Refactoring Applications for the XK7 and Future Hybrid Architectures

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&
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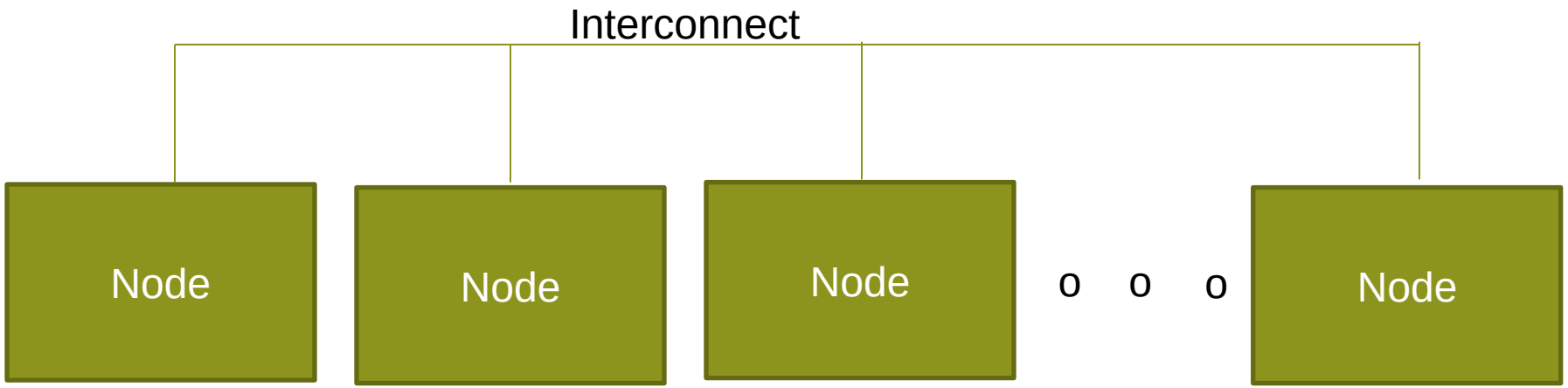
Are you ready for the future?

- **You must move to a hybrid (MPI, threading & vector) architecture to prepare for the future**
- **You must start considering how to manage your arrays to have them close to the computational engine when you need them there**
  - We are moving to a more complex memory hierarchy that will require user intervention to achieve good performance.
- **You must design your application to be performance portable across a wide range of systems**
  - Fortunately they will be similar enough that this will be possible
- **Bottom Line – you must understand your application extremely well to achieve acceptable performance on today's and tomorrow's architectures**

Outline of Tutorial

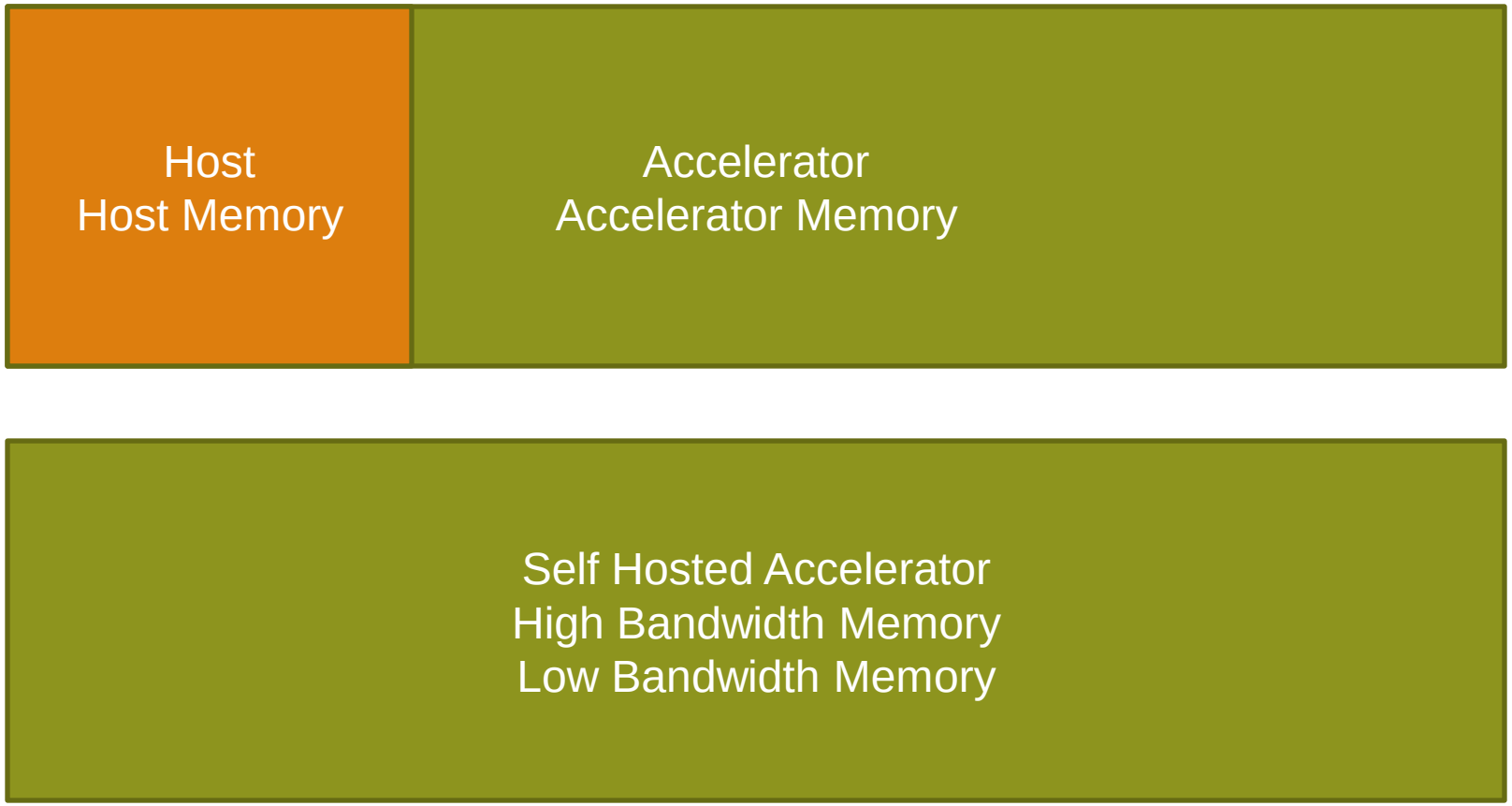
- **Future hardware trends (Levesque) (15 m)**
- **Analyzing an application (Levesque) (45 m)**
  - All MPI
  - Partial hybrid code
  - OpenACC and OpenMP
  - Tools to assist
- **Architecture of the XK7 (Larkin) (45 m)**
- **Strategy for refactoring the application (Levesque) (45 m)**
  - Tools to assist
- **Using Cuda/Cuda Fortran with OpenACC (Larkin) (45 m)**
  - Tools to assist
- **Looking forward (Levesque) (15 m)**
  - Trends

Future hardware trends

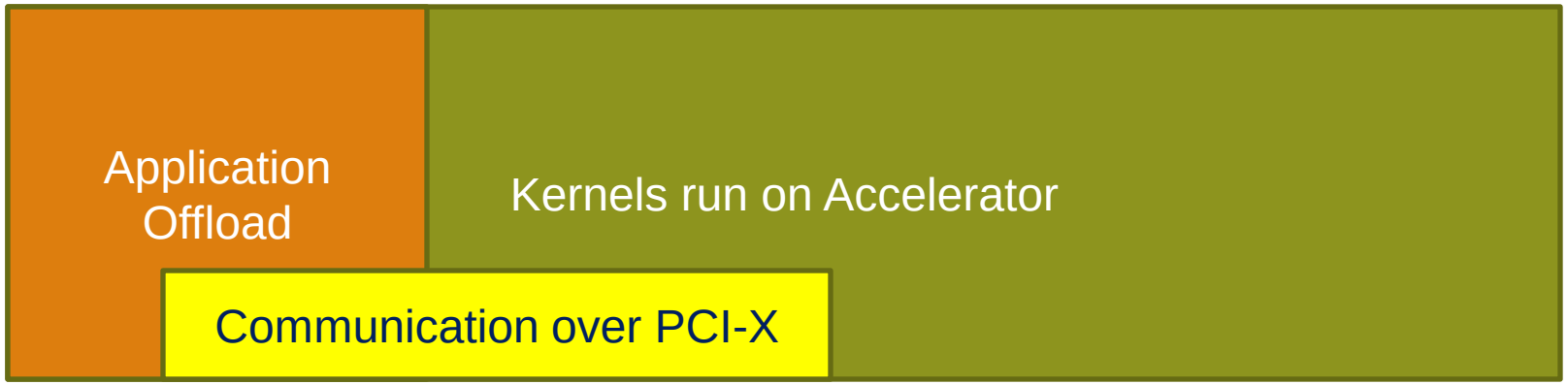


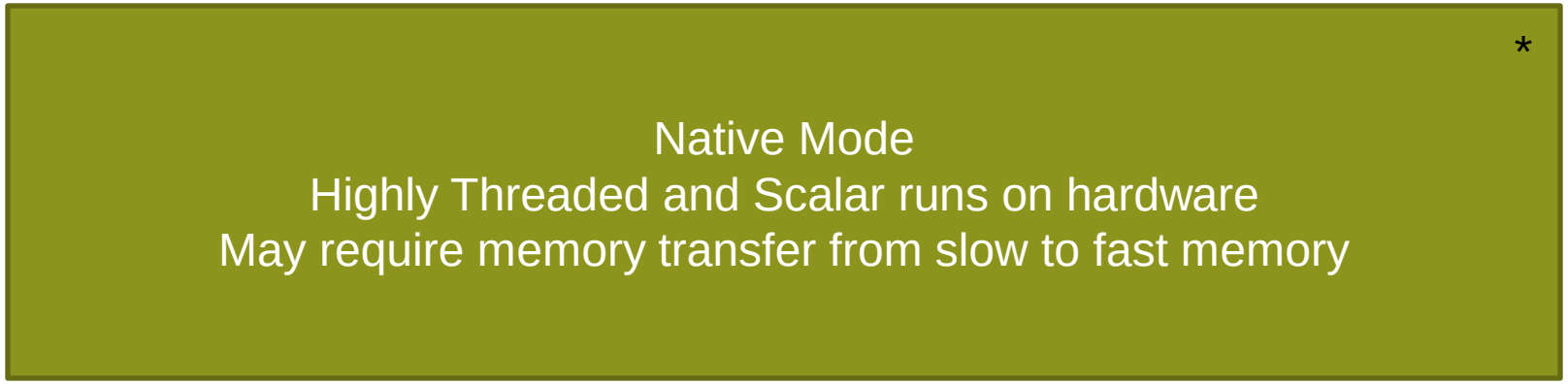
Everyone will be doing this

Node Architectures



Node Programming Paradigm's





* May include Multi-die multi-core node

Advantages & Disadvantages of the Node Architectures

	Off Load	Native - Accelerator	Native – Multi-core
Scalar Performance	Uses State of art Scalar Processor	Uses much slower scalar processor	Uses State of art Scalar Processor
Parallel Performance	Uses State of art Parallel Processor	Uses State of art Parallel Processor	Uses multi-core for performance
Data movement today	Significant Data Motion between Host/Accelerator	Minimal Data Motion	Minimal Data Motion
Data movement tomorrow	Significant Data Motion between Host/Accelerator	Significant Data Motion between Memory Levels	Minimal Data Motion
Amount of Memory	Limited on Accelerator	Limited fast Memory	Sufficient

Analyzing an application

- **What goes on within the time step loop?**
  - Where is computation
  - Where is communication
  - What data is used
- **What, if any computation can be moved?**
- **What, if any communication can be moved?**
- **Identification of potential overlap**
- **Where should OpenMP be used?**
- **Identification of potential streams**
  - What is a stream?
- **Where should OpenACC be used?**
- **What about I/O**

Things we need to know about the application

- **Where are the major arrays and how are they accessed**

  WHY – We need to understand how arrays can be allocated to assure most efficient access by major computational loops. (First touch, alignment, etc)

- **Where are the major computational and communication regions**

  WHY – We want to maintain a balance between computation and communication. How much time is spent in a computational region, what if any communication can be performed during that time

- **Where is the major I/O performed**

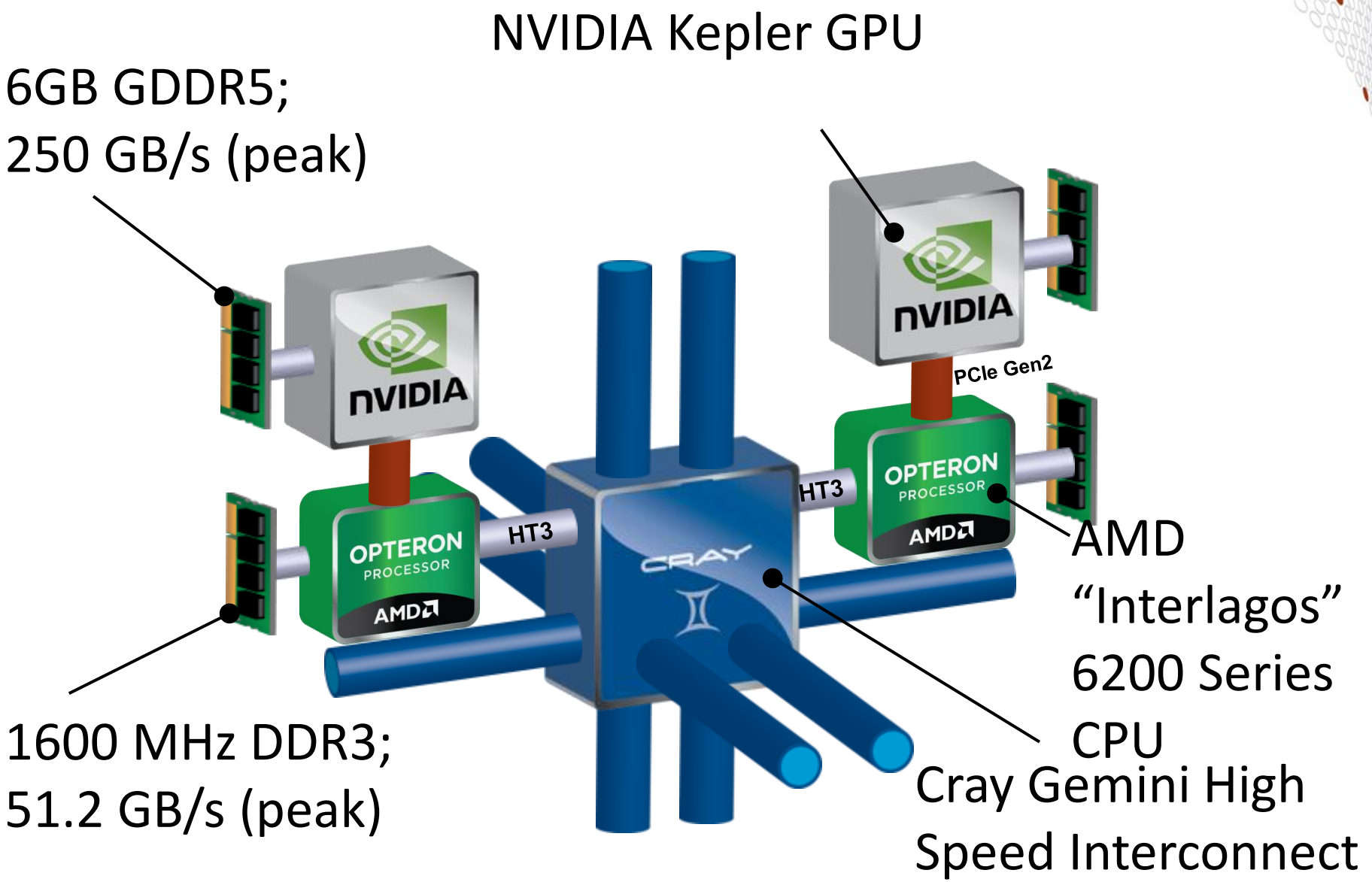
  WHY – Can we perform I/O asynchronously with computation/communication

Goals

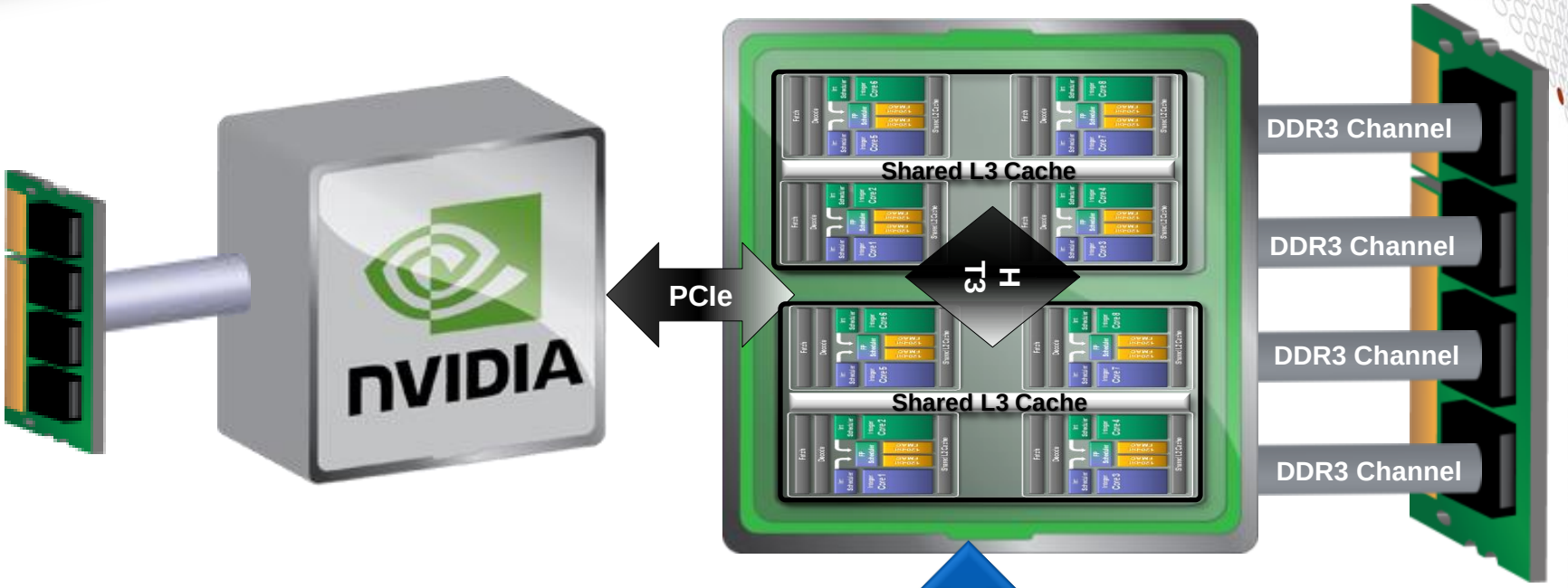
- **Develop a single source code that implements OpenMP and OpenACC in such a way that application can be efficiently run on:**
  - Multi-core MPP systems
  - Multi-core MPP systems with companion accelerator
    - Nvida
    - Intel
    - AMD
    - Whatever
- **Clearly identify three levels of parallelism**
  - MPI/PGAS between NUMA/UMA memory regions
  - Threading within the NUMA/UMA memory region
    - How this is implemented is important – OpenMP/OpenACC is most portable
  - SIMDization at a low level
    - How this is coded is important – compilers have different capability
- **We do want a performance/portable application at the end**

Cray XK7 Architecture

Cray XK7 Architecture



XK7 Node Details



- **1 Interlagos Processor, 2 Dies**
  - 8 “Compute Units”
  - 8 256-bit FMAC Floating Point Units
  - 16 Integer Cores
- **4 Channels of DDR3 Bandwidth to 4 DIMMs**
- **1 Nvidia Kepler Accelerator**
  - Connected via PCIe Gen 2

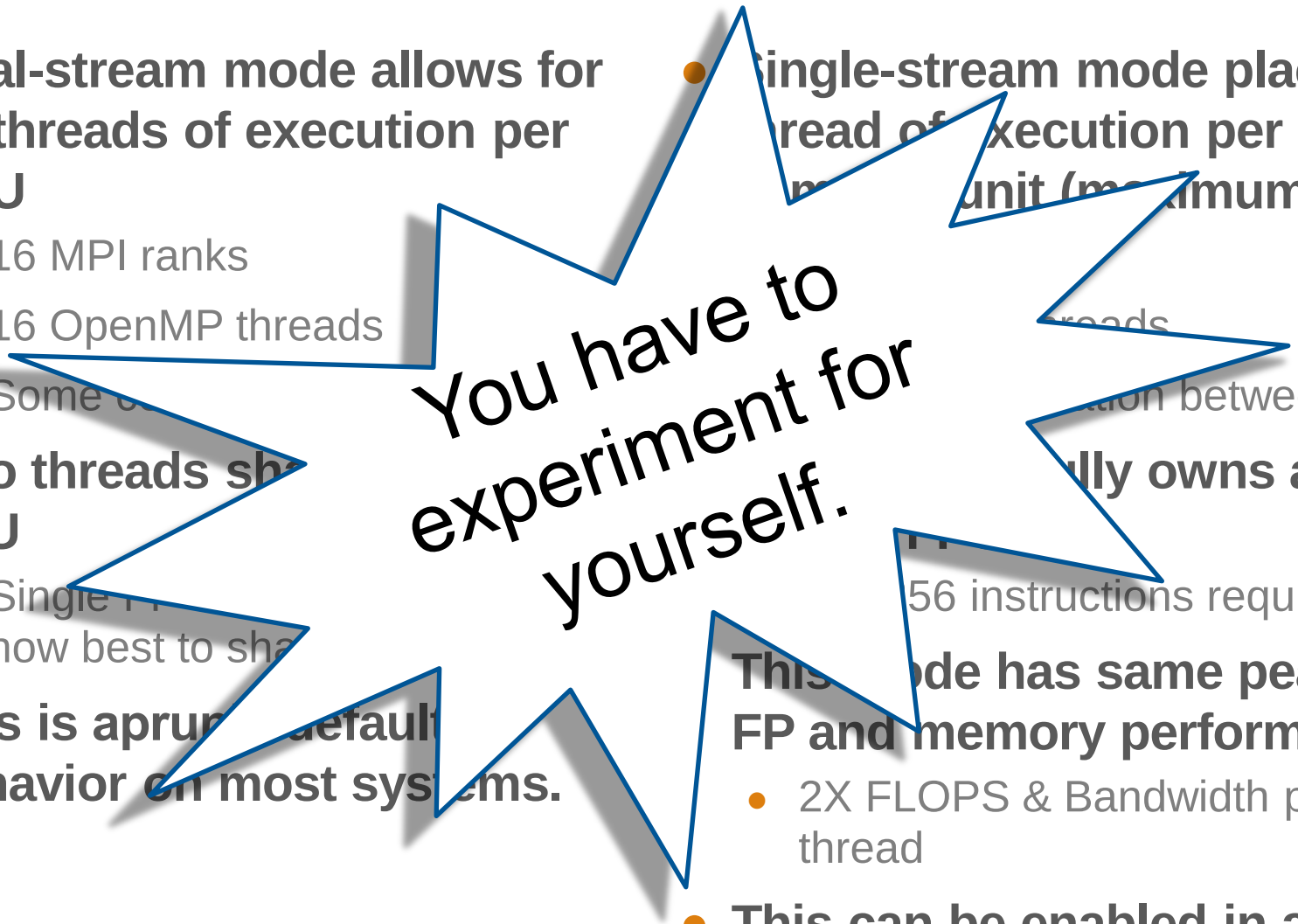
AMD Interlagos Single vs. Dual-Stream

- **Dual-stream mode allows for 16 threads of execution per CPU**
  - 16 MPI ranks
  - 16 OpenMP threads
  - Some combination between
- **Two threads share a 256-bit FPU**
  - Single FP scheduler determines how best to share
- **This is aprun's default behavior on most systems.**

- **Single-stream mode places 1 thread of execution per compute unit (maximum 8)**
  - 8 MPI ranks
  - 8 OpenMP threads
  - Some combination between
- **Each thread fully owns a 256-bit FPU**
  - AVX256 instructions required
- **This mode has same peak FP and memory performance**
  - 2X FLOPS & Bandwidth per thread
- **This can be enabled in aprun with –j1 flag**

AMD Interlagos Single vs. Dual-Stream

- **Dual-stream mode allows for 16 threads of execution per CPU**
  - 16 MPI ranks
  - 16 OpenMP threads
  - Some c…
- **Two threads sh… FPU**
  - Single F… how best to sha…
- **This is aprun … default behavior on most sys…ms.**



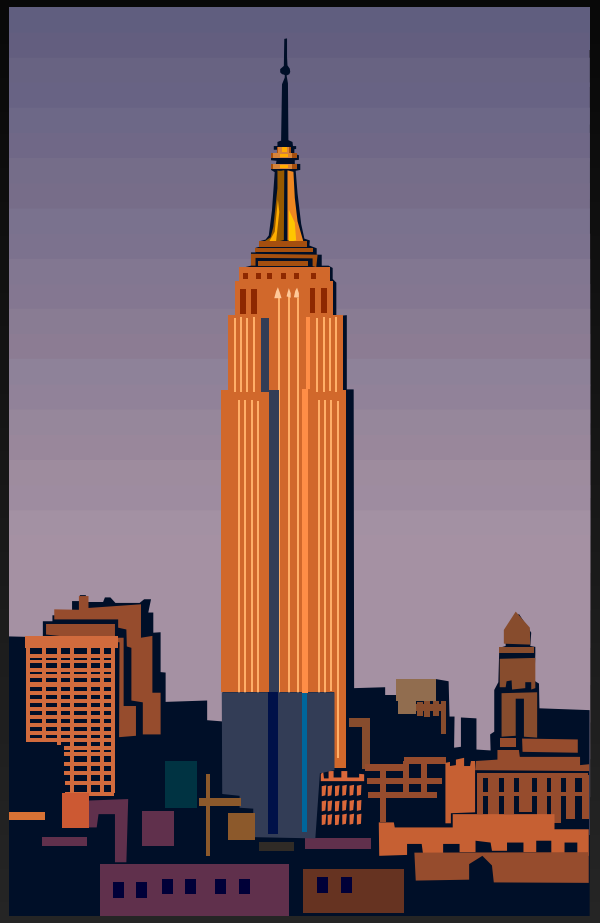
- **Single-stream mode places 1 …read of …xecution per …unit (m…imum 8)**
  - …reads
  - …tion between
- **…lly owns a …**
  - …56 instructions required
- **This …ode has same peak FP and memory performance**
  - 2X FLOPS & Bandwidth per thread
- **This can be enabled in aprun with –j2 flag**


How to Think Like a
GPU
NVIDIA

You've been hired to paint a building

You've been hired to paint a building

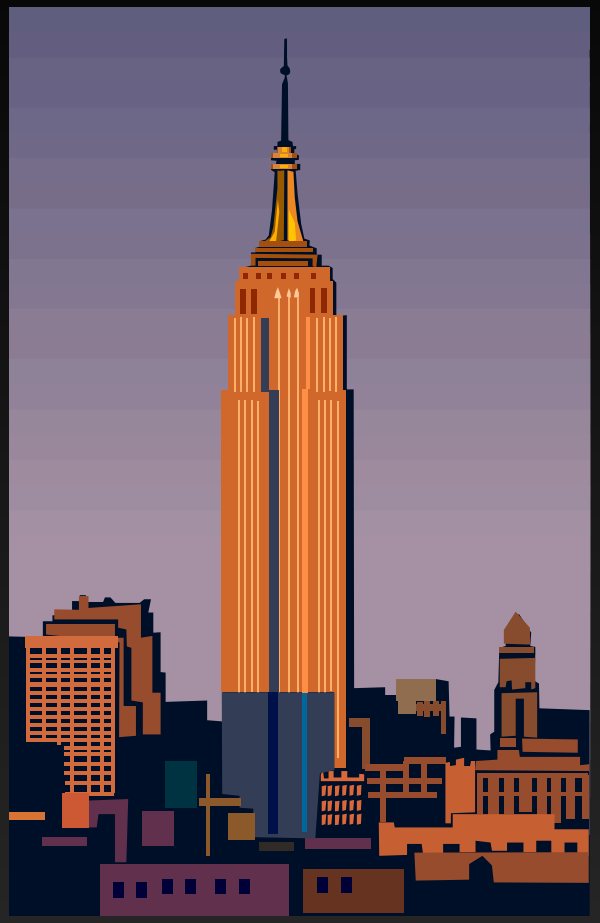
(A Big Building)



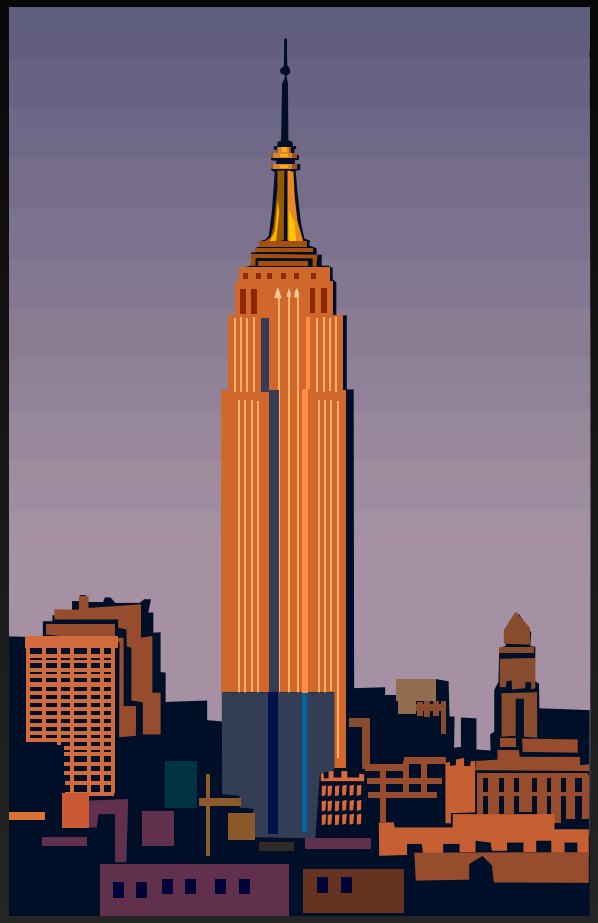
How can 1 painter paint faster?

1. Paint faster
   - One person's arm can only move so fast
2. Paint wider
   - A wider roller will cover more area, but rollers can only be made so wide
3. Minimize trips to paint bucket
   - A paint tray can be kept close by, but it can only realistically be so big

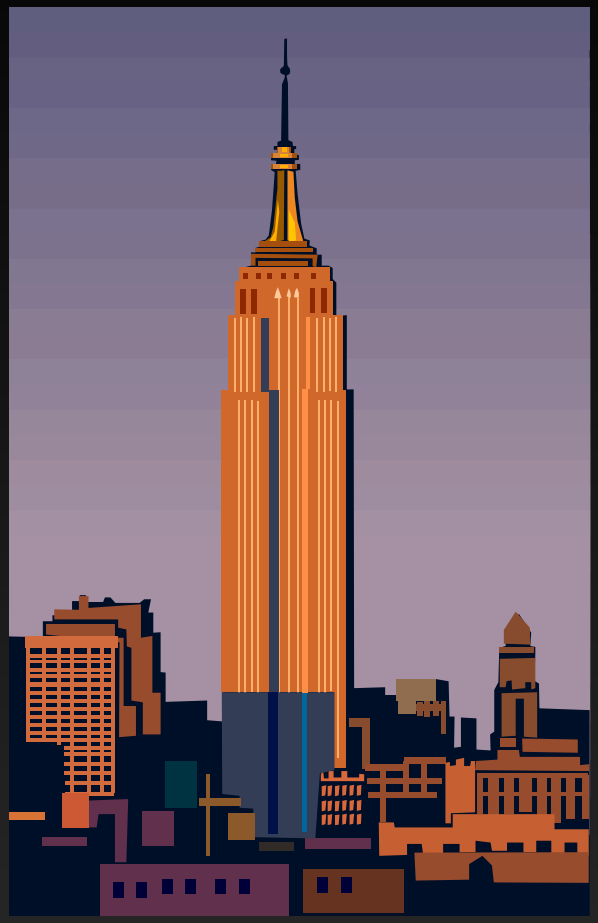
In order to paint it quickly, you keep your roller and paint close by and roll as quickly as possible



But, there's a limit to how quickly you can roll and how much paint you can keep near by.

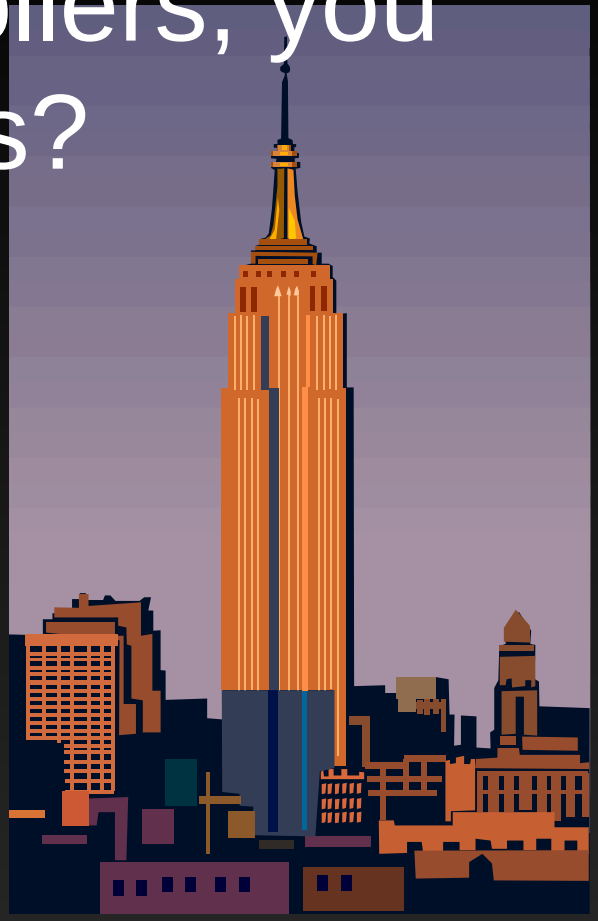


So you hire some help.



A well-organized team can paint nearly 4X faster.

What if, instead of buying more paint cans and wider rollers, you hire even more painters?



Now each painter is slower, but…

If we have enough painters, there will always be someone painting, so this won't matter.

Thread Performance vs. Throughput

- CPUs optimize for maximum performance from each thread.
  - Fast clocks
  - Big caches

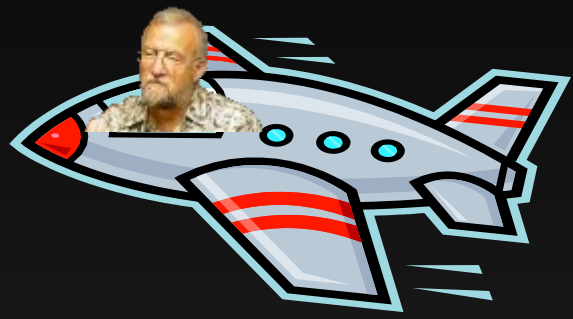
- GPUs optimize for maximum throughput.
  - Slower threads and smaller caches
  - Lots of threads active at once.

Another Example

Latency vs. Throughput

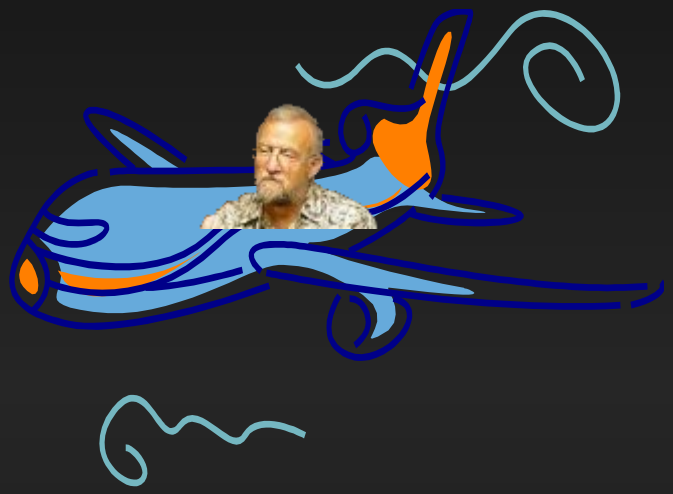
F-22 Rapter

- 1500 mph
- Knoxville to San Francisco in 1:25
- Seats 1



Boeing 737

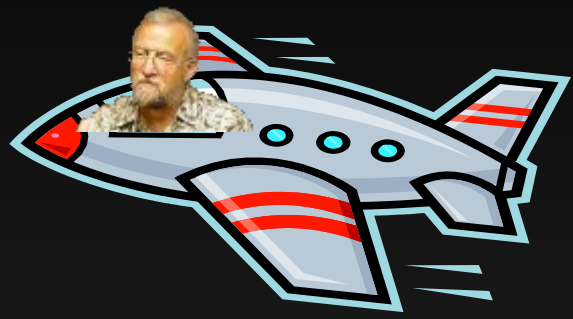
- 485 mph
- Knoxville to San Francisco in 4:20
- Seats 200



Latency vs. Throughput

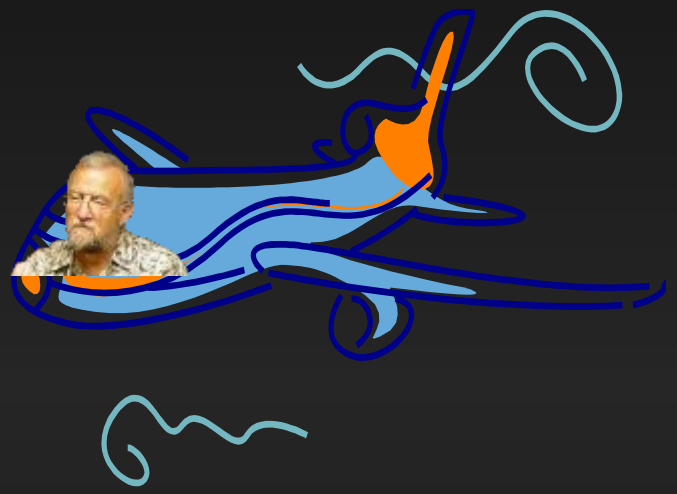
F-22 Rapter

- Latency – 1:25
- Throughput – 1 / 1.42 hours = 0.7 people/hr.



Boeing 737

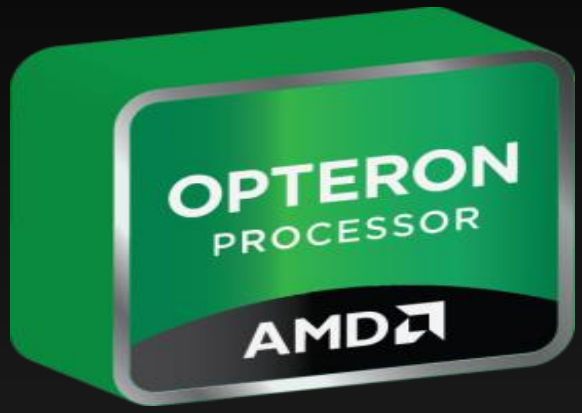
- Latency – 4:20
- Throughput – 200 / 4.33 hours = 46.2 people/hr.



Latency vs. Throughput

AMD Opteron

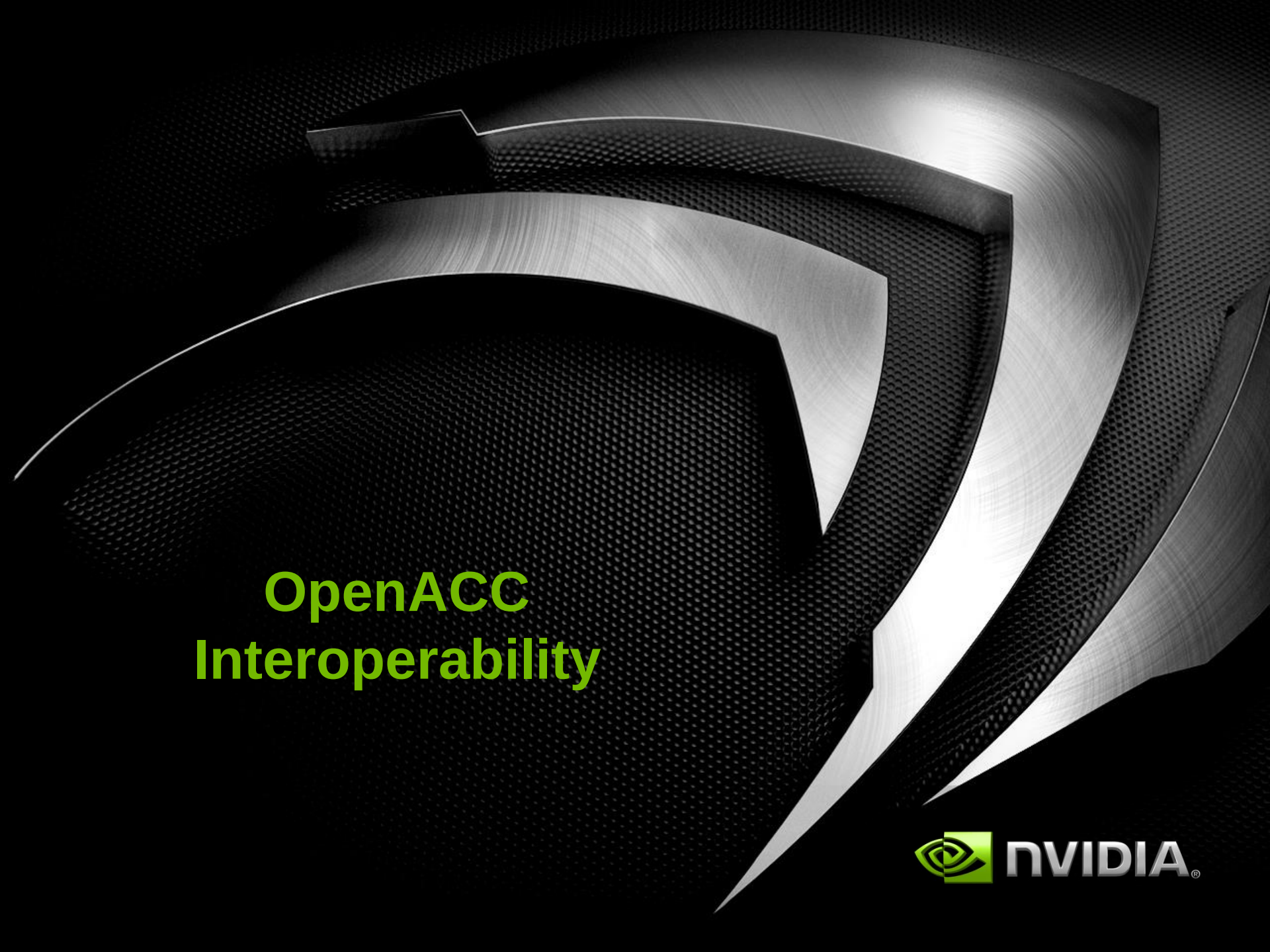
- Optimized for low latency
- For when time to complete an individual operation matters



NVIDIA Kepler

- Optimized for high throughput
- For when time to complete an operation on a lot of data matters

OpenACC Interoperability



OpenACC is not an Island

- OpenACC allows very high level expression of parallelism and data movement.
- It's still possible to leverage low-level approaches such as CUDA C, CUDA Fortran, and GPU Libraries.

Why Interoperate?

- Don’t reinvent the wheel
  - Lots of CUDA code and libraries already exist and can be leveraged.
- Maximum Flexibility
  - Some things can just be represented more easily in one approach or another.
- Maximum Performance
  - Sometimes hand-tuning achieves the most performance.

CUDA C Primer

Standard C

```
void saxpy(int n, float a,
           float *x, float *y)
{
  for (int i = 0; i < n; ++i)
    y[i] = a*x[i] + y[i];
}


int N = 1<<20;



// Perform SAXPY on 1M elements
saxpy(N, 2.0, x, y);
```

- Serial loop over 1M elements, executes 1M times sequentially.
- Data is resident on CPU.

Parallel C

```
__global__
void saxpy(int n, float a,
           float *x, float *y)
{
  int i = blockIdx.x*blockDim.x + threadIdx.x;
  if (i < n) y[i] = a*x[i] + y[i];
}

int N = 1<<20;
cudaMemcpy(d_x, x, N, cudaMemcpyHostToDevice);
cudaMemcpy(d_y, y, N, cudaMemcpyHostToDevice);

// Perform SAXPY on 1M elements
saxpy<<<4096,256>>>(N, 2.0, d_x, d_y);

cudaMemcpy(y, d_y, N, cudaMemcpyDeviceToHost);
```

- Parallel kernel, executes 1M times in parallel in groups of 256 elements.
- Data must be copied to/from GPU.

http://developer.nvidia.com/cuda-toolkit

CUDA C Interoperability

OpenACC Main

```
program main
  integer, parameter :: N = 2**20
  real, dimension(N) :: X, Y
  real               :: A = 2.0

  !$acc data
  ! Initialize X and Y
  ...

  !$acc host_data use_device(x,y)
  call saxpy(n, a, x, y)
  !$acc end host_data
  !$acc end data

end program
```

CUDA C Kernel & Wrapper

```
__global__
void saxpy_kernel(int n, float a,
                  float *x, float *y)
{
  int i = blockIdx.x*blockDim.x + threadIdx.x;
  if (i < n) y[i] = a*x[i] + y[i];
}

void saxpy(int n, float a, float *dx, float *dy)
{
  // Launch CUDA Kernel
  saxpy_kernel<<<4096,256>>>(N, 2.0, dx, dy);
}
```

- It's possible to interoperate from C/C++ or Fortran.
- OpenACC manages the data and passes device pointers to CUDA.

- CUDA kernel launch wrapped in function expecting device arrays.
- Kernel is launch with arrays passed from OpenACC in main.

CUDA C Interoperability (Reversed)

OpenACC Kernels

```
void saxpy(int n, float a, float *
restrict x, float * restrict y)
{
  #pragma acc kernels
deviceptr(x[0:n],y[0:n])
  {
    for(int i=0; i<n; i++)
    {
      y[i] += 2.0*x[i];
    }
  }
}
```

By passing a device pointer to an OpenACC region, it's possible to add OpenACC to an existing CUDA code.

CUDA C Main

```
int main(int argc, char **argv)
{
  float *x, *y, tmp;
  int n = 1<<20, i;

  cudaMalloc((void*)&x,(size_t)n*sizeof(float));
  cudaMalloc((void*)&y,(size_t)n*sizeof(float));

  ...

  saxpy(n, 2.0, x, y);
  cudaMemcpy(&tmp,y,(size_t)sizeof(float),
             cudaMemcpyDeviceToHost);
  return 0;
}
```

Memory is managed via standard CUDA calls.

CUDA Fortran

Standard Fortran

```
module mymodule contains
  subroutine saxpy(n, a, x, y)
    real :: x(:), y(:), a
    integer :: n, i
    do i=1,n
      y(i) = a*x(i)+y(i)
    enddo
  end subroutine saxpy
end module mymodule

program main
  use mymodule
  real :: x(2**20), y(2**20)
  x = 1.0, y = 2.0

  ! Perform SAXPY on 1M elements
  call saxpy(2**20, 2.0, x, y)

end program main
```

- Serial loop over 1M elements, executes 1M times sequentially.
- Data is resident on CPU.

Parallel Fortran

```
module mymodule contains
  attributes(global) subroutine saxpy(n, a, x, y)
    real :: x(:), y(:), a
    integer :: n, i
    attributes(value) :: a, n
    i = threadIdx%x+(blockIdx%x-1)*blockDim%x
    if (i<=n) y(i) = a*x(i)+y(i)
  end subroutine saxpy
end module mymodule

program main
  use cudafor; use mymodule
  real, device :: x_d(2**20), y_d(2**20)
  x_d = 1.0, y_d = 2.0

  ! Perform SAXPY on 1M elements
  call saxpy<<<4096,256>>>(2**20, 2.0, x_d, y_d)

end program main
```

- Parallel kernel, executes 1M times in parallel in groups of 256 elements.
- Data must be copied to/from GPU (implicit).

http://developer.nvidia.com/cuda-fortran

CUDA Fortran Interoperability

OpenACC Main

```
program main
  use mymodule
  integer, parameter :: N =
2**20
  real, dimension(N) :: X, Y

  X(:) = 1.0
  Y(:) = 0.0

  !$acc data copy(y) copyin(x)
  call saxpy(N, 2.0, x, y)
  !$acc end data

end program
```

CUDA Fortran Kernel & Launcher

```
module mymodule
  contains
  attributes(global) &
  subroutine saxpy_kernel(n, a, x, y)
    real :: x(:), y(:), a
    integer :: n, i
    attributes(value) :: a, n
    i = threadIdx%x+(blockIdx%x-1)*blockDim%x
    if (i<=n) y(i) = a*x(i)+y(i)
  end subroutine saxpy_kernel
  subroutine saxpy (n, a, x, y)
    use cudafor
    real, device :: x(:), y(:)
    real :: a
    integer :: n
    call saxpy_kernel<<<4096,256>>>(n, a, x, y)
  end subroutine saxpy
end module mymodule
```

- Thanks to the “device” attribute in saxpy, no host_data is needed.
- OpenACC manages the data and passes device pointers to CUDA.

- CUDA kernel launch wrapped in function expecting device arrays.
- Kernel is launch with arrays passed from OpenACC in main.

OpenACC with CUDA Fortran Main

Using the “deviceptr” data clause makes it possible to integrate OpenACC into an existing CUDA application.

CUDA C takes a few more tricks to compile, but can be done.

In theory, it should be possible to do the same with C/C++ (including Thrust), but in practice compiler incompatibilities make this difficult.

CUDA Fortran Main w/ OpenAcc Region

```
program main
  use cudafor
  integer, parameter :: N = 2**20
  real, device, dimension(N) :: X, Y
  integer :: i
  real :: tmp

  X(:) = 1.0
  Y(:) = 0.0

  !$acc kernels deviceptr(x,y)
  y(:) = y(:) + 2.0*x(:)
  !$acc end kernels

  tmp = y(1)
  print *, tmp
end program
```

CUBLAS Library

Serial BLAS Code

```
int N = 1<<20;


...

// Use your choice of blas library

// Perform SAXPY on 1M elements
blas_saxpy(N, 2.0, x, 1, y, 1);
```

Parallel cuBLAS Code

```
int N = 1<<20;


cublasInit();
cublasSetVector(N, sizeof(x[0]), x, 1, d_x, 1);
cublasSetVector(N, sizeof(y[0]), y, 1, d_y, 1);

// Perform SAXPY on 1M elements
cublasSaxpy(N, 2.0, d_x, 1, d_y, 1);

cublasGetVector(N, sizeof(y[0]), d_y, 1, y, 1);

cublasShutdown();
```

You can also call cuBLAS from Fortran, C++, Python, and other languages

http://developer.nvidia.com/cublas

CUBLAS Library & OpenACC

OpenACC can interface with existing GPU-optimized libraries (from C/C++ or Fortran).

This includes…

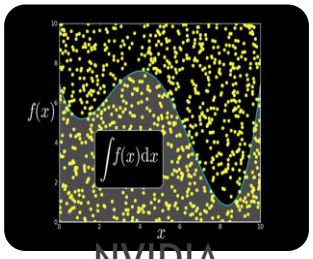
- CUBLAS
- Libsci_acc
- CUFFT
- MAGMA
- CULA
- …

OpenACC Main Calling CUBLAS

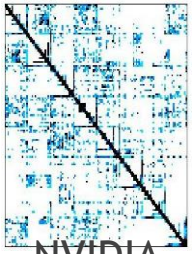
```
int N = 1<<20;
float *x, *y
// Allocate & Initialize X & Y
...

cublasInit();

#pragma acc data copyin(x[0:N]) copy(y[0:N])
{
  #pragma acc host_data use_device(x,y)
  {
    // Perform SAXPY on 1M elements
    cublasSaxpy(N, 2.0, d_x, 1, d_y, 1);
  }
}

cublasShutdown();
```

Some GPU-accelerated Libraries

NVIDIA cuBLAS



NVIDIA cuRAND



NVIDIA cuSPARSE

NVIDIA NPP

GPU VSIPL

Vector Signal Image Processing

CULA tools

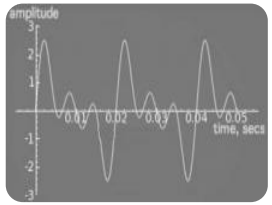
GPU Accelerated Linear Algebra

MAGMA

ICL UT

Matrix Algebra on GPU and Multicore

open source initiative



NVIDIA cuFFT

ROGUE WAVE SOFTWARE

IMSL Library

ArrayFire Matrix Computations

CUSP

Sparse Linear Algebra

open source initiative

Thrust

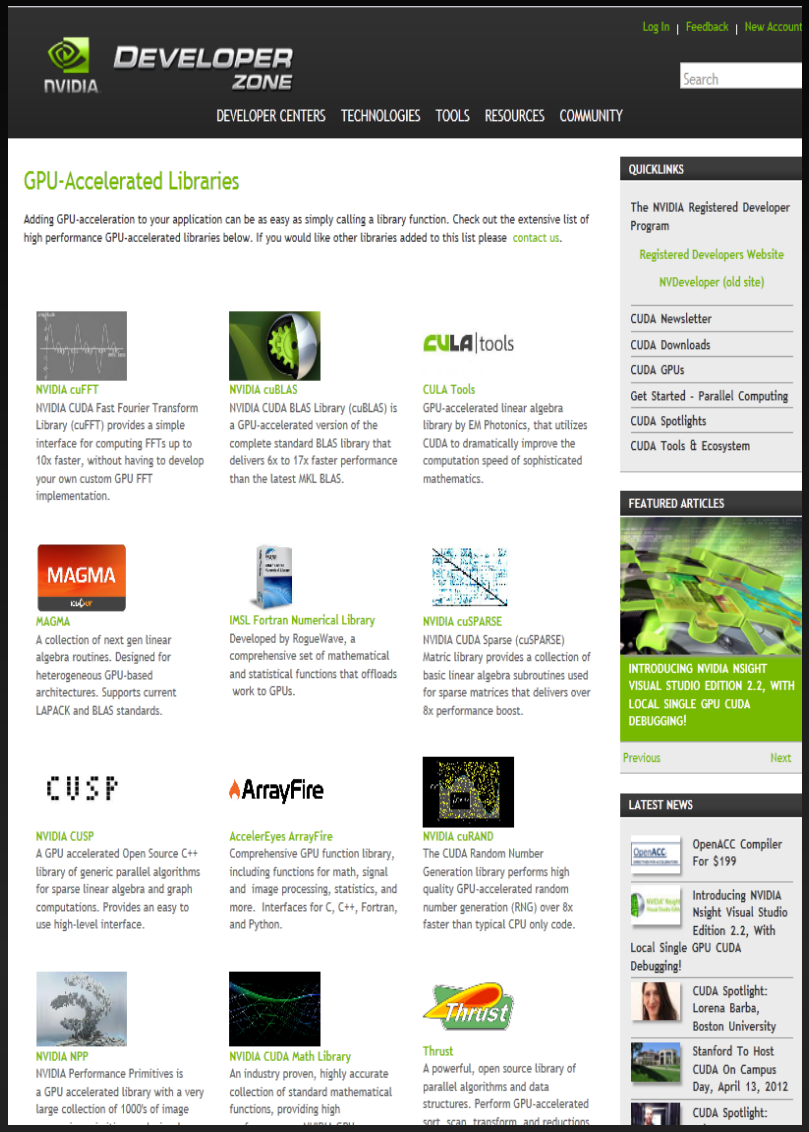
C++ STL Features for CUDA

open source initiative

Explore the CUDA (Libraries) Ecosystem

- CUDA Tools and Ecosystem described in detail on NVIDIA Developer Zone:

developer.nvidia.com/cuda-tools-ecosystem



Thrust C++ Template Library

Serial C++ Code with STL and Boost

```
int N = 1<<20;
std::vector<float> x(N), y(N);

...



// Perform SAXPY on 1M elements
std::transform(x.begin(), x.end(),
               y.begin(), y.end(),
                2.0f * _1 + _2);
```

www.boost.org/libs/lambda

Parallel C++ Code

```
int N = 1<<20;
thrust::host_vector<float> x(N), y(N);

...

thrust::device_vector<float> d_x = x;
thrust::device_vector<float> d_y = y;


// Perform SAXPY on 1M elements
thrust::transform(d_x.begin(), d_x.end(),
                  d_y.begin(),
d_y.begin(),
                  2.0f * _1 + _2);
```

http://thrust.github.com

Thrust C++ and OpenACC??

OpenACC Saxpy

```
void saxpy(int n, float a, float *
restrict x, float * restrict y)
{
#pragma acc kernels
deviceptr(x[0:n],y[0:n])
  {
    for(int i=0; i<n; i++)
    {
      y[i] += 2.0*x[i];
    }
  }
}
```

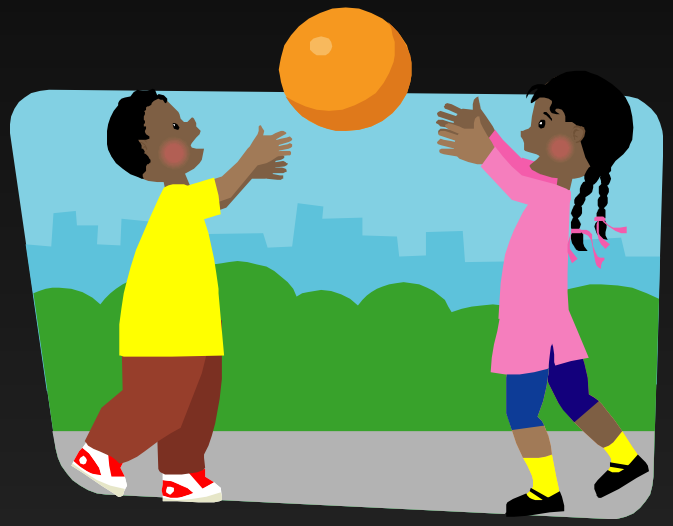
Thrust Main

```
int main(int argc, char **argv)
{
  int N = 1<<20;
  thrust::host_vector<float> x(N), y(N);
  for(int i=0; i<N; i++)
  {
    x[i] = 1.0f;
    y[i] = 1.0f;
  }

  thrust::device_vector<float> d_x = x;
  thrust::device_vector<float> d_y = y;
  thrust::device_ptr<float> p_x = &d_x[0];
  thrust::device_ptr<float> p_y = &d_y[0];

  saxpy(N,2.0,p_x.get(),p_y.get());

  y = d_y;
  return 0;
}
```

How to play well with others

My advice is to do the following:

1. Start with OpenACC
   - Expose high-level parallelism
   - Ensure correctness
   - Optimize away data movement last
2. Leverage other work that's available (even if it's not OpenACC)
   - Common libraries (good software engineering practice)
   - Lots of CUDA already exists
3. Share your experiences
   - OpenACC is still very new, best practices are still forming.
   - Allow others to leverage your work.




GPU Tools
I’m on the GPU, now what?
NVIDIA

CUDA-Memcheck

- You're hitting an error or getting wrong results, try cuda-memcheck first.
  - Reports OOB memory accesses
  - Reports errors from CUDA calls
  - https://developer.nvidia.com/cuda-memcheck
- Works with CUDA and OpenACC

```
$ aprun cuda-memcheck app.exe
```

CUDA-memcheck Output


```
========= CUDA-MEMCHECK
0.000000
========= Invalid __global__ read of size 4
=========     at 0x00000098 in saxpy$ck_L5_2
=========     by thread (0,0,0) in block (0,0,0)
=========     Address 0xb00c00000 is out of bounds
=========     Device Frame:<1 frames were hidden>
=========     Saved host backtrace up to driver entry point at kernel launch time
=========     Host Frame:<9 frames were hidden>
=========     Host Frame:/opt/cray/nvidia//default/lib64/libcuda.so.1 (cuLaunchKernel +
0x3ae) [0xc863e]
=========     Host Frame:/opt/cray/cce/8.1.7/craylibs/x86-64/libcrayacc.so.0
(__cray_acc_hw_start_kernel + 0x1072) [0x1b0a6]
=========     Host Frame:/opt/cray/cce/8.1.7/craylibs/x86-64/libcrayacc.so.0 [0x7c47]
=========     Host Frame:/opt/cray/cce/8.1.7/craylibs/x86-64/libcrayacc.so.0
(cray_start_acc_kernel + 0x114) [0x807e]
=========     Host Frame:./a.out [0xf01]
=========     Host Frame:./a.out [0xd81]
=========     Host Frame:/lib64/libc.so.6 (__libc_start_main + 0xe6) [0x1ec36]
=========     Host Frame:./a.out [0xac9]
========= ERROR SUMMARY: 3 errors
Application 219996 resources: utime ~6s, stime ~1s
```

Compiler Profiling Variables

- The Cray compiler provides automatic instrumentation when `CRAY_ACC_DEBUG=<1,2,3>` at runtime

```
ACC: Initialize CUDA
ACC: Get Device 0
ACC: Create Context
ACC: Set Thread Context
ACC: Start transfer 2 items from saxpy.c:17
ACC:       allocate, copy to acc 'x' (4194304 bytes)
ACC:       allocate, copy to acc 'y' (4194304 bytes)
ACC: End transfer (to acc 8388608 bytes, to host 0 bytes)
ACC: Execute kernel saxpy$ck_L17_1 blocks:8192 threads:128
async(auto) from saxpy.c:17
ACC: Wait async(auto) from saxpy.c:18
ACC: Start transfer 2 items from saxpy.c:18
ACC:       free 'x' (4194304 bytes)
ACC:       copy to host, free 'y' (4194304 bytes)
ACC: End transfer (to acc 0 bytes, to host 4194304 bytes)
```

Compiler Profiling Variables

- The PGI compiler provides automatic instrumentation when `PGI_ACC_TIME=1` at runtime

```
Accelerator Kernel Timing data
/home/jlarkin/kernels/saxpy/saxpy.c
  saxpy  NVIDIA  devicenum=0
        time(us): 3,256
        11: data copyin reached 2 times
             device time(us): total=1,619 max=892 min=727 avg=809
        11: kernel launched 1 times
            grid: [4096]  block: [256]
             device time(us): total=714 max=714 min=714 avg=714
            elapsed time(us): total=724 max=724 min=724 avg=724
        15: data copyout reached 1 times
             device time(us): total=923 max=923 min=923 avg=923
```

CUDA Profiler (nvprof)

- At its most basic, nvprof will instrument your application and provide information about all CUDA-related activity.
- It's also possible to use nvprof to gather data for the CUDA Visual Profiler for viewing on your machine.

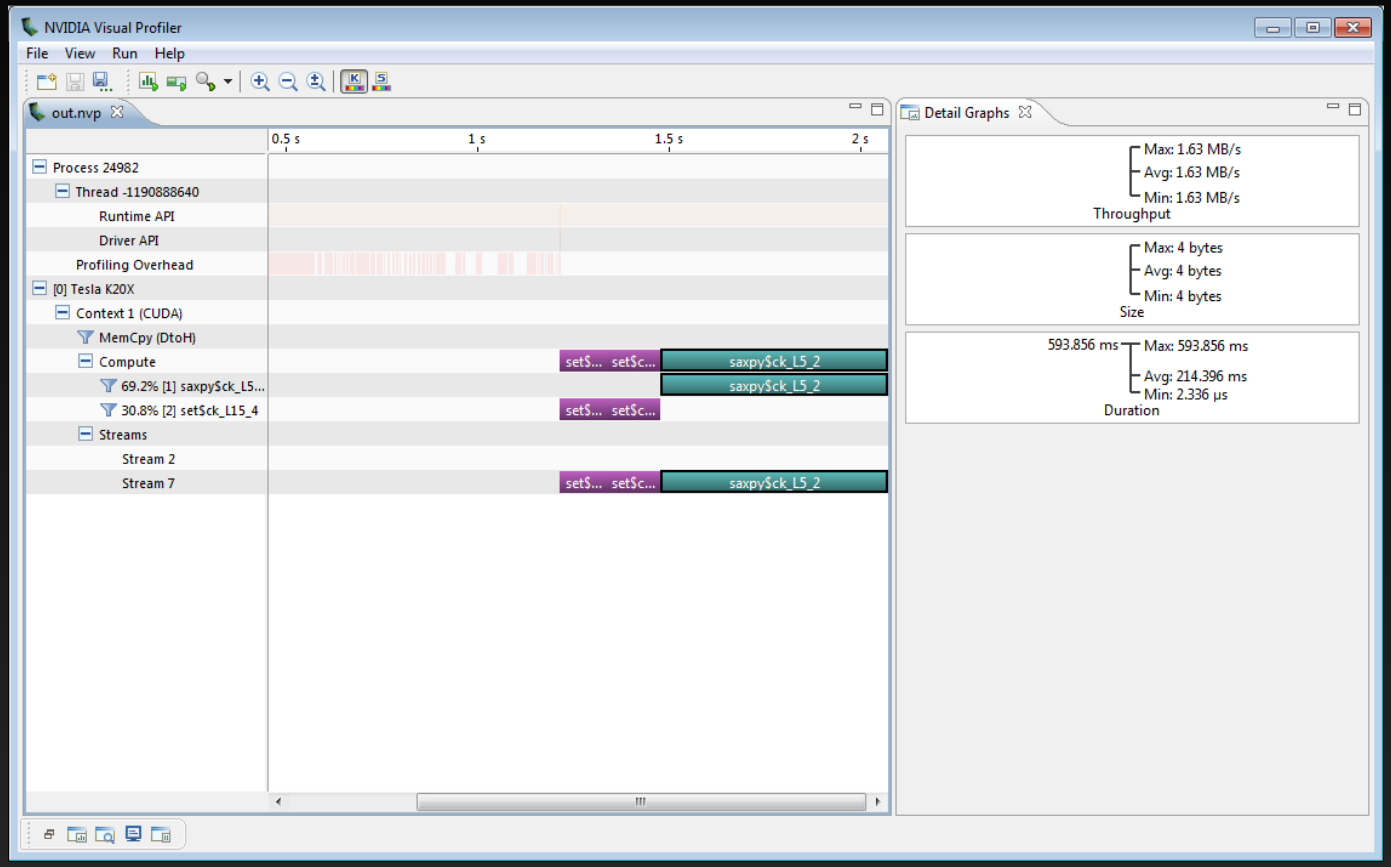
- NOTE: On Cray XK7, it's necessary to set the environment variable below to gather data.

```
export PMI_NO_FORK=1
setenv PMI_NO_FORK 1
```

NVProf Basic Output


```
$ aprun nvprof ./a.out
======== NVPROF is profiling a.out...
======== Command: a.out
2.000000
======== Profiling result:
 Time(%)      Time   Calls       Avg       Min       Max
Name
   70.20  594.27ms       1  594.27ms  594.27ms  594.27ms
saxpy$ck_L5_2
   29.80  252.26ms       2  126.13ms  126.13ms  126.13ms
set$ck_L15_4
    0.00    2.34us       1    2.34us    2.34us    2.34us
[CUDA memcpy DtoH]
```

Nvidia Visual Profiler



Instrument on compute node with: `aprun nvprof –o out.nvp a.out`
Then import into Visual Profiler on your local machine to analyze.

NVProf XK7 Trick

- When running a MPI app, all processes will write to the same file, but try this trick to get 1 per node:

```
#!/bin/bash
# USAGE: Add between aprun options and executable
# For Example: aprun -n 16 -N 1 ./foo arg1 arg2
# Becomes: aprun -n 16 -N 1 ./nvprof.sh ./foo arg1 arg2

# Give each *node* a separate file
LOG=profile_$(hostname).nvp

# Stripe each profile file by 1 to share the load on large runs
lfs setstripe -c 1 $LOG

# Execute the provided command.
exec nvprof -o $LOG $*
```

- Explanation: this script intercepts the call to your executable, determines a unique filename based on the compute node, and calls nvprof.

https://gist.github.com/jefflarkin/5503716

CUDA Command-Line Profiler

- Any CUDA or OpenACC program can also get a more detailed profile via the command-line profiler.

```
export COMPUTE_PROFILE=1
```

- Many performance counters are available.

```
export COMPUTE_PROFILE_CONFIG=events.txt
```

- Outputting to CSV allows importing into Visual Profiler

```
export COMPUTE_PROFILE_CSV=1
```

CLI Profiler Trick

- This trick matches the nvprof trick for getting a unique log file for each XK7 node.

```
#!/bin/bash
# USAGE: Add between aprun options and executable
# For Example: aprun -n 16 -N 1 ./foo arg1 arg2
# Becomes: aprun -n 16 -N 1 ./profile.sh ./foo arg1 arg2

# Enable command-line profiler
export COMPUTE_PROFILE=1

# Set output to CSV (optional)
export COMPUTE_PROFILE_CSV=1

# Give each *node* a separate file
export COMPUTE_PROFILE_LOG=cuda_profile_$(hostname).log

# Stripe each profile file by 1 to share the load on large runs
lfs setstripe -c 1 $COMPUTE_PROFILE_LOG

# Execute the provided command.
exec $*
```

https://gist.github.com/jefflarkin/5356512

What goes on within time step loop?

DO WHILE TIME < MAXIMUM TIME

- Compute
- Communicate
- Compute
- I/O
- Communicate
- Compute
- Compute
- Compute
- I/O
- Compute
- Communicate
- Compute
- Communicate

END DO

Where are the looping structures

```
DO WHILE TIME < MAXIMUM TIME

    call crunch0 (Contains loops )
     DO
       call crunch1
       call crunch2
    END DO

      call crunch3 (Contains loops )
      call communicate0 (Contains MPI)

    DO
     call crunch4 (Contains loops, I/O and/or MPI )
    END DO
      call Inputouput (Contains I/O)

END DO
```

Possible Approaches

- **Botton Up (Aim to parallelize some of the computation)**
  1. Identify looping structures that use the most time
  2. Identify what arrays are used in those loops
  3. Identify other loops that utilize those arrays
  4. Go to 2
  5. Can computation and/or communication be reorganized
- **Top Down (Aim to parallelize all computation)**
  1. Identify all arrays used within the time step loop
  2. Identify which loops access arrays
  3. Can computation and/or communication be reorganized

Analyze the code

- **Considering getting the maximum overlap of computation and communication**
  - Can some computation be delayed to allow for overlap of computation and communication

```
  call get_mass_frac( q, volum, yspecies )              ! get Ys from rho*Ys, volum from rho
  call get_velocity_vec( u, q, volum )                  ! fill the velocity vector
  call calc_inv_avg_mol_wt( yspecies, avmolwt )         ! set inverse of mixture MW
  call calc_temp(temp, q(:,:,:,5)*volum, u, yspecies )  ! set T, Cp_mix
  call calc_gamma( gamma, cpmix, mixMW )                ! set gamma
  call calc_press( pressure, q(:,:,:,4), temp, mixMW )  ! set pressure
!!!  Initiate Communication of temp, u and yspecies,mixMW
!!!  Wait for communication of halos of temp, u, yspecies,mixMW
```

  - Originally in S3D, all of the above computation was grouped and then halos temp,u and yspecies where communicated

```
  call get_mass_frac( q, volum, yspecies )              ! get Ys from rho*Ys, volum from rho
  call get_velocity_vec( u, q, volum )                  ! fill the velocity vector
  call calc_temp(temp, q(:,:,:,5)*volum, u, yspecies )  ! set T, Cp_mix
!!!  Initiate Communication of temp, u and yspecies
  call calc_inv_avg_mol_wt( yspecies, avmolwt )         ! set inverse of mixture MW
  call calc_gamma( gamma, cpmix, mixMW )                ! set gamma
  call calc_press( pressure, q(:,:,:,4), temp, mixMW )  ! set pressure
!!!  Wait for communication of halos of temp, u, yspecies
!!!  Initiate Communication of mixMW
```

Tools for performing this difficult task

- **Cray Perftool tool box has many elements that will be useful for this analysis**
  - ftn -h profile_generate
    - Tremendous overhead for instrumentation, only want to run this a few timestep.
    - Identifies loop characteristics – average, min, max loop iteration count
  - pat_build –u –g mpi,io
    - Identifies major routines, where MPI is used, where I/O is used, etc
- **Tools we need and are looking at**
  - Given an array or a set of arrays, show everywhere they are accessed and how they are accessed
    - This is difficult for Fortran, must consider aliasing through structures, routine arguments
    - This is extremely difficult and extremely useful for C and C++

Relationship between OpenMP and OpenACC

```
DO WHILE TIME < MAXIMUM TIME
  !$omp parallel default(shared) private(……)
            call crunch0 (Contains OpenMP  )
    !$omp do

            call crunch1
            call crunch2

    !$omp end do
          call communicate0 (Contains MPI)

     !$omp do
    call crunch3 (Contains OpenMP  )
  !$omp end parallel

END DO
```

Relationship between OpenMP and OpenACC

```
!$acc data copyin(OpenMP shared data…
!$acc        present_or_create( OpenMP private data…
DO WHILE TIME < MAXIMUM TIME
  !$omp parallel default(shared)  private(……)
              call crunch0 (Contains OpenMP and OpenACC)
    !$omp do
    !$acc parallel loop
              call crunch1
              call crunch2
    !$acc parallel loop
    !$omp end do
          call communicate0 (Contains MPI)

     !$omp do
    call crunch3 (Contains OpenMP and OpenACC)
  !$omp end parallel

END DO
!$acc end data
```

Relationship between OpenMP and OpenACC

```
DO WHILE TIME < MAXIMUM TIME
  !$omp parallel do default(shared) private(……)
     DO K = 1, KMAX
        call crunch0

        DO J = 1, JMAX
           call crunch1
           call crunch2
        END DO

     call communicate0 (Contains MPI)
     call crunch3
     END DO
  !$omp end parallel do
END DO
```

Relationship between OpenMP and OpenACC

```
!$acc data copyin(OpenMP shared data…
!$acc        present_or_create( OpenMP private data…
DO WHILE TIME < MAXIMUM TIME
  !$omp parallel do default(shared) private(……)
     DO K = 1, KMAX
          call crunch0(Contains OpenACC with ASYNC(K))
    !$ acc parallel loop present(….)  ASYNC(K)
          DO J = 1, JMAX
               call crunch1
               call crunch2
          END DO
    !$acc end parallel loop
    !$acc wait(K)
     call communicate0 (Contains MPI)
     call crunch3   (Contains OpenACC with ASYNC(K) )
  !$omp end parallel loop
END DO
```

1. First and foremost – Profile the application

Table 1: Profile by Function Group and Function

Time%	Time	Imb. Time	Imb. Time%	Calls	Group Function PE=HIDE
100.0%	74.343236	--	--	6922221.1	Total
68.0%	50.560859	--	--	6915004.0	USER
15.0%	11.125597	1.127372	9.2%	288000.0	remap_
14.4%	10.742300	1.092106	9.2%	288000.0	ppmlr_
13.0%	9.629421	1.156963	10.7%	2592000.0	parabola_
7.0%	5.200492	0.573247	9.9%	288000.0	evolve_
5.4%	3.978226	1.112412	21.9%	288000.0	riemann_
2.5%	1.877102	0.244424	11.5%	288000.0	states_
2.1%	1.554790	0.279146	15.2%	576000.0	paraset_
1.8%	1.349213	0.395894	22.7%	864000.0	volume_
1.3%	0.969134	0.324846	25.1%	864000.0	forces_
1.1%	0.834536	0.144497	14.8%	288000.0	flatten_
1.0%	0.759212	0.091074	10.7%	500.0	sweepx1_
0.9%	0.671678	0.067951	9.2%	500.0	sweepx2_
0.8%	0.576190	0.067274	10.5%	1000.0	sweepy_
0.8%	0.569666	0.045713	7.4%	500.0	sweepz_
0.5%	0.368043	0.120640	24.7%	288000.0	boundary_
0.4%	0.331896	0.046669	12.3%	1.0	vhone_
0.0%	0.015684	0.004329	21.6%	500.0	dtcon_
0.0%	0.006907	1.146796	99.4%	1.0	prin_
0.0%	0.000706	0.000916	56.5%	1.0	init_
0.0%	0.000064	0.000660	91.2%	1.0	exit

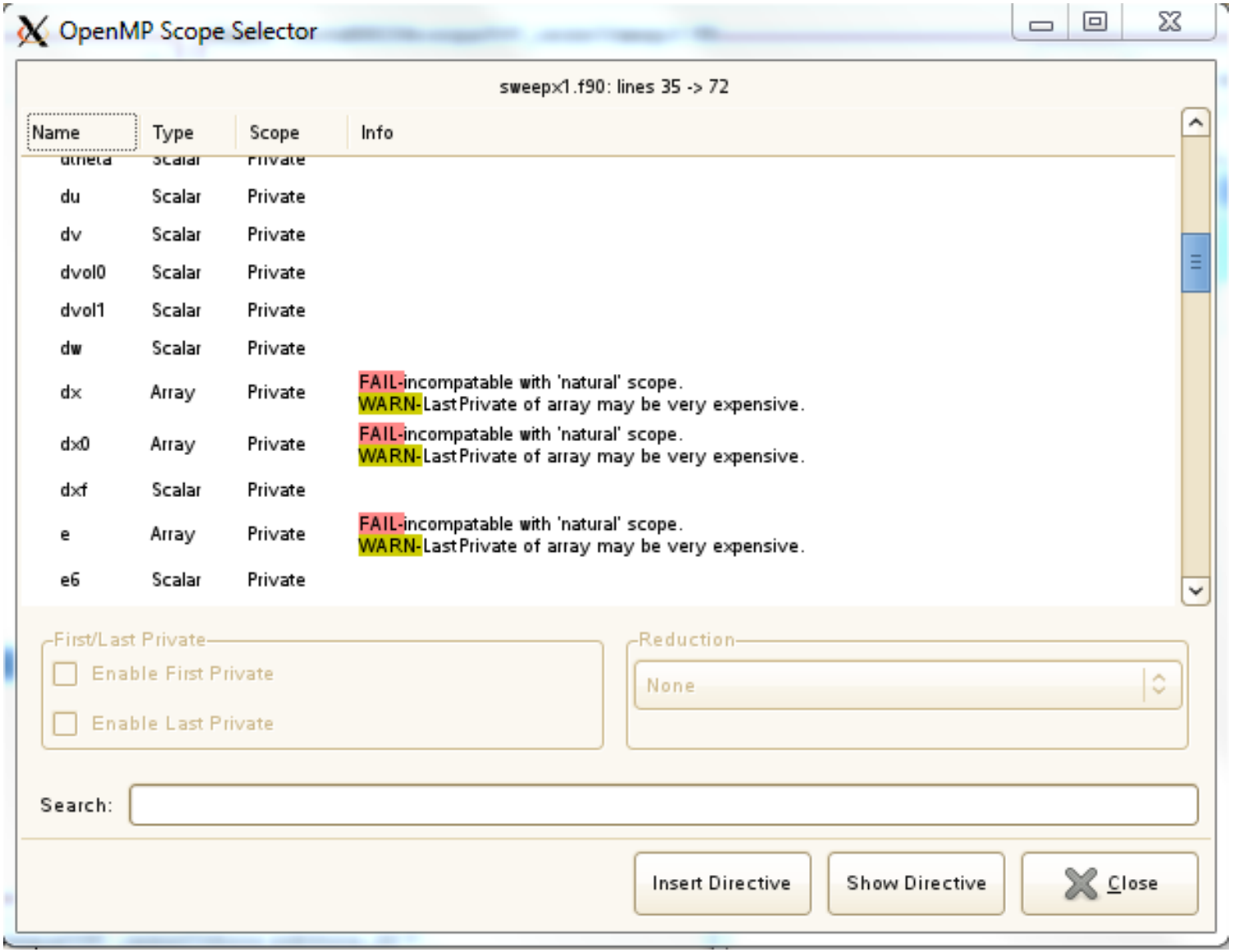
1. Continued

```
Table 1:  Function Calltree View

 Time%  |     Time  |    Calls  |Calltree
        |           |           | PE=HIDE

 100.0% | 53.513557 | 6627213.1 |Total
|-------------------------------------------------------
| 100.0% | 53.513427 | 6627009.0 |vhone_
||------------------------------------------------------
||  28.8% | 15.419074 |  368500.0 |sweepz_
3|        |           |           | sweepz_.LOOPS
||||-----------------------------------------------------
4|||  16.0% |  8.553538 |     500.0 |sweepz_.LOOPS(exclusive)
4|||  12.8% |  6.865537 |  368000.0 |sweepz_.LOOP.05.li.54
5|||        |           |           | sweepz_.LOOP.06.li.55
6|||        |           |           |  ppmlr_
|||||||-----------------------------------------------------
7||||||   5.0% |  2.701293 |  144000.0 |remap_
8||||||        |           |           | remap_.LOOPS
|||||||||-----------------------------------------------------
9||||||||   3.4% |  1.832297 |   96000.0 |parabola_
10|||||||       |           |           | parabola_.LOOPS
9||||||||   1.2% |  0.665167 |   16000.0 |remap_.LOOPS(exclusive)
|||||||||=====================================================
7||||||   4.1% |  2.192975 |   16000.0 |riemann_
8||||||        |           |           | riemann_.LOOPS
7||||||   1.8% |  0.941416 |   48000.0 |parabola_
8||||||        |           |           | parabola_.LOOPS
||||=======================================================
```

1. Continued

```
Table 1:  Profile by Function and Callers

 Time%  |     Time  |    Calls  |Group
        |           |           | Function
        |           |           |  Caller
        |           |           |   PE=HIDE
||  21.0% | 11.235866 | 2592000.0 |parabola_.LOOPS
3|       |           |           | parabola_
||||-------------------------------------------------
4|||  13.8% |  7.371909 | 1728000.0 |remap_.LOOPS
5|||       |           |           | remap_
6|||       |           |           |  ppmlr_
|||||||-------------------------------------------------
7||||||   3.5% |  1.876054 |   96000.0 |sweepy_.LOOP.2.li.39
8||||||       |           |           | sweepy_.LOOP.1.li.38
9||||||       |           |           |  sweepy_.LOOPS
10|||||       |           |           |   sweepy_
11|||||       |           |           |    vhone_
7||||||   3.4% |  1.839313 |  768000.0 |sweepx2_.LOOP.2.li.35
8||||||       |           |           | sweepx2_.LOOP.1.li.34
9||||||       |           |           |  sweepx2_.LOOPS
10|||||       |           |           |   sweepx2_
11|||||       |           |           |    vhone_
7||||||   3.4% |  1.832297 |   96000.0 |sweepz_.LOOP.06.li.55
8||||||       |           |           | sweepz_.LOOP.05.li.54
9||||||       |           |           |  sweepz_.LOOPS
10|||||       |           |           |   sweepz_
11|||||       |           |           |    vhone_
7||||||   3.4% |  1.824246 |  768000.0 |sweepx1_.LOOP.2.li.35
8||||||       |           |           | sweepx1_.LOOP.1.li.34
9||||||       |           |           |  sweepx1_.LOOPS
10|||||       |           |           |   sweepx1_
11|||||       |           |           |    vhone_
|||||||=================================================
```

2. Use Reveal to identify scoping of variables in the major loop – may call subroutines and functions



2. Continued

```
! module sweeps
!=======================================================================
! Data structures used in 1D sweeps, dimensioned maxsweep  (set in sweepsize.mod)
!-----------------------------------------------------------------------

use sweepsize

character(len=1) :: sweep                                  ! direction of sweep: x,y,z
integer :: nmin, nmax, ngeom, nleft, nright                ! number of first and last real zone
real, dimension(maxsweep) :: r, p, e, q, u, v, w           ! fluid variables
real, dimension(maxsweep) :: xa, xa0, dx, dx0, dvol        ! coordinate values
real, dimension(maxsweep) :: f, flat                       ! flattening parameter
real, dimension(maxsweep,5) :: para                        ! parabolic interpolation coefficients
real :: radius, theta, stheta

end module sweeps
```

For OpenMP these need to be made task_private, for OpenACC they must be passed down the call chain.

2. Continued

Original

```
hdt    = 0.5*dt
do n = nmin-4, nmax+4
  Cdtdx (n) = sqrt(gam*p(n)/r(n))/(dx(n)*radius)
  svel      = max(svel,Cdtdx(n))
  Cdtdx (n) = Cdtdx(n)*hdt
  fCdtdx(n) = 1. - fourthd*Cdtdx(n)
enddo
```

Restructured

```
hdt    = 0.5*dt
Svel0 = 0.0
do n = nmin-4, nmax+4
  Cdtdx (n) = sqrt(gam*p(n)/r(n))/(dx(n)*radius)
  svel0(n)      = max(svel(n),Cdtdx(n))
  Cdtdx (n) = Cdtdx(n)*hdt
  fCdtdx(n) = 1. - fourthd*Cdtdx(n)
Enddo
!$omp critical
Do n = nmin-4, nmax +4
Svel = max(svel0(n),svel)
Enddo
!$omp end critical
```

For OpenMP need to have a critical region around setting of svel, for OpenACC This needs to be pulled up chain and made a reduction variable.

2. Continued

```
! Directive inserted by Cray Reveal.  May be incomplete.
!$OMP  parallel do default(none)                                          &
!$OMP&   unresolved (f,flat,p,q,radius)                                   &
!$OMP&   private (i,j,k,n,dxf,xaf,xwag,temp1,d,np,umidr,umidl,zrgh,zlft,  &
!$OMP&            pmold,l,uold,dm,dm0,fractn2,nn,fluxq,fluxe,fluxw,       &
!$OMP&            fluxv,fluxu,fluxr,delp2,delp1,shock,temp2,old_flat,     &
!$OMP&            onemfl,hdt,sinxf0,gamfac1,gamfac2,dtheta,deltx,fractn,  &
!$OMP&            ekin)                                                   &
!$OMP&   shared  (gamm,js,ks,ngeomx,nleftx,nrightx,send1,zdx,zfl,zpr,     &
!$OMP&            zro,zux,zuy,zuz,zxa)                                    &
!$OMP&   firstprivate (dx,dx0,e,r,u,v,w,xa,xa0,umid,pmid,rrgh,urgh,prgh,  &
!$OMP&            rlft,ulft,plft,ul,u6,du,rl,r6,dr,pl,p6,dp,steep,ci,c,   &
!$OMP&            bi,b,ai,a,scrch3,scrch2,scrch1,ar,da,diffa,fict,grav,   &
!$OMP&            fcdtdx,cdtdx,wrgh,wlft,prghi,plfti,crgh,clft,amid,       &
!$OMP&            fict1,grav1,fict0,grav0,xa3,xa2,upmid,xa1,dtbdm,dvol1,  &
!$OMP&            delta,dvol0,el,e6,de,ql,q6,dq,wl,w6,dw,vl,v6,dv)        &
!$OMP&   lastprivate (dx,dx0,e,r,u,v,w,xa,xa0)
```

3. Use OpenACC to identify data motion require to run with companion accelerator

```
46.  + G-------------< !$acc parallel loop private( k,j,i,n,r, p, e, q, u, v, w, svel0,&
47.    G               !$acc&      xa, xa0, dx, dx0, dvol, f, flat, para,radius, theta, stheta)&
48.    G               !$acc&      reduction(max:svel)
49.    G               #else
50.    G               !$omp parallel do private( k,j,i,n,r, p, e, q, u, v, w, svel0,&
51.    G               !$omp&      xa, xa0, dx, dx0, dvol, f, flat, para,radius, theta, stheta)&
52.    G               !$omp&      reduction(max:svel)
53.    G               #endif
54.  + G g-----------< do k = 1, ks
55.  + G g 3---------<  do j = 1, js
56.    G g 3               theta=0.0
57.    G g 3               stheta=0.0
58.    G g 3               radius=0.0
59.    G g 3
60.    G g 3             ! Put state variables into 1D arrays, padding with 6 ghost zones
61.  + G g 3 4-------<    do m = 1, npey
62.  + G g 3 4 r4----<     do i = 1, isy
63.    G g 3 4 r4             n = i + isy*(m-1) + 6
64.    G g 3 4 r4             r(n) = recv2(1,k,i,j,m)
65.    G g 3 4 r4             p(n) = recv2(2,k,i,j,m)
66.    G g 3 4 r4             u(n) = recv2(3,k,i,j,m)
67.    G g 3 4 r4             v(n) = recv2(4,k,i,j,m)
68.    G g 3 4 r4             w(n) = recv2(5,k,i,j,m)
69.    G g 3 4 r4             f(n) = recv2(6,k,i,j,m)
70.    G g 3 4 r4---->     enddo
71.    G g 3 4------->    enddo
72.    G g 3
73.    G g 3 g-------<    do i = 1,imax
74.    G g 3 g              n = i + 6
75.    G g 3 g              xa0(n) = zxa(i)
76.    G g 3 g              dx0(n) = zdx(i)
77.    G g 3 g              xa (n) = zxa(i)
78.    G g 3 g              dx (n) = zdx(i)
79.    G g 3 g              p  (n) = max(smallp,p(n))
80.    G g 3 g              e  (n) = p(n)/(r(n)*gamm)+0.5*(u(n)**2+v(n)**2+w(n)**2)
```

3. Continued

```
 72.     G g 3
 73.     G g 3 g-------<     do i = 1,imax
 74.     G g 3 g               n = i + 6
 75.     G g 3 g               xa0(n) = zxa(i)
 76.     G g 3 g               dx0(n) = zdx(i)
 77.     G g 3 g               xa (n) = zxa(i)
 78.     G g 3 g               dx (n) = zdx(i)
 79.     G g 3 g               p  (n) = max(smallp,p(n))
 80.     G g 3 g               e  (n) = p(n)/(r(n)*gamm)+0.5*(u(n)**2+v(n)**2+w(n)**2)
 81.     G g 3 g------->     enddo
 82.     G g 3
 83.     G g 3               ! Do 1D hydro update using PPMLR
 84.   + G g 3 gr2 Ip-->     call ppmlr (svel0, sweep, nmin, nmax, ngeom, nleft, nright,r, p, e, q, u, v,
 85.     G g 3                  xa, xa0, dx, dx0, dvol, f, flat, para,radius, theta, stheta)
 86.     G g 3 g-------<   do n = nmin-4, nmax+4
 87.     G g 3 g           svel      = max(svel,svel0(n))
 88.     G g 3 g------->   enddo
 89.     G g 3           #ifdef DEBUGX
 90.     G g 3             print *,'In sweepx2',svel
 91.     G g 3           #endif
 92.     G g 3
 93.     G g 3               ! Put updated values back into 3D arrays, dropping ghost zones
 94.     G g 3 g-------<     do i = 1, imax
 95.     G g 3 g               n = i + 6
 96.     G g 3 g               zro(i,j,k) = r(n)
 97.     G g 3 g               zpr(i,j,k) = p(n)
 98.     G g 3 g               zux(i,j,k) = u(n)
 99.     G g 3 g               zuy(i,j,k) = v(n)
100.     G g 3 g               zuz(i,j,k) = w(n)
101.     G g 3 g               zfl(i,j,k) = f(n)
102.     G g 3 g------->     enddo
103.     G g 3
104.     G g 3--------->  enddo
105.     G g----------> enddo
```

3. Continued

```
ftn-6405 ftn: ACCEL File = sweepx2.f90, Line = 46
  A region starting at line 46 and ending at line 107 was placed on the accelerator.

ftn-6418 ftn: ACCEL File = sweepx2.f90, Line = 46
  If not already present: allocate memory and copy whole array "recv2" to accelerator, free at line 107
  (acc_copyin).

ftn-6418 ftn: ACCEL File = sweepx2.f90, Line = 46
  If not already present: allocate memory and copy whole array "zxa" to accelerator, free at line 107
  (acc_copyin).

ftn-6418 ftn: ACCEL File = sweepx2.f90, Line = 46
  If not already present: allocate memory and copy whole array "zdx" to accelerator, free at line 107
  (acc_copyin).

ftn-6416 ftn: ACCEL File = sweepx2.f90, Line = 46
  If not already present: allocate memory and copy whole array "zro" to accelerator, copy back at line 107
  (acc_copy).

ftn-6416 ftn: ACCEL File = sweepx2.f90, Line = 46
  If not already present: allocate memory and copy whole array "zpr" to accelerator, copy back at line 107
  (acc_copy).

ftn-6416 ftn: ACCEL File = sweepx2.f90, Line = 46
  If not already present: allocate memory and copy whole array "zux" to accelerator, copy back at line 107
  (acc_copy).
```

4. Once one loop is analyze, now look at next highest compute loop, perform steps 2 and 3.

```
Table 1:  Profile by Function and Callers

 Time%  |     Time  |    Calls  |Group
        |           |           | Function
        |           |           |  Caller
        |           |           |   PE=HIDE
||  21.0% | 11.235866 | 2592000.0 |parabola_.LOOPS
3|       |           |           | parabola_
||||-------------------------------------------------
4|||  13.8% |  7.371909 | 1728000.0 |remap_.LOOPS
5|||        |           |           | remap_
6|||        |           |           |  ppmlr_
|||||||-------------------------------------------------
7||||||   3.5% |  1.876054 |   96000.0 |sweepy_.LOOP.2.li.39
8||||||        |           |           | sweepy_.LOOP.1.li.38
9||||||        |           |           |  sweepy_.LOOPS
10|||||        |           |           |   sweepy_
11|||||        |           |           |    vhone_
7||||||   3.4% |  1.839313 |  768000.0 |sweepx2_.LOOP.2.li.35
8||||||        |           |           | sweepx2_.LOOP.1.li.34
9||||||        |           |           |  sweepx2_.LOOPS
10|||||        |           |           |   sweepx2_
11|||||        |           |           |    vhone_
7||||||   3.4% |  1.832297 |   96000.0 |sweepz_.LOOP.06.li.55
8||||||        |           |           | sweepz_.LOOP.05.li.54
9||||||        |           |           |  sweepz_.LOOPS
10|||||        |           |           |   sweepz_
11|||||        |           |           |    vhone_
7||||||   3.4% |  1.824246 |  768000.0 |sweepx1_.LOOP.2.li.35
8||||||        |           |           | sweepx1_.LOOP.1.li.34
9||||||        |           |           |  sweepx1_.LOOPS
10|||||        |           |           |   sweepx1_
11|||||        |           |           |    vhone_
|||||||=================================================
```

5. Soon multiple loops can be combined within a OpenACC data region for elminating transfers to and from the host.

```
!###############################################################################
!                          MAIN COMPUTATIONAL LOOP
#ifdef GPU
!$acc data copy(zro,zpr,zux,zuy,zuz,zfl,zxa,zdx,zxc,zya,zdy,zyc,zza,zdz,zzc)
#endif
do while (ncycle < ncycend)
!  if(mype == 0) write(*,*) 'STEP = ',ncycle
  ncycle = ncycle + 2
  ncycp  = ncycp  + 2
  ncycd  = ncycd  + 2
  ncycm  = ncycm  + 2
  olddt  = dt
  svel   = 0.
  if ( time + 2*dt > endtime ) then ! set dt to land on endtime
    if(mype==0) write(8,*) 'cutting to the end...', ncycle, ncycend
    dt = 0.5*(endtime - time)
    ncycend = ncycle-1
    ncycp   = nprin
    ncycd   = ndump
  else if ( timep+2.0*dt > tprin ) then ! set dt to land on tprin
    dt = 0.5*(tprin - timep)
    ncycp = nprin
  else if ( timem+2*dt > tmovie ) then ! set dt to land on tmovie
    dt = 0.5*(tmovie - timem)
    ncycm = nmovie
  endif
! Alternate sweeps to approximate 2nd order operator splitting
  call sweepx1(svel)
  call sweepy(svel)
  if (ndim==3) then
   call sweepz  (svel)
   call sweepy(svel)
  endif
  call sweepx2(svel)
```

6. Work outward until a data region encompasses a communication, I/O or looping structure more suited for the host

- **Now the hard part**
  - Must now account for update host and device
    - When message passing is done by the host, must update the host prior to the transfer and update the device after the transfer
    - When any computation is performed on the host, must update the host prior to the transfer and update the device after the transfer
    - When I/O is performed on the host, must update the host prior to the transfer and update the device after the transfer

!$acc host_data use_device

```
#ifdef GPU
!$acc data present(f)
!$acc host_data use_device(f)
#endif
  if( deriv_z_list(idx)%packed ) then
    deriv_z_list(idx)%packed = .false.
    if(deriv_z_list(idx)%neg_nbr>=0) then
       call MPI_ISend(f(1,1,1),(mx*my*iorder/2),&
                      MPI_REAL8,deriv_z_list(idx)%neg_nbr,deriv_list_size + idx, &
                      gcomm,deriv_z_list(idx)%req(2),ierr)
    endif
    if(deriv_z_list(idx)%pos_nbr>=0) then
     ! send ghost cells to neighbor on (+z) side
       nm = mz + 1 - iorder/2
       call MPI_ISend(f(1,1,nm),(mx*my*iorder/2), &
                      MPI_REAL8,deriv_z_list(idx)%pos_nbr,idx, &
                      gcomm,deriv_z_list(idx)%req(4),ierr)
    endif
  else
    if(deriv_z_list(idx)%neg_nbr>=0) then
       call MPI_ISend(f(1,1,1),(mx*my*iorder/2),&
                      MPI_REAL8,deriv_z_list(idx)%neg_nbr,deriv_list_size + idx, &
                      gcomm,deriv_z_list(idx)%req(2),ierr)
    endif

    if(deriv_z_list(idx)%pos_nbr>=0) then
     ! send ghost cells to neighbor on (+z) side
       nm = mz + 1 - iorder/2
       call MPI_ISend(f(1,1,nm),(mx*my*iorder/2), &
                      MPI_REAL8,deriv_z_list(idx)%pos_nbr,idx, &
                      gcomm,deriv_z_list(idx)%req(4),ierr)
    endif
  endif
#ifdef GPU
!$acc end host_data
!$acc end data
#endif
```

7. Move data region outside time step loop

8. Test versions after each step – don't worry about performance yet – just accuracy

9. The compiler may introduce data transfer so look at –rm listing for each individual OpenACC loop.

```
ftn-6417 ftn: ACCEL File = computeCoefficients_r.f90, Line = 151
  Allocate memory and copy whole array "sqrtq" to accelerator, free at line 1752 (acc_copyin).

ftn-6418 ftn: ACCEL File = computeCoefficients_r.f90, Line = 151
  If not already present: allocate memory and copy whole array "wt" to accelerator,
  free at line  1752 (acc_copyin).

ftn-6422 ftn: ACCEL File = computeCoefficients_r.f90, Line = 151
  If not already present: allocate memory for whole array "xxwt" on accelerator,
  free at line 1752 (acc_share).

ftn-6422 ftn: ACCEL File = computeCoefficients_r.f90, Line = 151
  If not already present: allocate memory for whole array "y" on accelerator,
  free at line 1752 (acc_share).

ftn-6422 ftn: ACCEL File = computeCoefficients_r.f90, Line = 151
  If not already present: allocate memory for whole array "x" on accelerator,
  free at line 1752 (acc_share).

ftn-6405 ftn: ACCEL File = computeCoefficients_r.f90, Line = 156
  A region starting at line 156 and ending at line 223 was placed on the accelerator.

ftn-6416 ftn: ACCEL File = computeCoefficients_r.f90, Line = 156
  If not already present: allocate memory and copy whole array "lambdax" to accelerator,
  copy back at line 223 (acc_copy).

ftn-6416 ftn: ACCEL File = computeCoefficients_r.f90, Line = 156
  If not already present: allocate memory and copy whole array "vscsty" to accelerator,
  copy back at line 223 (acc_copy).

ftn-6418 ftn: ACCEL File = computeCoefficients_r.f90, Line = 156
  If not already present: allocate memory and copy whole array "mixmx" to accelerator,
  free at line 223 (acc_copyin).
```

9. Useful information can be obtained by using setenv CRAY_ACC_DEBUG 1 or 2 or 3

```
ACC: Start transfer 1 items async(auto) from ../source/f90_files/solve/integrate_erk.f90:99
ACC:   flags: AUTO_ASYNC
ACC:    async_info: 0x2aaab89bb720
ACC:
ACC:   Trans 1
ACC:       Simple transfer of 'q' (168 bytes)
ACC:            host ptr 7fffffff6ab8
ACC:            acc  ptr b28f80000
ACC:            flags: DOPE_VECTOR DV_ONLY_DATA COPY_ACC_TO_HOST
ACC:            Transferring dope vector
ACC:              dim:1 lowbound:1 extent:48 stride_mult:1
ACC:              dim:2 lowbound:1 extent:48 stride_mult:48
ACC:              dim:3 lowbound:1 extent:48 stride_mult:2304
ACC:              dim:4 lowbound:1 extent:56 stride_mult:110592
ACC:              dim:5 lowbound:3 extent:1 stride_mult:6193152
ACC:              DV size=49545216 (scale:8, elem_size:8)
ACC:              total mem size=49545216 (dv:0 obj:49545216)
ACC:            async copy acc to host (b28f80000 to 100324f08c0) async_info 0x2aaab89bb720
ACC:                split copy acc to host (100324f08c0 to b28f80000) size = 49545216
ACC:
ACC: End transfer (to acc 0 bytes, to host 49545216 bytes)
```

9. Useful information can be obtained by using setenv CRAY_ACC_DEBUG 1 or 2 or 3

```
ACC: Start transfer 89 items async(auto) from ../source/f90_files/solve/rhsf.f90:256
ACC:       allocate, copy to acc 'aex' (8 bytes)
ACC:       allocate, copy to acc 'aey' (8 bytes)
ACC:       allocate, copy to acc 'aez' (8 bytes)
ACC:       present 'avmolwt' (884736 bytes)
ACC:       allocate, copy to acc 'bex' (8 bytes)
ACC:       allocate, copy to acc 'bey' (8 bytes)
ACC:       allocate, copy to acc 'bez' (8 bytes)
ACC:       allocate 'buffer31' (110592 bytes)
ACC:       allocate 'buffer32' (110592 bytes)
ACC:       allocate 'buffer33' (110592 bytes)
ACC:       allocate 'buffer34' (110592 bytes)
ACC:       allocate 'buffer35' (110592 bytes)
ACC:       allocate 'buffer36' (110592 bytes)
ACC:       allocate 'buffer37' (110592 bytes)
ACC:       allocate 'buffer41' (6193152 bytes)
ACC:       allocate 'buffer42' (6193152 bytes)
ACC:       allocate 'buffer43' (6193152 bytes)
ACC:       allocate 'buffer44' (6193152 bytes)
ACC:       allocate 'buffer45' (6193152 bytes)
ACC:       allocate, copy to acc 'cex' (8 bytes)
ACC:       allocate, copy to acc 'cey' (8 bytes)
ACC:       allocate, copy to acc 'cez' (8 bytes)
ACC:       present 'cpcoef_aa' (832416 bytes)
ACC:       present 'cpcoef_bb' (832416 bytes)
ACC:       present 'cpmix' (884736 bytes)
ACC:       allocate, copy to acc 'dex' (8 bytes)
```

9. Useful information can be obtained by using setenv CRAY_ACC_DEBUG 1 or 2 or 3

```
ACC: Transfer 46 items (to acc 831869196 bytes, to host 0 bytes) async(auto)
from ../source/drivers/solve_driver.f90:176
ACC: Transfer 49 items (to acc 0 bytes, to host 0 bytes) async(auto)
from ../source/f90_files/solve/integrate_erk.f90:68
ACC: Transfer 7 items (to acc 0 bytes, to host 204374016 bytes) async(auto)
from ../source/f90_files/solve/integrate_erk.f90:75
ACC: Wait async(auto) from ../source/f90_files/solve/integrate_erk.f90:75
ACC: Execute kernel integrate_$ck_L86_1 async(auto)
from ../source/f90_files/solve/integrate_erk.f90:86
ACC: Transfer 1 items (to acc 0 bytes, to host 49545216 bytes) async(auto)
from ../source/f90_files/solve/integrate_erk.f90:99
ACC: Wait async(auto) from ../source/f90_files/solve/integrate_erk.f90:99
ACC: Transfer 89 items (to acc 1260 bytes, to host 0 bytes) async(auto)
from ../source/f90_files/solve/rhsf.f90:256
ACC: Transfer 15 items (to acc 0 bytes, to host 0 bytes) async(auto)
from ../source/f90_files/solve/calc_primitive_var.f90:42
ACC: Transfer 4 items (to acc 0 bytes, to host 0 bytes) async(auto)
from ../source/f90_files/solve/calc_primitive_var.f90:47
ACC: Execute kernel calc_primary_vars_$ck_L47_1 async(auto)
from ../source/f90_files/solve/calc_primitive_var.f90:47
ACC: Wait async(auto) from ../source/f90_files/solve/calc_primitive_var.f90:157
ACC: Transfer 4 items (to acc 0 bytes, to host 0 bytes) async(auto)
from ../source/f90_files/solve/calc_primitive_var.f90:157
```

9. Useful information can be obtained by using setenv CUDA_PROFILE 1

```
method=[ integrate_$ck_L86_1 ] gputime=[ 1265.536 ] cputime=[ 26.000 ] occupancy=[ 1.000 ]
method=[ memcpyDtoHasync ] gputime=[ 7381.152 ] cputime=[ 8.000 ]
method=[ memcpyHtoDasync ] gputime=[ 4.672 ] cputime=[ 13.000 ]
method=[ memcpyHtoDasync ] gputime=[ 2.496 ] cputime=[ 6.000 ]
method=[ memcpyHtoDasync ] gputime=[ 2.496 ] cputime=[ 6.000 ]
method=[ memcpyHtoDasync ] gputime=[ 2.528 ] cputime=[ 6.000 ]
method=[ memcpyHtoDasync ] gputime=[ 2.496 ] cputime=[ 10.000 ]
method=[ memcpyHtoDasync ] gputime=[ 2.528 ] cputime=[ 6.000 ]
method=[ memcpyHtoDasync ] gputime=[ 3.616 ] cputime=[ 8.000 ]
method=[ memcpyHtoDasync ] gputime=[ 2.528 ] cputime=[ 6.000 ]
method=[ memcpyHtoDasync ] gputime=[ 2.528 ] cputime=[ 6.000 ]
method=[ memcpyHtoDasync ] gputime=[ 2.528 ] cputime=[ 6.000 ]
method=[ memcpyHtoDasync ] gputime=[ 2.528 ] cputime=[ 6.000 ]
method=[ memcpyHtoDasync ] gputime=[ 2.528 ] cputime=[ 6.000 ]
method=[ memcpyHtoDasync ] gputime=[ 3.616 ] cputime=[ 8.000 ]
method=[ memcpyHtoDasync ] gputime=[ 3.808 ] cputime=[ 8.000 ]
method=[ memcpyHtoDasync ] gputime=[ 3.872 ] cputime=[ 8.000 ]
method=[ memcpyHtoDasync ] gputime=[ 2.688 ] cputime=[ 6.000 ]
method=[ memcpyHtoDasync ] gputime=[ 2.624 ] cputime=[ 6.000 ]
```

10. Optimize/Minimize data transfers first by using present on data clause.

- **PRESENT**
  - This is for variables that have been copyin, copy or created up the call chain
    - If you forget this – you could be creating an error. Compiler will copy in the host version when you are expecting the device version
- **PRESENT_OR_CREATE**
  - This is for variables that are only going to be used on the device
- **PRESENT_OR_COPYIN**
  - This is for variables that must be copied in from the host; however, they do not change after the first copyin

11. Gather perftools statistics on code and identify bottlenecks

Table 1: Time and Bytes Transferred for Accelerator Regions

Acc Time%	Acc Time	Host Time	Acc Copy In (MBytes)	Acc Copy Out (MBytes)	Events	Function Thread=HIDE
100.0%	130.491	140.390	50831	96209	897204	Total
17.1%	22.301	0.118	--	--	600	reaction_rate_vec_.ACC_ASYNC_KERNEL@li.167
8.9%	11.634	0.069	--	--	600	rhsf_.ACC_ASYNC_KERNEL@li.916
5.1%	6.594	0.810	6961	--	8400	derivative_xyz_wait_np$derivative_m_.ACC_ASYNC_COPY@li.
4.5%	5.815	0.004	--	--	100	computecoefficients_r_.ACC_ASYNC_KERNEL@li.155
3.7%	4.829	0.820	6961	--	8400	derivative_xyz_wait_np$derivative_m_.ACC_ASYNC_COPY@li.
3.5%	4.503	0.872	6961	--	8400	derivative_xyz_wait_np$derivative_m_.ACC_ASYNC_COPY@li.
3.1%	4.022	0.176	--	6497	1800	derivative_z_pack_np_.ACC_ASYNC_COPY@li.577
2.9%	3.842	0.241	--	6497	1800	derivative_z_pack_np_.ACC_ASYNC_COPY@li.619
2.9%	3.809	0.018	--	--	600	rhsf_.ACC_ASYNC_KERNEL@li.1737
2.8%	3.598	0.071	--	--	600	rhsf_.ACC_ASYNC_KERNEL@li.1680
2.7%	3.517	2.074	6961	--	8400	derivative_xyz_wait_np$derivative_m_.ACC_ASYNC_COPY@li.
2.3%	3.060	0.009	--	19491	100	integrate_.ACC_ASYNC_COPY@li.75
2.2%	2.856	0.174	--	6497	1800	derivative_y_pack_np_.ACC_ASYNC_COPY@li.650
2.1%	2.801	0.175	--	6497	1800	derivative_y_pack_np_.ACC_ASYNC_COPY@li.608
1.9%	2.529	0.068	--	--	600	rhsf_.ACC_ASYNC_KERNEL@li.624
1.9%	2.526	0.080	--	--	600	rhsf_.ACC_ASYNC_KERNEL@li.1636
1.8%	2.402	0.084	--	--	600	rhsf_.ACC_ASYNC_KERNEL@li.400
1.8%	2.399	0.066	--	--	600	rhsf_.ACC_ASYNC_KERNEL@li.450
1.8%	2.375	2.799	--	7341	600	save_bc_deriv1$rhsf_.ACC_ASYNC_COPY@li.248
1.7%	2.251	0.777	6961	--	8400	derivative_xyz_wait_np$derivative_m_.ACC_ASYNC_COPY@li.
1.6%	2.145	0.770	6961	--	8400	derivative_xyz_wait_np$derivative_m_.ACC_ASYNC_COPY@li.
1.6%	2.043	0.043	--	--	100	computecoefficients_r_.ACC_ASYNC_KERNEL@li.225
1.5%	1.938	0.066	--	--	600	rhsf_.ACC_ASYNC_KERNEL@li.493
1.4%	1.877	0.172	--	6497	1800	derivative_x_pack_np_.ACC_ASYNC_COPY@li.640
1.3%	1.734	1.674	3544	--	600	rhsf_.ACC_ASYNC_COPY@li.2436
1.1%	1.444	1.270	--	464.062	6600	derivative_x_pack_.ACC_ASYNC_COPY@li.463
1.0%	1.254	0.027	--	--	700	calc_primary_vars_.ACC_ASYNC_KERNEL@li.47
1.0%	1.247	0.160	--	6497	1800	derivative_x_pack_np_.ACC_ASYNC_COPY@li.598

11. Continued

```
Table 1:  Profile by Function Group and Function

 Time%  |      Time  |    Imb.   |  Imb.   |    Calls  |Group
        |            |    Time   | Time%   |           | Function
        |            |           |         |           |  Thread=HIDE

 100.0% | 174.160022 |       -- |     -- | 4867603.0 |Total
|-------------------------------------------------------------------------------------------------------------
|  92.4% | 160.926071 |       -- |     -- | 2676780.0 |USER
||------------------------------------------------------------------------------------------------------------
||  12.8% |  22.319336 | 0.000000 |   0.0% |     600.0 |reaction_rate_vec_.ACC_SYNC_WAIT@li.5008
||  10.3% |  17.997279 | 0.000000 |   0.0% |     600.0 |rhsf_.ACC_DATA_REGION@li.256
||   7.6% |  13.238744 | 0.000000 |   0.0% |    6600.0 |derivative_z_pack_.ACC_ASYNC_KERNEL@li.479
||   3.4% |   5.842934 | 0.000000 |   0.0% |    3000.0 |derivative_xyz_wait_np$derivative_m_.ACC_SYNC_WAIT@li.567
||   3.3% |   5.817360 | 0.000000 |   0.0% |     100.0 |computecoefficients_r_.ACC_SYNC_WAIT@li.222
||   2.7% |   4.743826 | 0.000321 |   0.0% |     600.0 |rhsf_.LOOP@li.2268
||   2.3% |   3.991119 | 0.000000 |   0.0% |    6600.0 |derivative_x_send_.ACC_SYNC_WAIT@li.717
||   1.8% |   3.072952 | 0.000000 |   0.0% |     100.0 |integrate_.ACC_SYNC_WAIT@li.75
||   1.7% |   3.040157 | 0.000000 |   0.0% |  201600.0 |deriv_inplane_1_
||   1.7% |   3.024576 | 0.000000 |   0.0% |     560.0 |filter$filter_m_
||   1.7% |   3.019308 | 0.000000 |   0.0% |     700.0 |calc_primary_vars_.ACC_SYNC_WAIT@li.157
||   1.6% |   2.798427 | 0.000000 |   0.0% |     600.0 |save_bc_deriv1$rhsf_.ACC_ASYNC_COPY@li.248
||   1.2% |   2.111812 | 0.000000 |   0.0% |  201600.0 |deriv_inplane_2_
||   1.2% |   2.071792 | 0.000000 |   0.0% |    8400.0 |derivative_xyz_wait_np$derivative_m_.ACC_ASYNC_COPY@li.544
||   1.2% |   2.006773 | 0.000000 |   0.0% |     100.0 |computecoefficients_r_.ACC_SYNC_WAIT@li.1748
||   1.1% |   1.975207 | 0.000000 |   0.0% |    6600.0 |derivative_z_pack_.ACC_ASYNC_COPY@li.454
||   1.1% |   1.914216 | 0.000000 |   0.0% |     100.0 |controller$rk_m_
||   1.0% |   1.673879 | 0.000000 |   0.0% |     600.0 |rhsf_.ACC_ASYNC_COPY@li.2436
||   0.9% |   1.615192 | 0.000000 |   0.0% |     600.0 |rhsf_.ACC_ASYNC_COPY@li.2187
||   0.9% |   1.598921 | 0.000000 |   0.0% |     600.0 |rhsf_.ACC_ASYNC_COPY@li.2189
||   0.9% |   1.586929 | 0.000000 |   0.0% |     600.0 |rhsf_.ACC_ASYNC_COPY@li.2191
||   0.7% |   1.268257 | 0.000000 |   0.0% |    6600.0 |derivative_x_pack_.ACC_ASYNC_COPY@li.463
||   0.6% |   1.080301 | 0.001090 |   0.1% |     600.0 |rhsf_.LOOP@li.2411
||   0.5% |   0.949635 | 0.000000 |   0.0% |     100.0 |integrate_.ACC_SYNC_WAIT@li.145
||   0.5% |   0.892484 | 0.000000 |   0.0% |   67200.0 |point_der1_y_
||   0.5% |   0.888298 | 0.000000 |   0.0% |   67200.0 |point_der1_x_
||   0.5% |   0.870532 | 0.000000 |   0.0% |     100.0 |integrate_.ACC_SYNC_WAIT@li.99
```

12. If bottleneck is data copies and you did a good job on 9. - look at packing buffers on the accelerator

```
if (vary_in_x==1) then
      call derivative_x_pack_np( nx,ny,nz, yspecies(1,1,1,1), 5, 'yspecies-x',n_spec,25)
   endif
   if (vary_in_y==1) then
      call derivative_y_pack_np( nx,ny,nz, yspecies(1,1,1,1),5, 'yspecies-y',n_spec,27)
   endif
   if (vary_in_z==1) then
      call derivative_z_pack_np( nx,ny,nz, yspecies(1,1,1,1),5, 'yspecies-z',n_spec,29)
   endif
   if (vary_in_x==1) then
      call derivative_x_pack( nx,ny,nz, temp(1,1,1),4,'temp-x',19)
      call derivative_x_pack( nx,ny,nz, u(1,1,1,1), 1,  'u-x1',1)
      call derivative_x_pack( nx,ny,nz, u(1,1,1,2), 2,  'u-x2',7)
      call derivative_x_pack( nx,ny,nz, u(1,1,1,3), 3,  'u-x3',13)
   endif
   if (vary_in_y==1) then
      call derivative_y_pack( nx,ny,nz, temp(1,1,1),4,'temp-y',21)
      call derivative_y_pack( nx,ny,nz, u(1,1,1,1), 1, 'u-y1',3)
      call derivative_y_pack( nx,ny,nz, u(1,1,1,2), 2, 'u-y2',9)
      call derivative_y_pack( nx,ny,nz, u(1,1,1,3), 3, 'u-y3',15)
   endif
   if (vary_in_z==1) then
      call derivative_z_pack( nx,ny,nz, temp(1,1,1),4,'temp-z',23)
      call derivative_z_pack( nx,ny,nz, u(1,1,1,1), 1, 'u-z1',5)
      call derivative_z_pack( nx,ny,nz, u(1,1,1,2), 2, 'u-z2',11)
      call derivative_z_pack( nx,ny,nz, u(1,1,1,3), 3, 'u-z3',17)
   endif
```

13. If bottleneck is kernel performance

- You absolutely have to vectorize on a good vector length; that is, greater than or equal to 32 (32 is a warp, 128 is 4 warps)
- You need to have thousands of the warps waiting to kick off to amortize latency to memory
- Watch out for register spills
- Watch out for overflowing shared memory
- Jeff – what the heck is occupancy?

A Simdized OpenACC loop

```
do i = 1, nx*ny*nz, ms
  ml = i
  mu =  min(i+ms-1, nx*ny*nz)
DIRECTION: do m=1,3
diffFlux(ml:mu,1,1,n_spec,m) = 0.0
grad_mixMW(ml:mu,1,1,m)=grad_mixMW(ml:mu,1,1,m)&
    *avmolwt(ml:mu,1,1)
SPECIES: do n=1,n_spec-1
   diffFlux(ml:mu,1,1,n,m)=-Ds_mixavg(ml:mu,1,1,n)&
     *(grad_Ys(ml:mu,1,1,n,m)+Ys(ml:mu,1,1,n)*&
       grad_mixMW(ml:mu,1,1,m) )
diffFlux(ml:mu,1,1,n_spec,m)=&
         diffFlux(ml:mu,1,1,n_spec,m)-&
         diffFlux(ml:mu,1,1,n,m)

enddo SPECIES
enddo DIRECTION
enddo
```

A Better Simdized OpenACC loop

```
do i = 1, nx*ny*nz, ms
  ml = i
  mu =  min(i+ms-1, nx*ny*nz)
   difftemp1 = 0.0
   difftemp2 = 0.0
   difftemp3 = 0.0
   grad_mixMW(i,1,1,1)= grad_mixMW(i,1,1,1)* avmolwt(i,1,1)
   grad_mixMW(i,1,1,2)= grad_mixMW(i,1,1,2)* avmolwt(i,1,1)
   grad_mixMW(i,1,1,3)= grad_mixMW(i,1,1,3)* avmolwt(i,1,1)
   do n=1,n_spec-1
     diffFlux(i,1,1,n,1)=- ds_mxvg(i,1,1,n)* ( grad_Ys(i,1,1,n,1) + yspecies(i,1,1,n)*grad_mixMW(i,1,1,1) )
     diffFlux(i,1,1,n,2) =-ds_mxvg(i,1,1,n)* ( grad_Ys(i,1,1,n,2) + yspecies(i,1,1,n)*grad_mixMW(i,1,1,2) )
     diffFlux(i,1,1,n,3) = - ds_mxvg(i,1,1,n)*( grad_Ys(i,1,1,n,3) +yspecies(i,1,1,n)*grad_mixMW(i,1,1,3) )
     difftemp1 = difftemp1-diffFlux(i,1,1,n,1)
     difftemp2 = difftemp2-diffFlux(i,1,1,n,2)
     difftemp3 = difftemp3-diffFlux(i,1,1,n,3)
   enddo      ! n
   diffFlux(i,1,1,n_spec,1) =  difftemp1
   diffFlux(i,1,1,n_spec,2) =  difftemp2
   diffFlux(i,1,1,n_spec,3) =  difftemp3
   grad_T(i,1,1,1)=-lambda(i,1,1)* grad_T(i,1,1,1)
   grad_T(i,1,1,2)=-lambda(i,1,1)* grad_T(i,1,1,2)
   grad_T(i,1,1,3)=-lambda(i,1,1)* grad_T(i,1,1,3)
   do n=1,n_spec
     grad_T(i,1,1,1)=grad_T(i,1,1,1)+ h_spec(i,1,1,n)*diffFlux(i,1,1,n,1)
     grad_T(i,1,1,2)=grad_T(i,1,1,2)+ h_spec(i,1,1,n)*diffFlux(i,1,1,n,2)
     grad_T(i,1,1,3)=grad_T(i,1,1,3)+ h_spec(i,1,1,n)*diffFlux(i,1,1,n,3)
enddo          ! i                                ! k
```

Temperature Interpolation loop

```
tmp1(ml:mu) = e0(ml:mu) - 0.5*tmp1(ml:mu)
LOOPM: DO m = ml, mu
   icount = 1
   r_gas = Ru*avmolwt(m)
   yspec(:) = ys(m, :)
   ITERATION: DO
    cpmix(m) = mixCp( yspec, temp(m) )
    enthmix  = mixEnth( yspec, temp(m) )
    deltat =   &
       ( tmp1(m) - (enthmix- &
         r_gas*temp(m)) )  &
          / ( cpmix(m) - r_gas )
    temp(m) = temp(m) + deltat
      IF( ABS(deltat) < atol ) THEN
         cpmix(m) = mixCp( yspec, &
     temp(m) )
      EXIT ITERATION
   ELSEIF( icount > icountmax ) THEN
     STOP
   ELSE
     icount = icount + 1
   ENDIF
  ENDDO ITERATION
ENDDO LOOPM
```

Temperature Interpolation loop

```
 ITERATION: do
do m = ml, mu
      !-- compute mixture heat capacity and enthalpy for this temperature
      n = max(1,min(2001,int((temp(m)-temp_lobound)*invEnthInc)+1))
      cpmix(m) = 0.0
      do mm=1,n_spec
        cpmix(m) = cpmix(m) +  &
            yspecies(m,mm)*(cpCoef_aa(mm,n) * temp(m) + cpCoef_bb(mm,n) )
      enddo
      enthmix(m) = 0.0
      do mm=1,n_spec
        enthmix(m) = enthmix(m) + yspecies(m,mm)*(enthCoef_aa(mm,n)*temp(m) + enthCoef_bb(mm,n))
      enddo

      !-- calculate deltat, new temp
      !   remember tmp1 holds the internal energy
      deltat(m) = ( tmp1(m) - (enthmix(m)-Ru*avmolwt(m)*temp(m)) )  &
                /( cpmix(m) - Ru*avmolwt(m) )
      if(iconverge(m).eq.0)temp(m) = temp(m) + deltat(m)
    enddo
    do m = ml, mu
      !-- check for convergence
!     if( abs(deltat(m)) < atol.and.iconverge(m).eq.0 ) then  ! converged
!          BUG- FIX AUG-16-04 - cpmix was not updated after successful convergence
        iconverge(m) = 1
        n = max(1,min(2001,int((temp(m)-temp_lobound)*invEnthInc)+1))
        cpmix(m) = 0.0
        do mm=1,n_spec
          cpmix(m) = cpmix(m) +  &
              yspecies(m,mm)*(cpCoef_aa(mm,n) * temp(m) + cpCoef_bb(mm,n) )
        enddo
!     endif
    enddo
```

Temperature Interpolation loop

```
if(all(iconverge(ml:mu).eq.1))EXIT ITERATION
        EXIT ITERATION
        do m = ml,mu
        if(iconverge(m).eq.0)then
         if( icount(m) > icountmax ) then  ! maximum count violation
           write(6,*)'calc_temp cannot converge after 100 iterations'
           write(6,*) 'for processor with rank =',myid
           write(6,*) 'm=',m
           stop  !ugly termination but that's the way it is without doing a broadcast
         else
           icount(m) = icount(m) + 1
         endif
        endif
        enddo
    enddo ITERATION
 end do
```

14. Consider introducing CUDA streams

```
if (vary_in_x==1) then
      call derivative_x_pack_np( nx,ny,nz, yspecies(1,1,1,1), 5, 'yspecies-x',n_spec,25)
   endif
   if (vary_in_y==1) then
      call derivative_y_pack_np( nx,ny,nz, yspecies(1,1,1,1),5, 'yspecies-y',n_spec,27)
   endif
   if (vary_in_z==1) then
      call derivative_z_pack_np( nx,ny,nz, yspecies(1,1,1,1),5, 'yspecies-z',n_spec,29)
   endif
   if (vary_in_x==1) then
      call derivative_x_pack( nx,ny,nz, temp(1,1,1),4,'temp-x',19)
      call derivative_x_pack( nx,ny,nz, u(1,1,1,1), 1,  'u-x1',1)
      call derivative_x_pack( nx,ny,nz, u(1,1,1,2), 2,  'u-x2',7)
      call derivative_x_pack( nx,ny,nz, u(1,1,1,3), 3,  'u-x3',13)
   endif
   if (vary_in_y==1) then
      call derivative_y_pack( nx,ny,nz, temp(1,1,1),4,'temp-y',21)
      call derivative_y_pack( nx,ny,nz, u(1,1,1,1), 1, 'u-y1',3)
      call derivative_y_pack( nx,ny,nz, u(1,1,1,2), 2, 'u-y2',9)
      call derivative_y_pack( nx,ny,nz, u(1,1,1,3), 3, 'u-y3',15)
   endif
   if (vary_in_z==1) then
      call derivative_z_pack( nx,ny,nz, temp(1,1,1),4,'temp-z',23)
      call derivative_z_pack( nx,ny,nz, u(1,1,1,1), 1, 'u-z1',5)
      call derivative_z_pack( nx,ny,nz, u(1,1,1,2), 2, 'u-z2',11)
      call derivative_z_pack( nx,ny,nz, u(1,1,1,3), 3, 'u-z3',17)
   endif
```

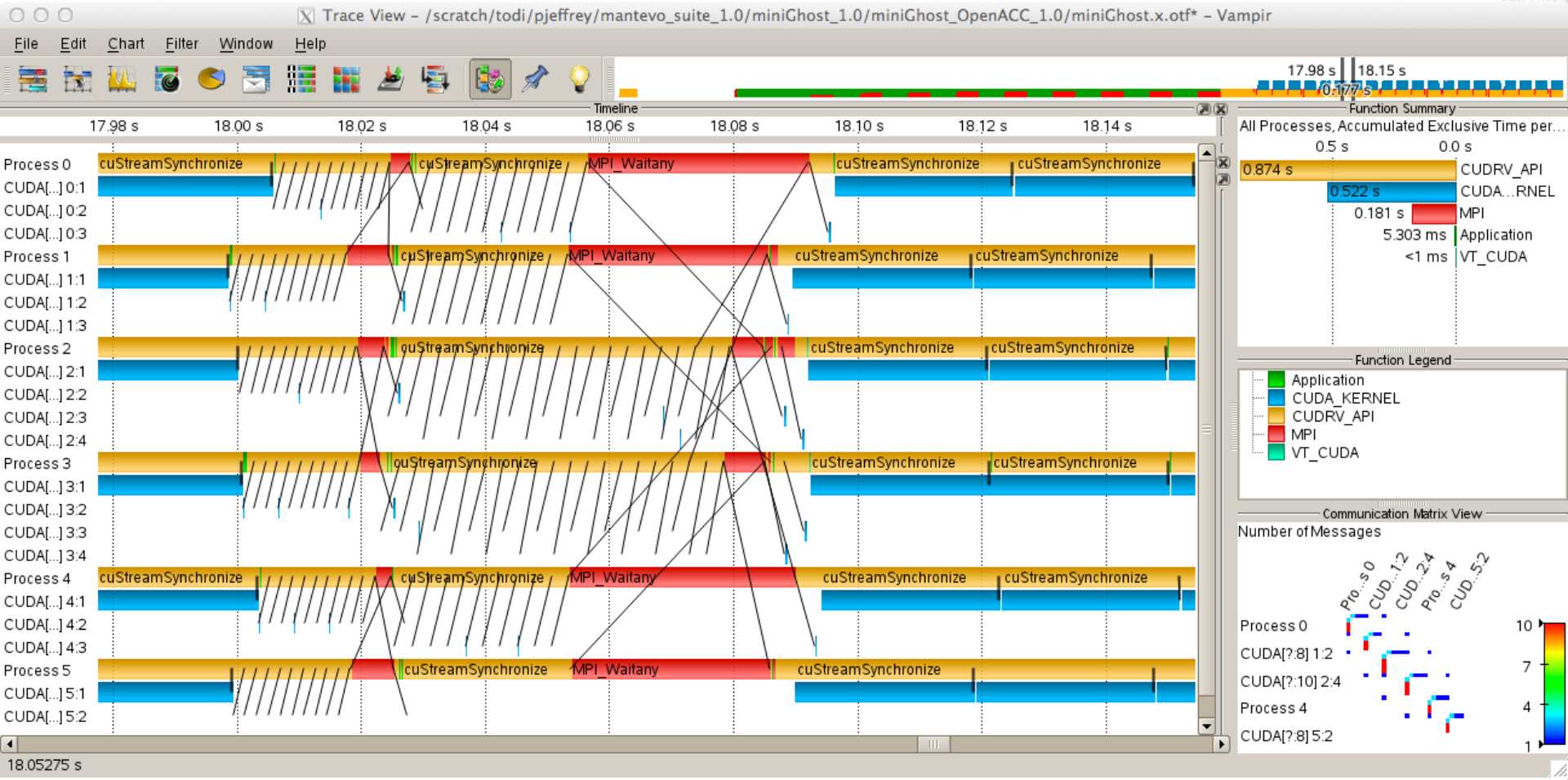
14. Continued

```
! Start communication - the _prep routines do posts and sends using buffer
! identified by itmp
call computeScalarGradient_prep_np(yspecies(1,1,1,1), 5,25,n_spec)
itmp = 4
istr = 19
call computeScalarGradient_prep( temp, itmp, istr )
itmp = 1
istr = 1
call computeVectorGradient_prep( u, itmp,istr )     endif
```

14. Continued

```
   do i = 1, reqcount
        call MPI_WAITANY(reqcount,req,index, stat, ierr )
if(direction(index).eq.1)then
!$acc update device(pos_f_x_buf(:,:,:,idx(index):idx(index)+nb(index)-1)) async(isync)
endif
if(direction(index).eq.2)then
!$acc update device(neg_f_x_buf(:,:,:,idx(index):idx(index)+nb(index)-1)) async(isync)
endif
if(direction(index).eq.3)then
!$acc update device(pos_f_y_buf(:,:,:,idx(index):idx(index)+nb(index)-1)) async(isync)
endif
if(direction(index).eq.4)then
!$acc update device(neg_f_y_buf(:,:,:,idx(index):idx(index)+nb(index)-1)) async(isync)
endif
if(direction(index).eq.5)then
!$acc update device(pos_f_z_buf(:,:,:,idx(index):idx(index)+nb(index)-1)) async(isync)
endif
if(direction(index).eq.6)then
!$acc update device(neg_f_z_buf(:,:,:,idx(index):idx(index)+nb(index)-1)) async(isync)
endif
isync=isync+1
    enddo
```

15. Start looking at timelines showing communication, host execution and accelerator



Strategy for refactoring the application

1. **First and foremost – Profile the application**
   Must identify looping structure within the time step loop
   Use –h profile_generate on compile and –Ocalltree or –Ocallers
2. **Use Reveal to identify scoping of variables in the major loop – may call subroutines and functions**
   The idea is to first generate OpenMP version of the loop and then add some OpenACC
3. **Use OpenACC to identify data motion require to run with companion accelerator**
   Once scoping is obtained, the OpenACC compiler will indicate what data would need to be moved to run on the accelerator – user must have the variable scoping correct
4. **Once one loop is analyze, now look at next highest compute loop, perform steps 2 and 3.**
5. **Soon multiple loops can be combined within a OpenACC data region for elminating transfers to and from the host.**

Strategy for refactoring the application

6. **Work outward until a data region encompasses a communication, I/O or looping structure more suited for the host**
   a. Must use updates to move data to and from the host to supply host with up-to-date data
7. **Move data region outside time step loop**
   a. Now must account for all updates to keep host and accelerator with consistent data
8. **Test versions after each step – don't worry about performance yet – just accuracy**
9. **The compiler may introduce data transfer so look at –rm listing for each individual OpenACC loop.**
10. **Optimize/Minimize data transfers first by using present on data clause.**

Strategy for refactoring the application

11. **Gather perftools statistics on code and identify bottlenecks**
12. **If bottleneck is data copies look at step 9**
13. **If bottleneck is kernel performance**
    A. Look at –rm and see what the compiler did to optimize the loop
    B. Ideally we want three levels of parallelism, gang, worker, vector
    C. Inner loop needs to be g on listing
    D. If inner loop is indicated by a loop level, that means that it is running in scalar – BAD
14. **Consider introducing CUDA streams**
    A. Either by taking an outer loop that cannot be parallelized due to communication and running that in a streaming mode
    B. Taking several independent operations and running that in a stream mode
15. **Start looking at timelines showing communication, host execution and accelerator**
    A. What can be overlapped