hydro kernel
- Only a few thousand lines of code, so it's easy to rewrite for new architectures and programming models





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What is OpenACC?

- C/C++/Fortran API that supports offloading work to accelerator devices
- Uses pragmas to provide the compiler hints for parallel regions
  - Familiar interface for OpenMP programmers!

```
1  /* A, B, and C currently on CPU */
2  #pragma acc parallel loop copyin(A[0:N], \
3                                   B[0:N]) \
4                            copyout(C[0:N])
5  for(int i = 0; i < N; ++i) {
6    C[i] = A[i] * B[i];
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OpenACC - Introduction

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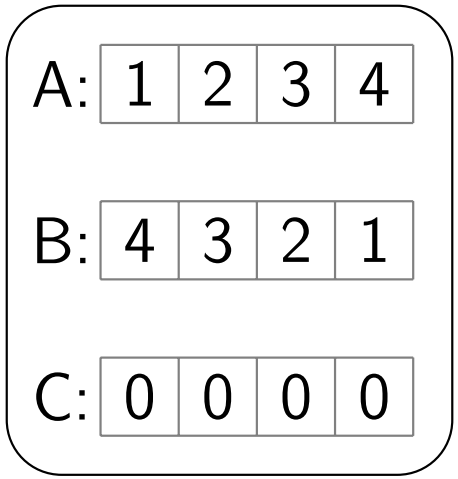
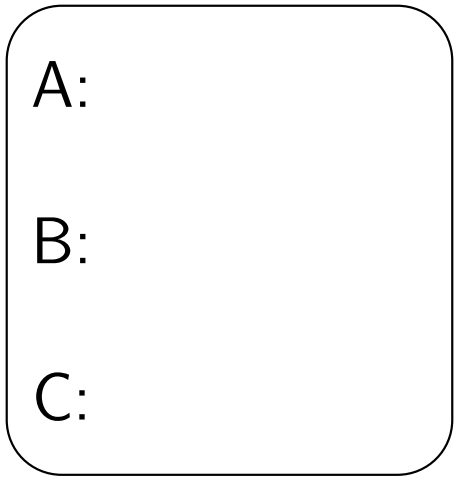


CPU



Accelerator

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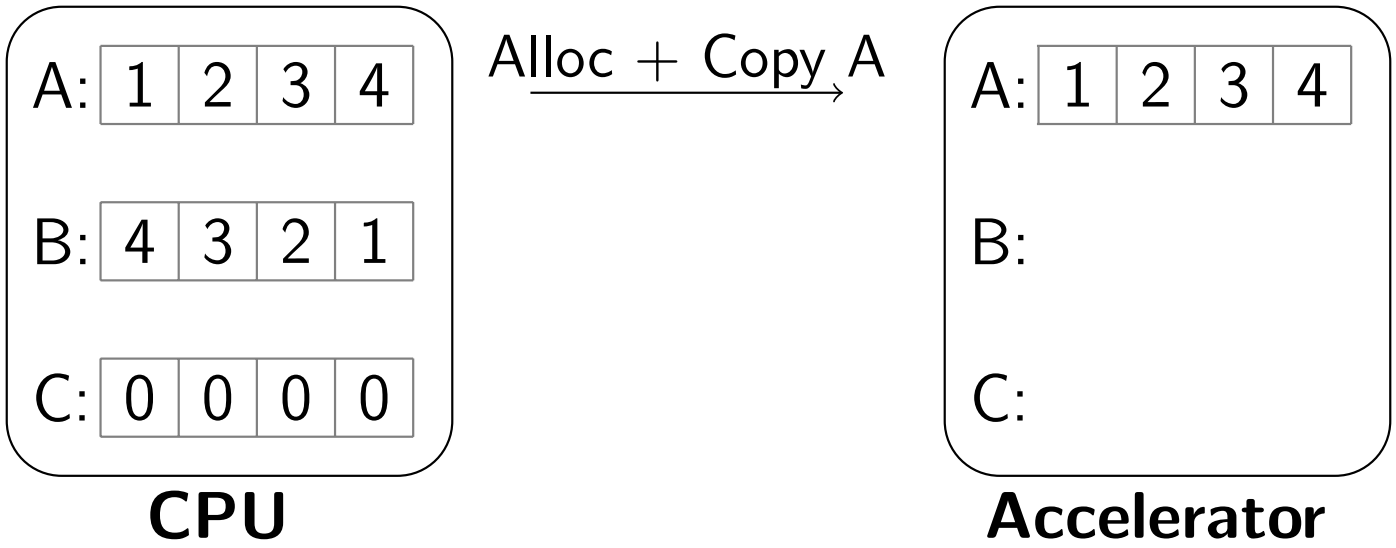

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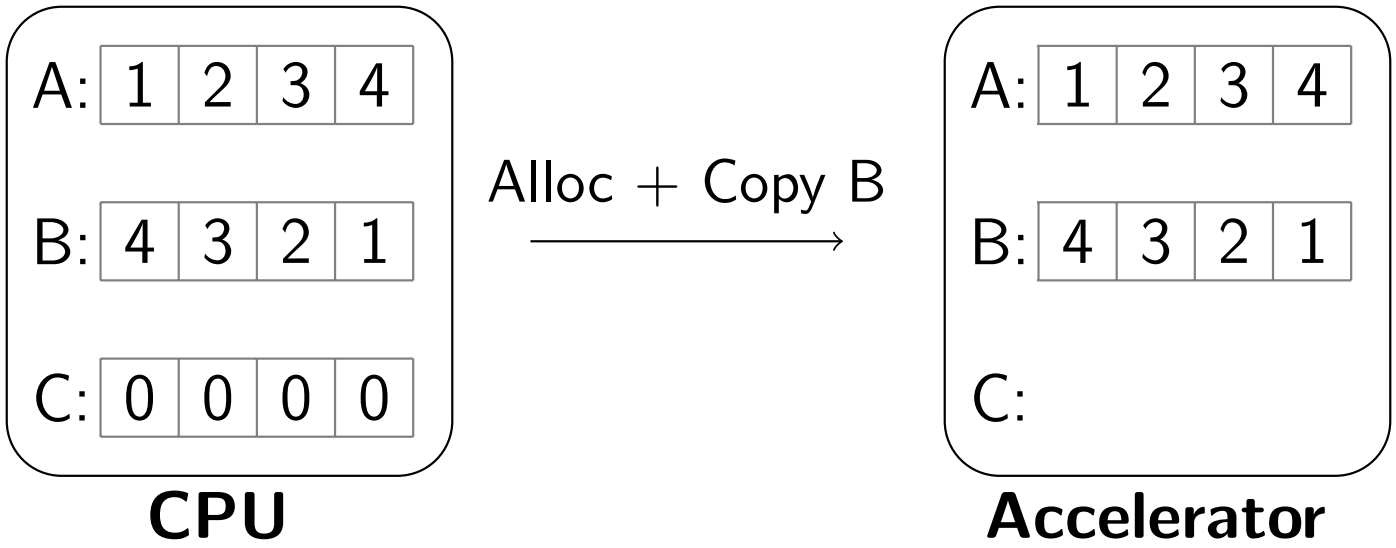

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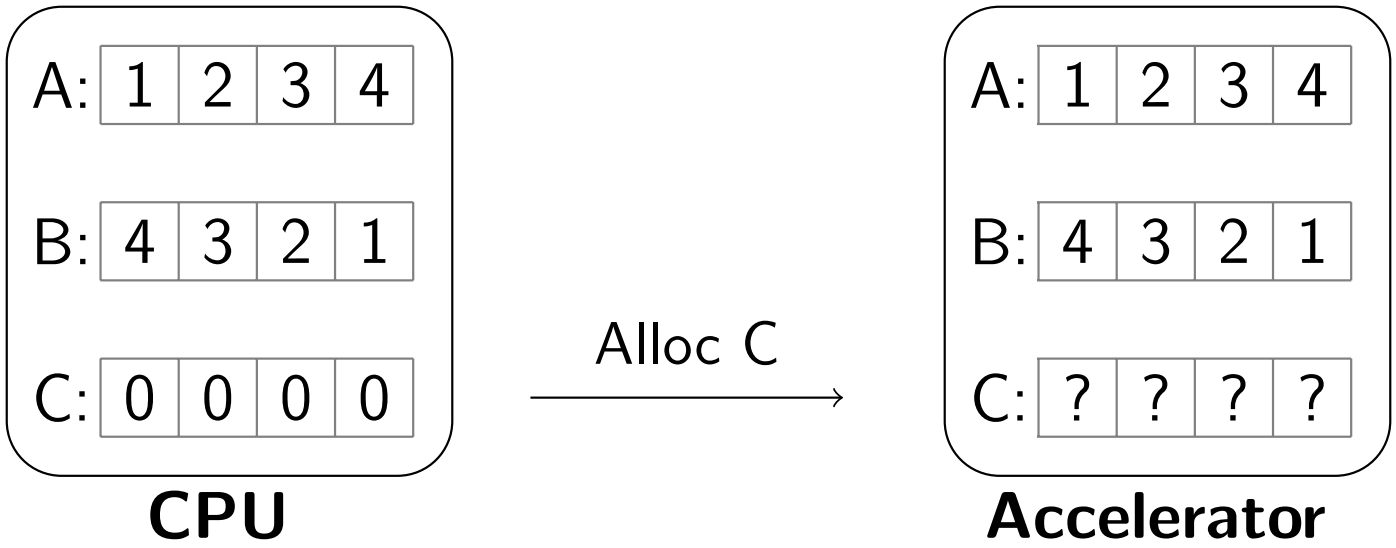

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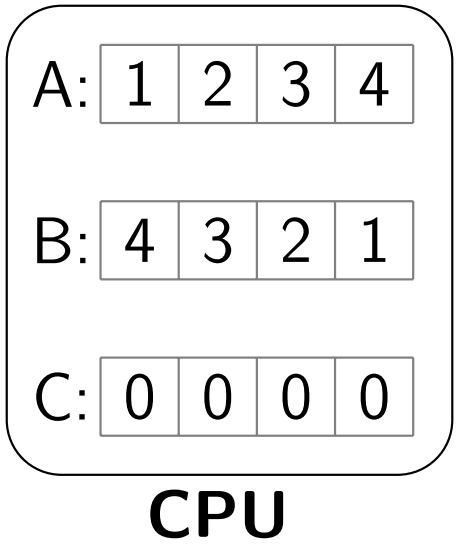

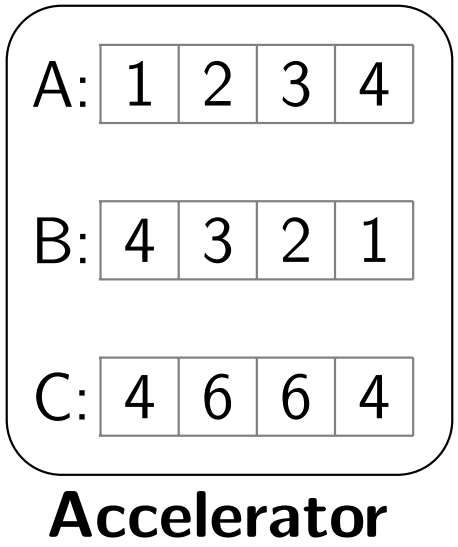

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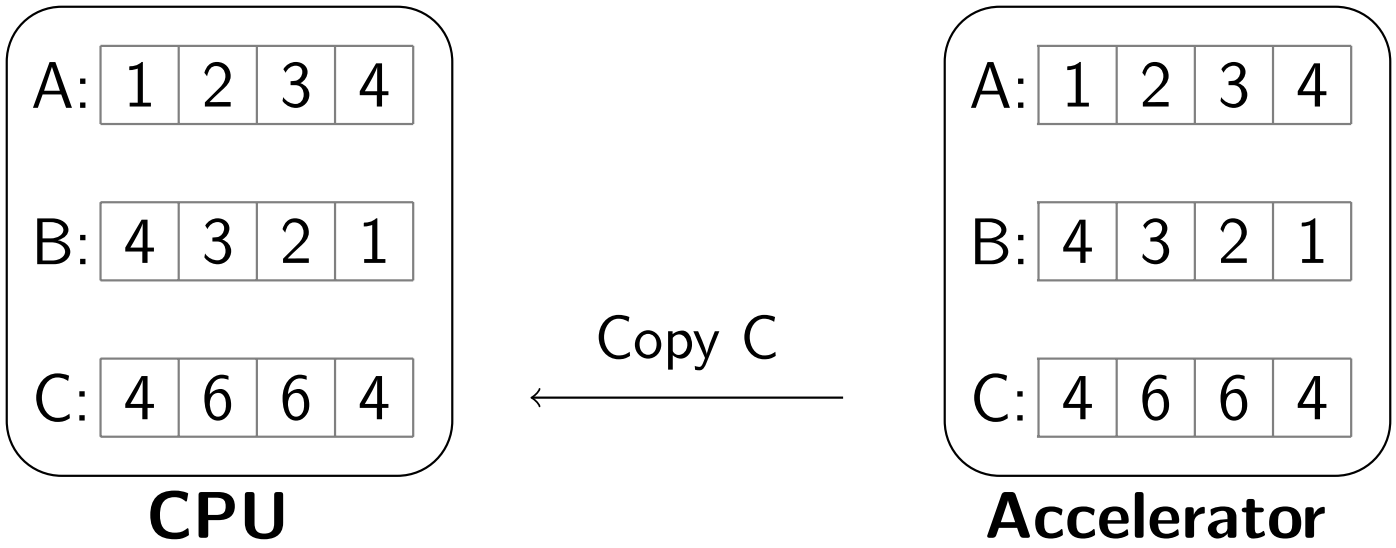

Data Regions

- Data regions provide a means of specifying memory transfers
- Minimizing data movement between the CPU and accelerator is essential for performance

```
1  /* A, B, and C allocated on CPU */
2  #pragma acc data copyin(A[0:N], \
3                          B[0:N]) \
4                  copyout(C[0:N])
5  {
6    /* A, B, and C are now on accelerator */
7    compute_C(A,B,C);
8    compute_more_C(A,B,C);
9  }
10 /* C has now been updated on CPU */
```

OpenACC - Availability

Compiler Support

- Three compilers have implementations of OpenACC
  - PGI, CAPS, Cray
- Our code has only been tested with PGI thus far

LLNL Support

- edge and rzgpu both have pgi-accelerator available
  - Compile on edge84 and rzgpu2

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Implicit Data Regions

- When functions are called from within a data region, the programmer must be aware of which memory is found on the accelerator
- It's easy to forget where your data is and instead access junk

```
1  #pragma acc data copyin(A[0:N], \
2                          B[0:N]) \
3                  copyout(C[0:N])
4  {
5    compute_C(A,B,C);
6    print_intermediate_results(C); /* OUCH! */
7    compute_more_C(A,B,C);
8  }
```

Thread-Local Arrays

- The OpenACC standard currently doesn't say what to do with local arrays in accelerated regions
- As of pgcc v13.6, these are treated as a shared resource among threads

Before

```
1   for(Index_t i = 0; i < N; ++i) {
2     Real_t scratch[4];
3     for(Index_t j = 0; j < 4; ++j) {
4       scratch[j] = x[i*4 + j];
5     }
6
7
8
9
10
11
12    /* do work */
13  }
```

After

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6
7
8
9
10
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12   /* do work */
13 }
```

After

```
#pragma acc parallel loop copy(x[0:N*4])
for(Index_t i = 0; i < N; ++i) {
  Real_t scratch0;
  Real_t scratch1;
  Real_t scratch2;
  Real_t scratch3;

  scratch0 = x[i*4 + 0];
  scratch1 = x[i*4 + 1];
  scratch2 = x[i*4 + 2];
  scratch3 = x[i*4 + 3];
  /* do work */
}
```

Runtime Errors

- Class members are often extracted before entering a data region
  - Currently you cannot access members within a pragma
- If these are not made `volatile`, they will be optimized away

```
1  volatile Real_t *x = domain.x();
2           Real_t *y = domain.y(); /* y is optimized away */
3  #pragma acc data copyin(x[0:N], \
4                          y[0:N]) /* runtime error! */
5  {
6    accelerated_physics(domain);
7  }
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Compiler Optimizations

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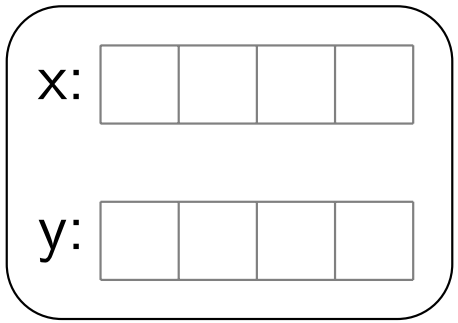

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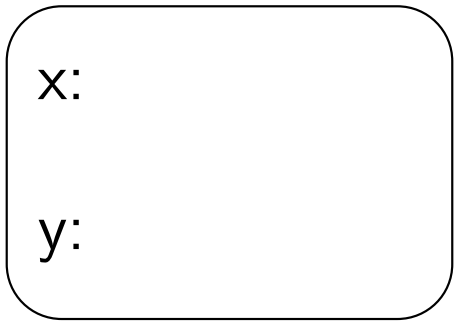

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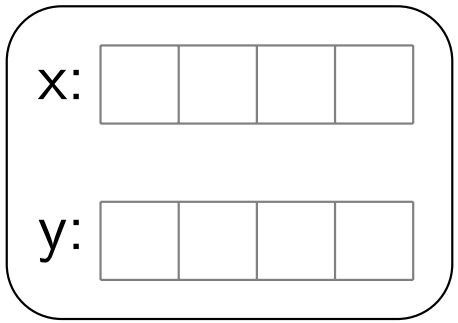

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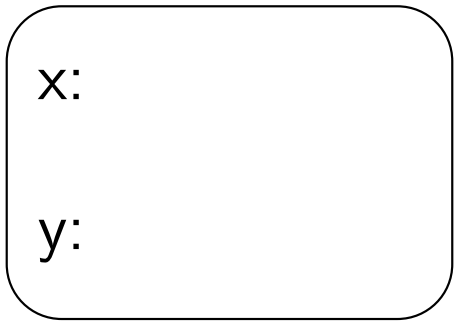

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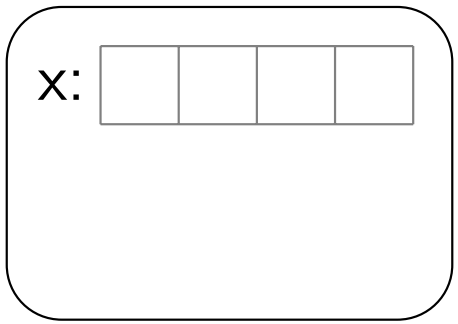

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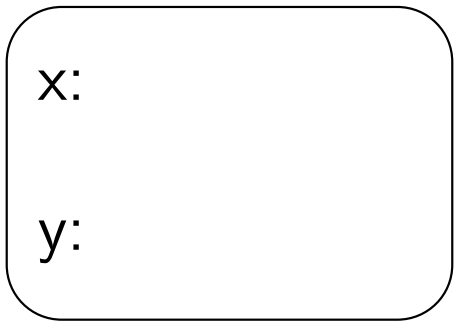

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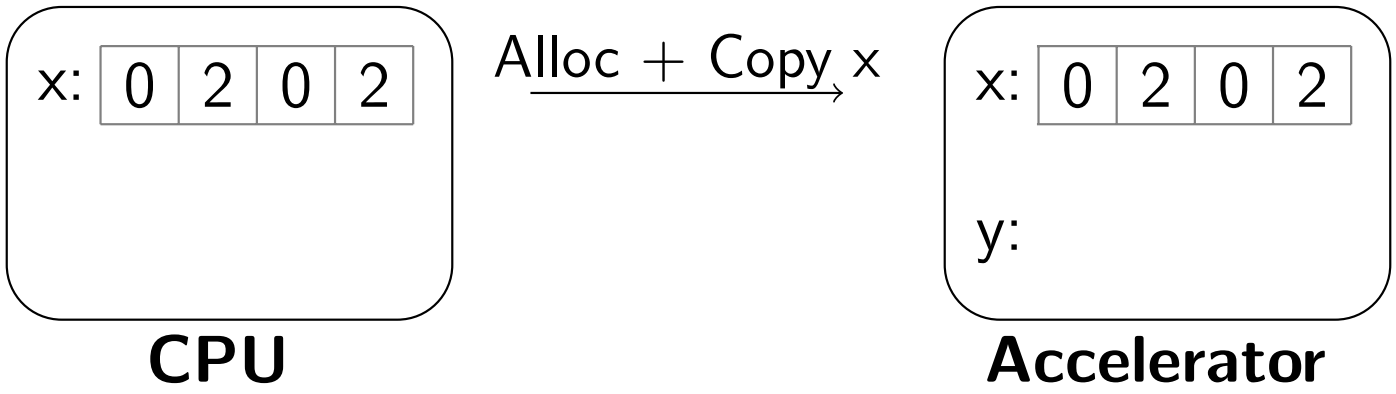

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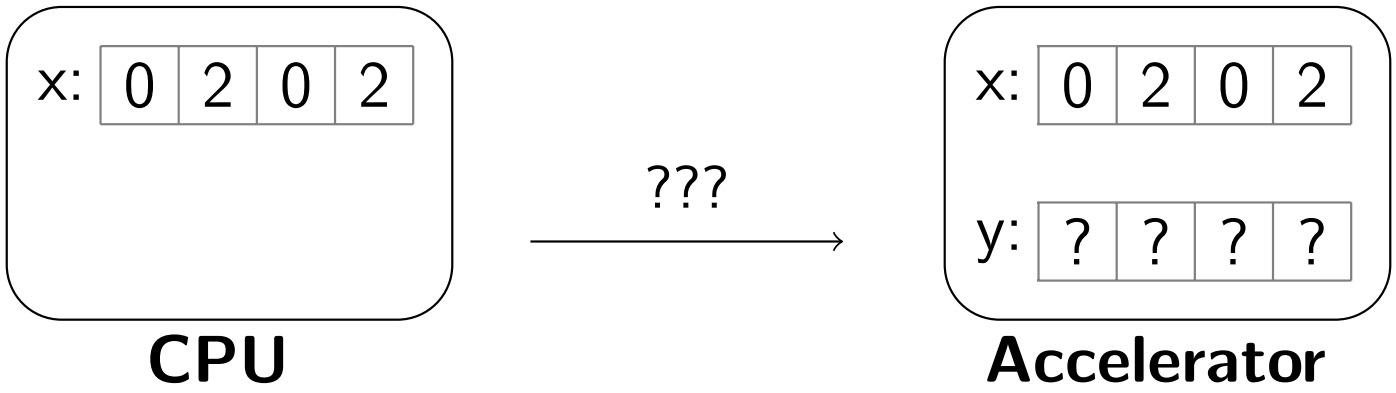

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Experimental Methodologies

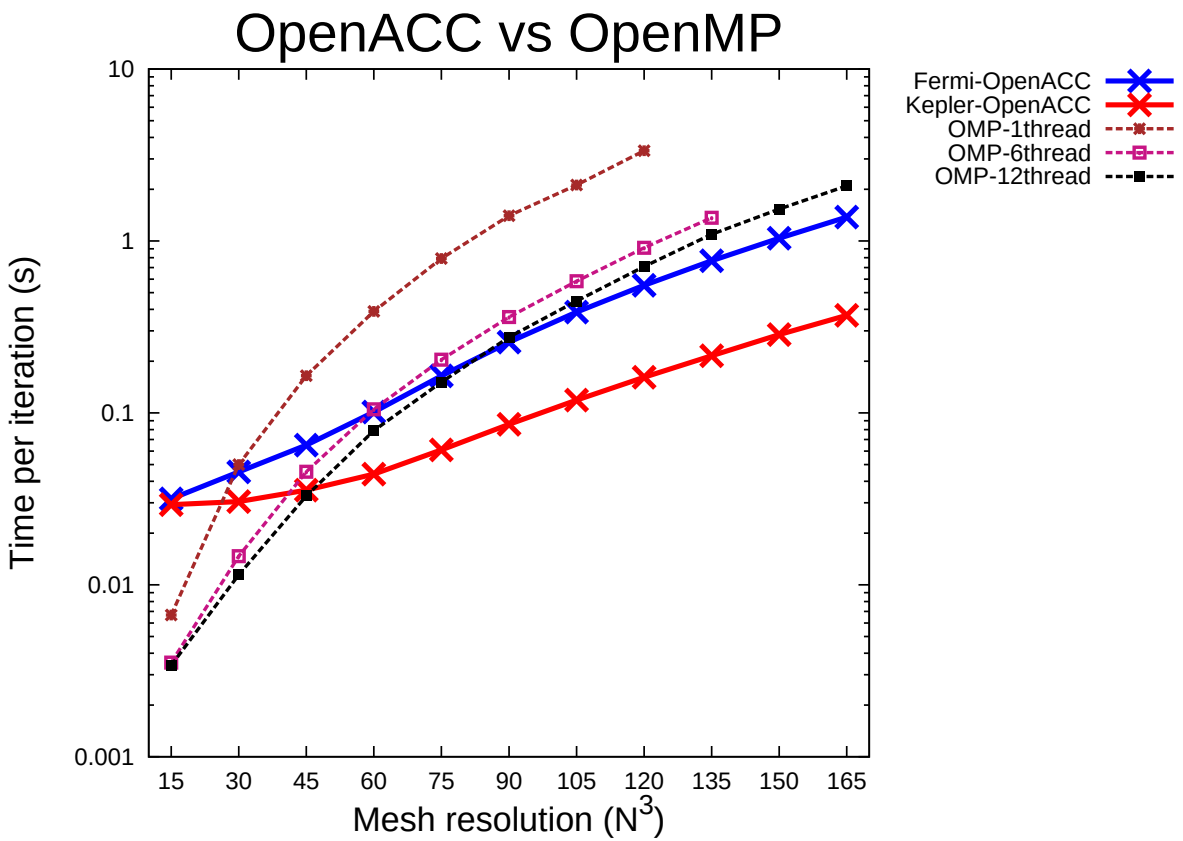
Completed Tasks

- OpenACC rewrite of LULESH
- Also supports MPI
- Falls back to OpenMP if not compiled with OpenACC
  - This lets us measure the runtime effects of the loop unrolling and other changes we made

Measurements of Interest

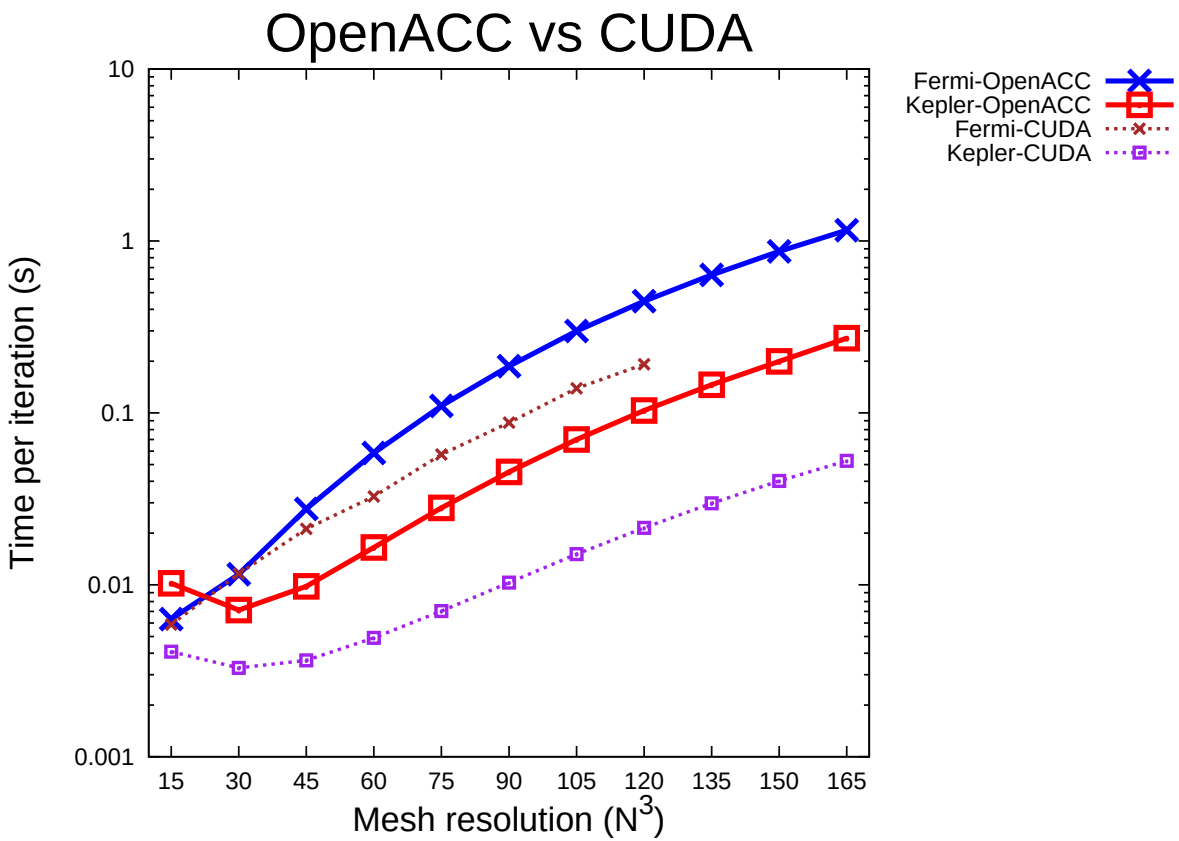
- OpenACC vs OpenMP
- OpenACC vs CUDA
- Weak scaling
- Strong scaling

Runtime Comparisons



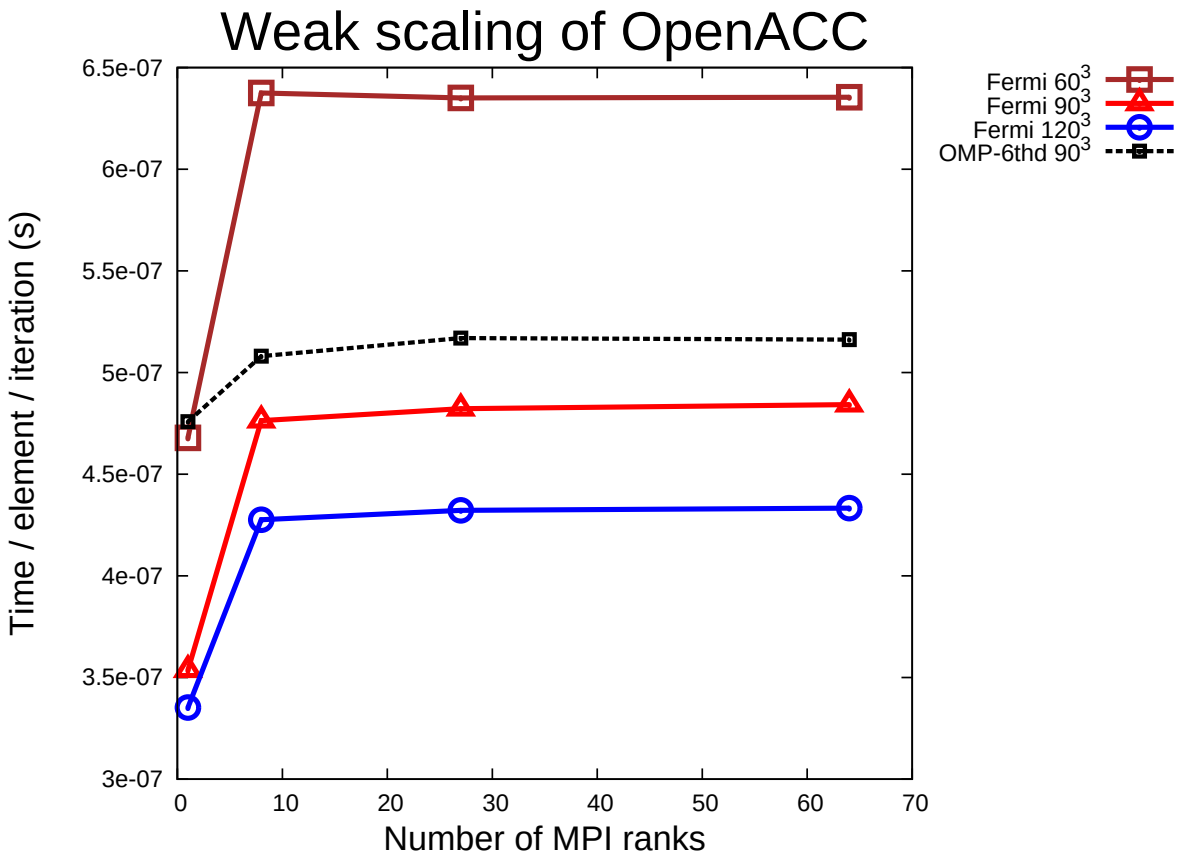
- OpenMP times were taken using up to 12 threads on a dual hex-core Intel Westmere system

Runtime Comparisons



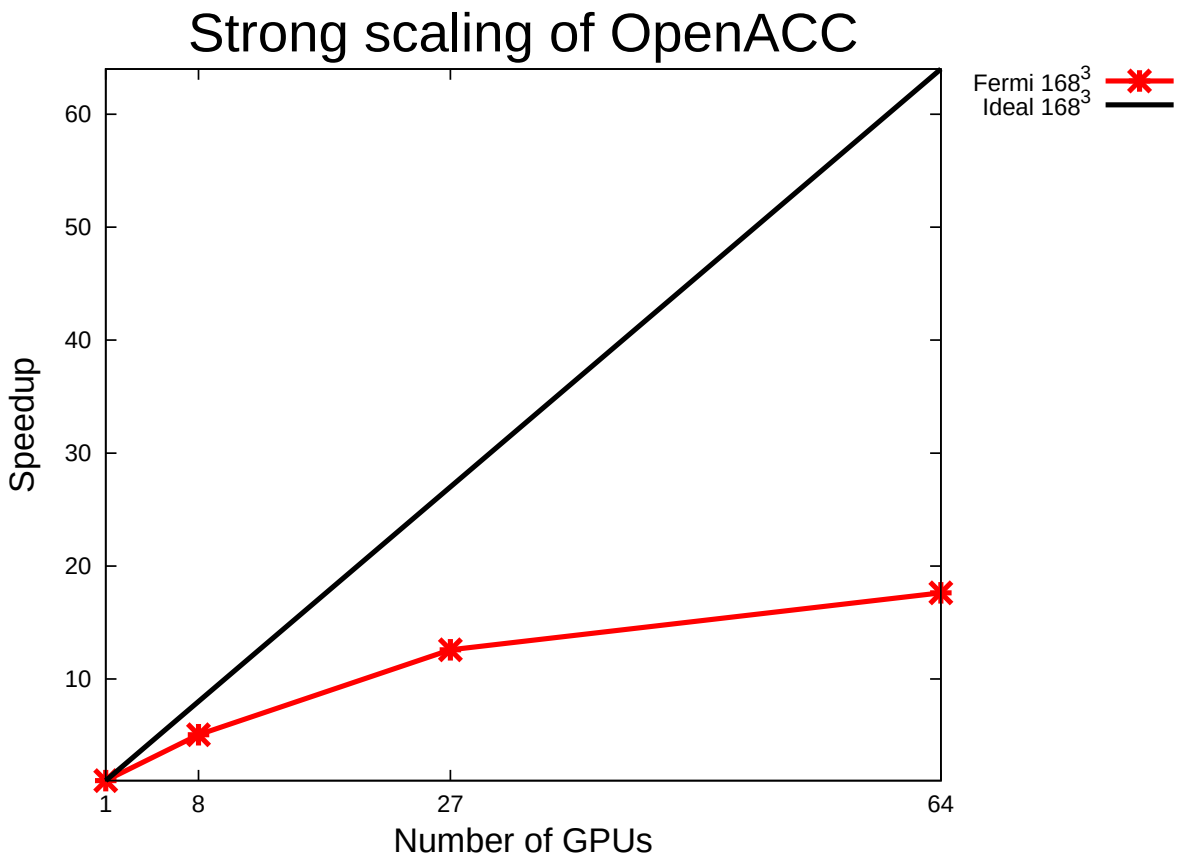
- We used a single, balanced region to emulate the computations done by the CUDA version of LULESH

Scaling Study



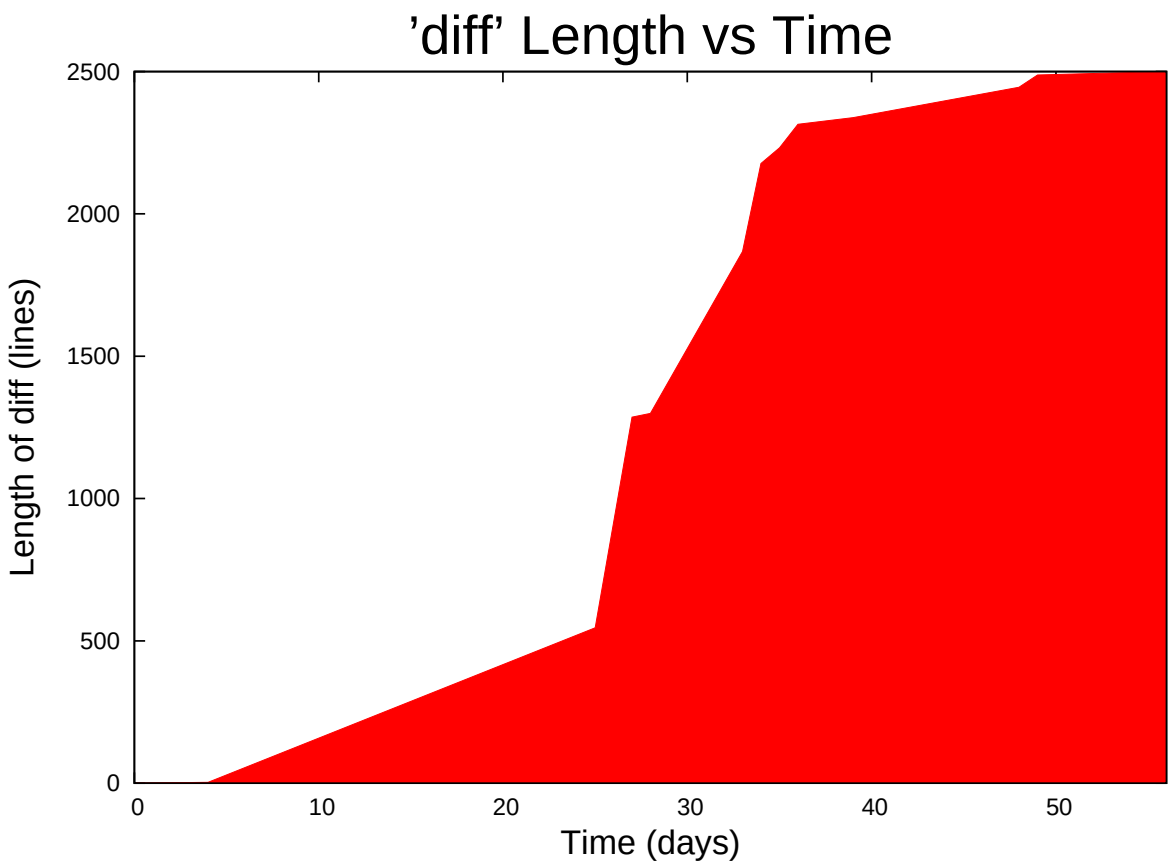
- For simplicity, LULESH's decomposition requires scaling with a cubic number of processes
- Weak scaling works well once hardware is fully saturated

Scaling Study



- Strong scaling is difficult due to decomposition and the large GPU overhead for small problem sizes

Programmability



- Due to large codebase changes (e.g. loop unrolling) large commits were often necessary

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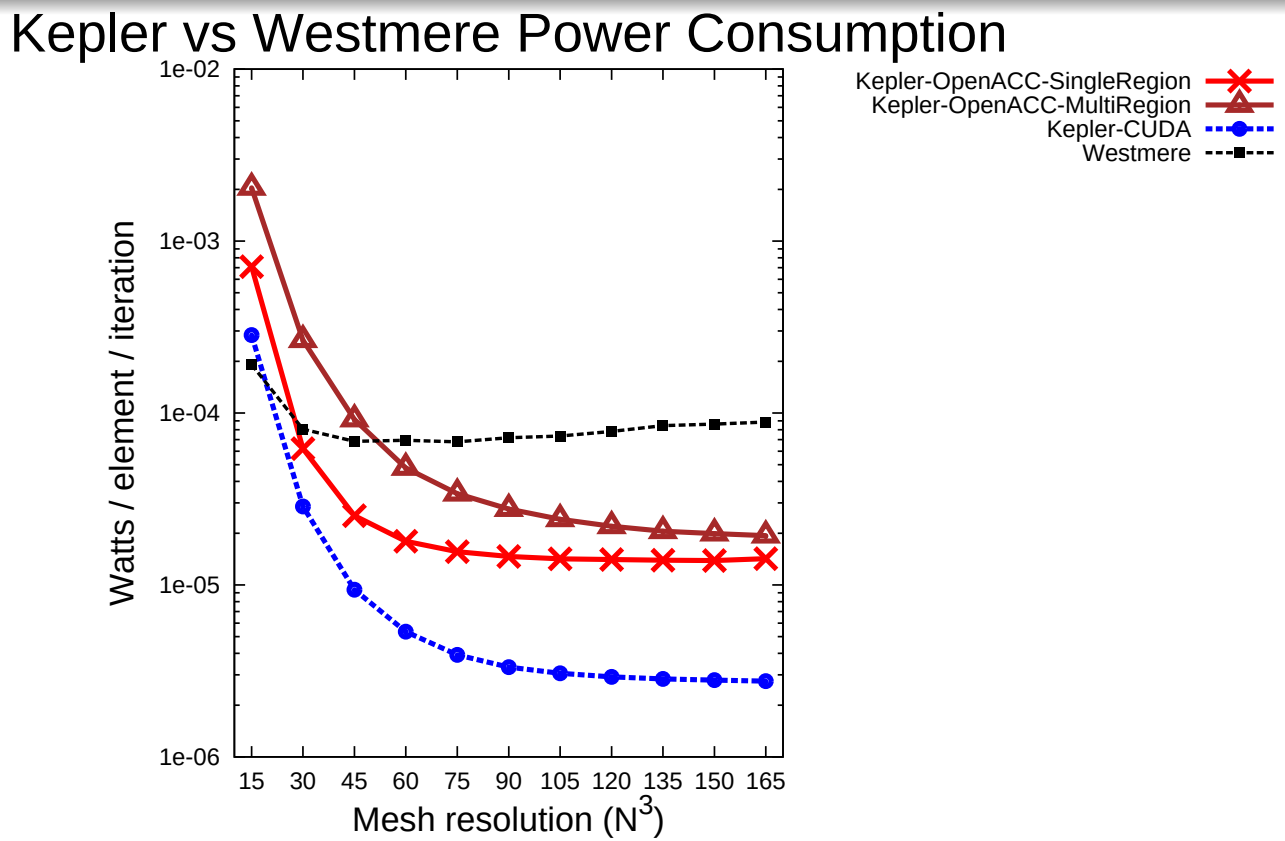
OpenACC Evaluation



Is OpenACC cost effective?

- Power is a major concern for future HPC systems
- Kepler K20Xm TDP: 235W
- Westmere Xeon E7 TDP: 95W * 2 sockets

OpenACC Evaluation

Do we recommend OpenACC?

- In the future, possibly
  - Let the standard and implementations mature first
  - Right now the required code changes are too expensive
- What about OpenMP v4?
  - The new OpenMP standard supports SIMD constructs as well
  - OpenACC is intended to be merged with OpenMP

Thank you!