Tool Chain For Co-Design

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Why worry about the tool chain?

Lets look at a simple dot product.

Dot Product on CPU: C

```
double * dotP(double *a, double *b, size_t length){
  double result = 0.0;
  for(size_t i=0; i < length; i++){
    result += a[i] * b[i];
  }
  return result;
}
```

Dot Product on CPU: OpenMP

```
double * dotP(double *a, double *b, size_t length){
  double result = 0.0;
#pragma omp parallel for reduction(+:result)
  for(size_t i=0; i < length; i++){
    result += a[i] * b[i];
  }
  return result;
}
```

Dot Product on GPU: CUDA

```
__global__ void dotP(double *g_a, double *g_b, int *g_odata) {
  extern __shared__ int sdata[];
  // each thread loads one element from global to shared mem
  unsigned int tid = threadIdx.x;
  unsigned int i = blockIdx.x * blockDim.x + threadIdx.x;
  sdata[tid] = g_a[i] * g_b[i];
  __syncthreads();
  // do reduction in shared memory
  for(unsigned int s=1; s < blockDim.x ; s *= 2) {
    if (tid % (2*s) == 0) {
      sdata[tid] += sdata[tid + s];
    }
    __syncthreads();
  }
  // write result for this block to global mem
  if (tid == 0) g_odata[ blockIdx.x ] = sdata[0];
}//Must be run 2-3 times to produce a final result
```

(Based on an example from "Optimizing Parallel Reduction in CUDA" by Mark Harris)

Library Dot Product

```
double * dotP(double *a, double *b, size_t length){
  double result = 0.0;
  accel_dotProd_reduce(a, b,
        {length,0,0}, {0,0,0}, {length,0,0},
        &result);
  return result;
}
```

Dot Product on GPU: OpenACC

```
double * dotP(double *a, double *b, size_t length){
  double result = 0.0;
#pragma acc kernels for copyin(a[0:length],b[0:length]) reduction(+:result)
  for(size_t i=0; i < length; i++){
    result += a[i] * b[i];
  }
  return result;
}
```

OpenACC vs OpenMP

```
double * dotP(double *a, double *b, size_t length){
  double result = 0.0;
- #pragma omp parallel for reduction(+:result)
+ #pragma acc kernels for copyin(a[0:length],b[0:length]) reduction(+:result)
  for(size_t i=0; i < length; i++){
    result += a[i] * b[i];
  }
  return result;
}
```

Advantages to OpenACC or OpenMP 4.0

- Little to no alteration of core code is required
- The CPU and GPU code are often the same
- Directives are portable, supporting CPU, GPU and potentially even FPGA devices given an appropriate compiler

What's the Catch?

OpenACC is new and evolving rapidly

Limitations to OpenACC

1. No support for atomic operations
2. Minimal support for routine calls
3. No device debugging support
4. Lack of support for deep memory copies
5. No automatic work-sharing across devices

The Upside of Rapid Evolution

PGI 2014 Update Improvements

1. Atomics are accessible from Fortran OpenACC
2. Preliminary support for routine calls
3. CUDA Fortran and OpenACC device and host debugging
4. C-style 2d array copy support, a first step toward deep copies

Device Debugging Support

- Before PGI 2014
  - OpenACC debugging is host-only
  - Device debugging can only check outputs
- With PGI 2014 and Allinea DDT
  - Debugging on host and device with:
    - Breakpoints
    - Individual thread stepping
    - Memory watchpoints on all CUDA memory spaces
  - Device memory debugging
    - Inspect values and arrays in global and even *shared* memory
    - Catch and debug out-of-range accesses

Deep Copies

Several projects, notably Sensei, have encountered the lack of support for arrays where each element contains, or is, a dynamic array.

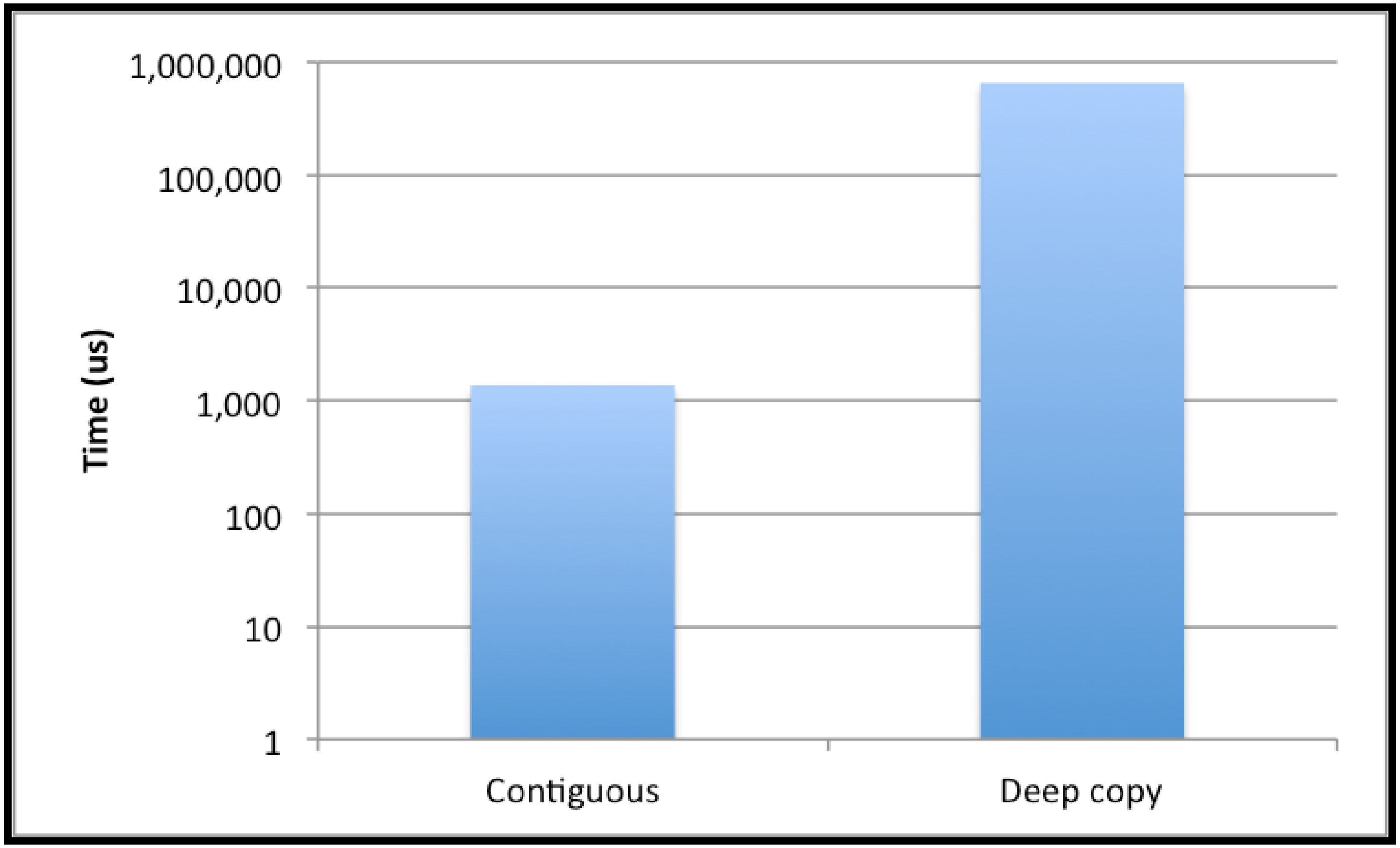
Deep Copies
C Example

```c
double ** a2 = (double**)calloc(y_length, sizeof(double*));
double ** b2 = (double**)calloc(y_length, sizeof(double*));

for (int i = 0; i < y_length; i++) {
  a2[i] = calloc(x_length, sizeof(double));
  b2[i] = calloc(x_length, sizeof(double));
}

#pragma acc kernels for copyin(a2[0:y_length][0:x_length],b2[0:y_length][0:x_length]
for (int i = 0; i < y_length; i++) {
  for (int j = 0; j < x_length; j++) {
    sum += a2[i][j] * b2[i][j];
  }
}
```

Deep Copies
Performance Consequences



Deep Copies

Performance Consequences

Note that the Y axis was log10, Contiguous is 483 *times* faster

Co-Design in the Tool Chain

Collaborations with PGI and the OpenMP Accelerator Working Group

OpenACC Optimization with PGI

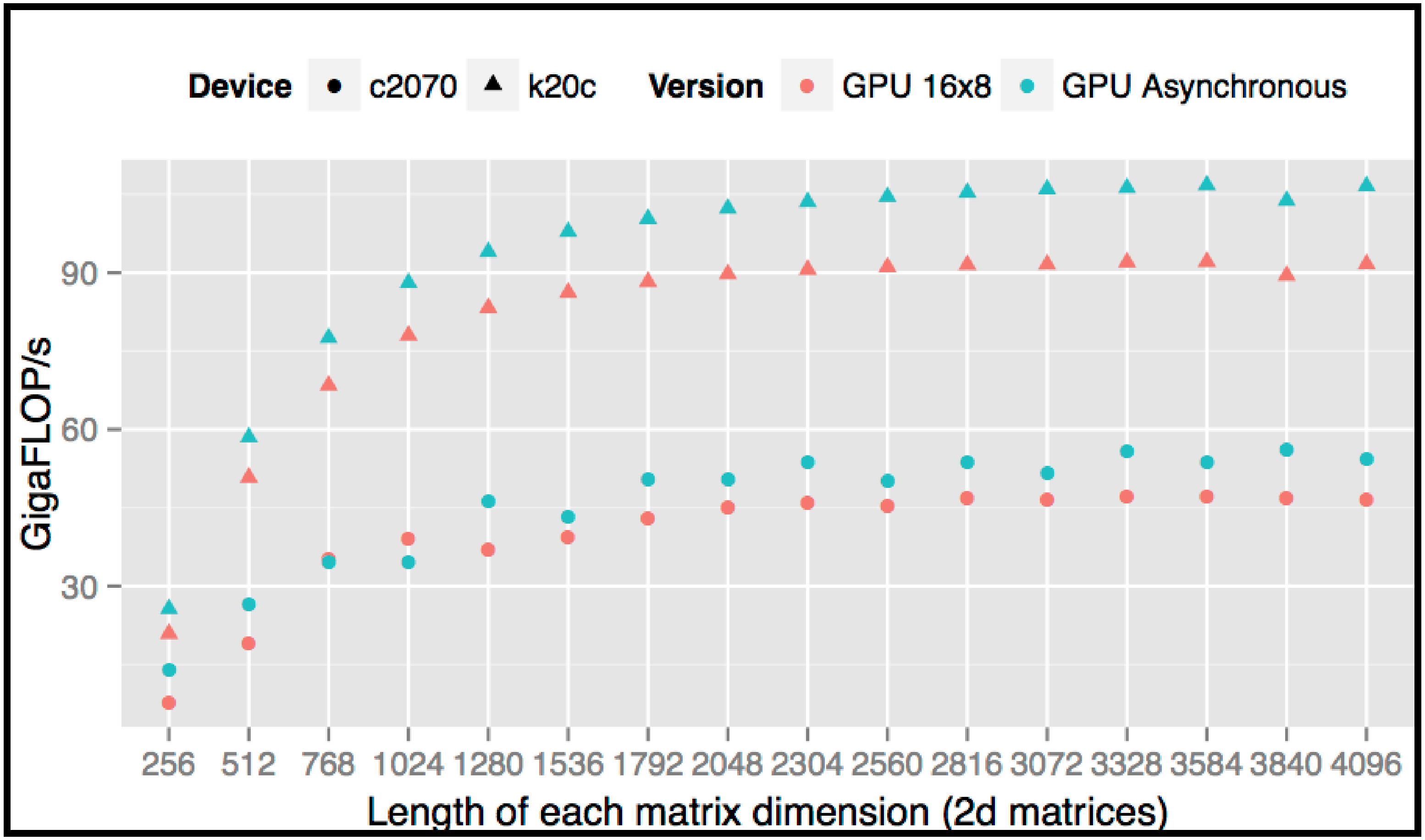
Sensei Lite

Unexpected Data Movement

- Data movement is one of the largest causes of overhead in heterogeneous applications
  - OpenACC reductions can be an unexpected source
  - Every region containing a reduction imposes a synchronous data copy of the reduction variable back to the host!
- Sensei Lite uses a reduction for almost all kernels
  - Error residuals detect algorithm convergence
  - Are they all necessary?

By testing for convergence less often, a full run can enqueue far more work between barriers.

Performance with Infrequent Reductions



Targeting Multiple Architectures with OpenACC

- OpenACC can, in principle, support:
  - CPUs
  - GPUs: NVIDIA and AMD
  - Co-processors: Xeon Phi, Tile64
  - Etc.

In practice, a single binary normally supports just one, and that one is usually NVIDIA GPUs with the possible addition of the host CPU.

PGI OpenACC -> AMD Radeon OpenCL

In private beta until January 24th, 2013

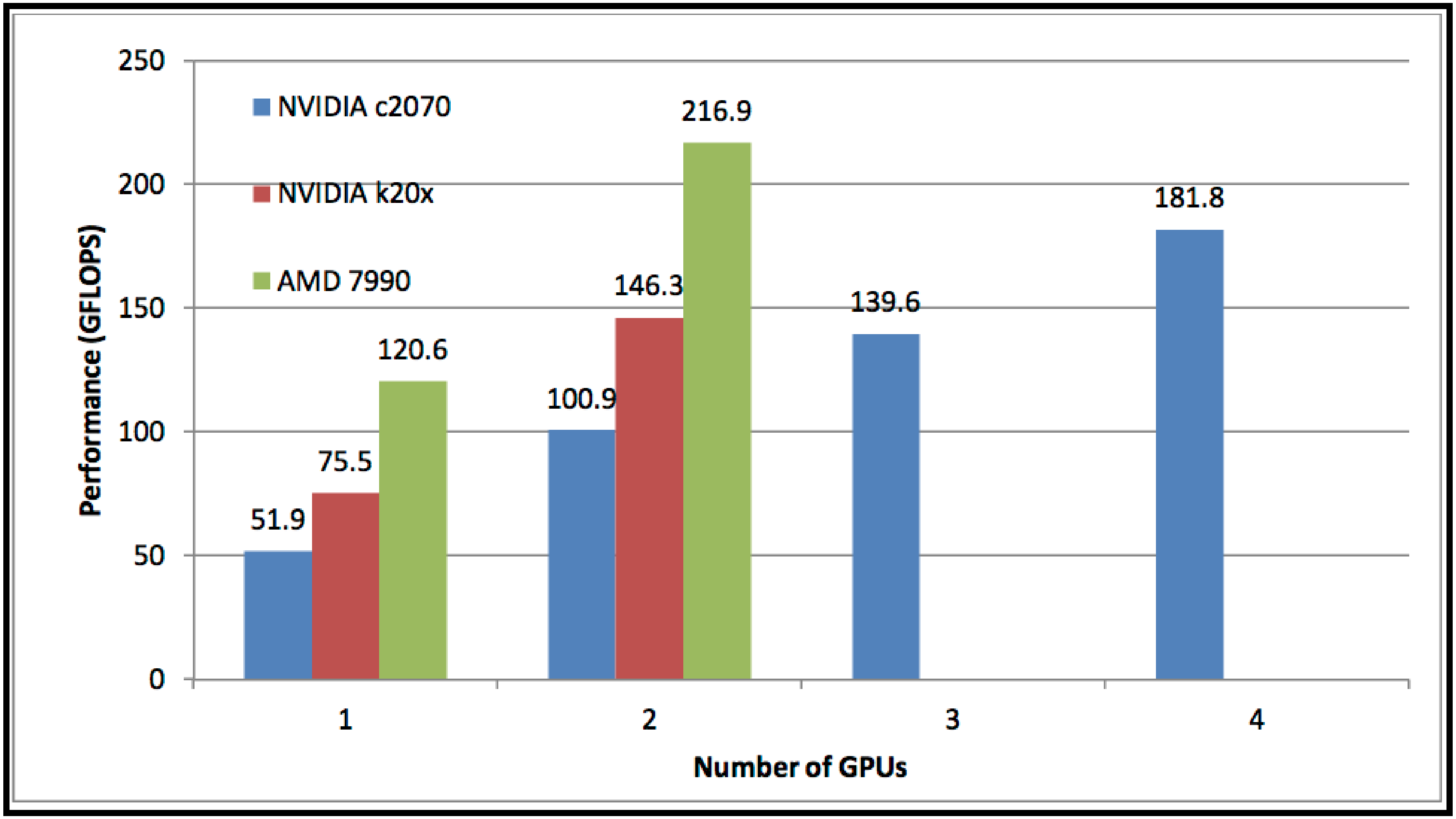
PGI 14.1 marks the release of official support

AMD Radeon evaluation for CFD

Required:

- Re-targeting Sensei Lite to support multiple devices
- Adding support for selecting multiple device types
- Backing out non-portable optimizations:
  - Custom gang and vector sizes
  - Synchronization between iterations returns, to exchange boundary values

Multi-GPU and AMD



- B. P. Pickering, C. W. Jackson, T. R. W. Scogland, W.-C. Feng, and C. J. Roy, "Directive-Based GPU Programming for Computational Fluid Dynamics," AIAA Paper 2014-1131, 52nd Aerospace Sciences Meeting, National Harbor, MD, January 13-17, 2014.

OpenMP 4.0

OpenACC is a target, and standard, of convenience.

OpenMP 4.0

OpenMP Accelerator directives are more likely to be long-lasting, but do not offer support for certain critical optimization tools.

OpenMP 4.0->4.1

We have been working directly with the OpenMP Accelerator working group on improved support for features critical to the performance of our designs including:

- Support for unstructured data lifetimes
- Asynchronous invocation of "target", or accelerator, regions
- Task-dependency resolution across both host and device tasks
- Work-sharing across devices

Summary

- The expressibility, stability and usability of the tool chain can have a significant effect on rate of progress
- Significant performance gains can be realized with directive-based programming models
- Neither OpenACC nor OpenMP 4.0 are perfect, but both can provide real advantages, and are improving quickly

Questions?