Using Kokkos for Performant Cross-Platform Acceleration of Liquid Rocket Simulations

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Viewgraph/Briefing Charts

Venke Sankaran

N/A
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Dr. Michael Carilli
Contractor, ERC Incorporated
RQRC
AFRL-West

May 8, 2017
SPACE-LRC: Scalable Physics-based Advanced Computational Engineering Platform for Liquid Rocket Combustion Simulation

SPACE simulation of rotating detonation engine
(courtesy of Dr. Christopher Lietz)
Components of SPACE-LRC

- **GEMS (Purdue University):** Unstructured near-body solver
- **CASTLES (AFRL-West):** High-order Cartesian off-body solver
  - Kokkos is integrated into CASTLES
- **PUNDIT (CREATE-AV):** Mesh communication between GEMS and CASTLES
- **SAMRAI (LLNL):** Adaptive meshing for off-body
Structure of CASTLES

Control API

Timestepping
Time derivatives for physical quantities

System
Specifies system of equations

Geometry
Handles spatial discretization

Equations
Physics-independent quantities

Physics
Turbulence models
Detailed chemical kinetics

Chung Viscosity Model (ported to Kokkos)
Peng-Robinson Equation of State (ported to Kokkos)
What is Kokkos?

“Performant cross platform parallelism”: write once, compile for anything.

Parallel patterns (for, reduce, scan) accept user-defined functors (like Thrust or Intel TBB)

Backends for Nvidia GPU, Intel Xeon, Xeon Phi, IBM Power8, others.

“View” data structure provides optimal layout: cache-order access when compiled for CPU, coalesced access when compiled for GPU.

Thrust offers similar multi-platform backends – but less low level control and does not abstract data layout.

Programming Guide:

At GTC 2017:
S7344 - Kokkos : The C++ Performance Portability Programming Model
S7253 - Kokkos Hierarchical Task-Data Parallelism for C++ HPC Applications
Enabling Kokkos in CASTLES

CASTLES is a Cartesian solver written in Fortran 90.

- Identify performance limiting subroutines
- Port Fortran subroutines to Kokkos C++
- Optimize ported routines
- Minimally invasive integration of Kokkos C++ with CASTLES ("code surgery")
Identify critical subroutines – CPU profile

Quick and easy single-process profile with nvprof:

nvprof --cpu-profiling on
--cpu-profiling-mode top-down ./CASTLES.x

I like the top-down view...
easy to see global structure and call chains.

Can also do bottom up profile (default)
Identify critical subroutines – CPU profile

Quick and easy single-process profile with nvprof:

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I like the top-down view...
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Can also do bottom up profile (default)

Looks like those “preos” and “chung” routines are burning a lot of CPU time

====== CPU profiling result (top down):
51.29% clone
| 51.29% start_thread
| 51.29% orte_progress_thread_engine
| | 51.29% opal_libevent2021_event_base_loop
| | 51.29% poll_dispatch
| | 51.29% poll
48.54% MAIN_
| 48.45% interfacetime_mp_maintimeexplicit_
| | 48.45% interfacetime_mp_rhstimesp34_
| | | 29.7% interfacegeom_mp_rhsgemomsescalcal_
| | | | 15.46% interfacegeom_mp_rhsgemom3redsadllr_
| | | | | 15.35% interfaceyexternal_mp_rhssyssupdisss_
| | | | | | 9.85% eosmodule_mp_eoscalcrhoh0fromrp_
| | | | | | | 9.64% eosmodule_mp_eosrhohfromrpfrompprop_
| | | | | | | | 9.64% preosmodule_mp_preosrhohfromrpfrompprop_
| | | | | | | | 5.1% eosmodule_mp_eosgammajacobianproperties_
| | | | | | | | | 5.1% preosmodule_mp_preosgammajacobianproperties_
| | | | 13.9% interfacegeom_mp_bcgeomrescalc_
| | | | | 14.7% interfacegeom_mp_bcgeoms菅isubin_
| | | | | | 14.7% interfaceeqnfluids_mp_bcfluidseqnsubin_velocity_
| | | | | | | 14.7% preosmodule_mp_preoscalctfromhp_
| | | | | | | | 3.5% interfaceyexternal_mp_stepsys3dcalcqadd_
| | | | | | | | | 3.5% eosmodule_mp_eosthermalproperties_
| | | | | | | | | | 3.5% preosmodule_mp_preosthermalproperties_
Peng-Robinson equation of state and Chung transport model

**Peng-Robinson Equation of State:**
Computes physical properties (density, enthalpy, etc.) for real gas mixtures at high pressure

**Chung Transport Model:**
Computes transport properties (viscosity, thermal conductivity, mass diffusivity) for real gas mixtures at high pressure

Many underlying subroutines shared between Chung and P-R.

Properties are computed individually per cell (or interpolated points at cell interfaces), so trivially parallel

Relatively small data transfer, lengthy computation => perfect for GPU offload

Input/output data scales linearly with number of species (NS)

Subroutines contain single loops, double loops, triple loops over NS => runtime scales like a*NS + b*NS² + c*NS³

Occupies significant majority of CASTLES runtime for ns >= 4ish

---

Cubic polynomial fits P-R scaling with number of chemical species

\[
y = 2\times 10^{-10}x^3 + 3\times 10^{-9}x^2 + 2\times 10^{-8}x + 6\times 10^{-9}
\]

\[
R^2 = 0.9999
\]

<table>
<thead>
<tr>
<th>Number of species (NS)</th>
<th>Seconds per grid point</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>0.00E+00</td>
</tr>
<tr>
<td>8</td>
<td>5.00E-06</td>
</tr>
<tr>
<td>11</td>
<td>1.00E-05</td>
</tr>
<tr>
<td>14</td>
<td>1.50E-05</td>
</tr>
<tr>
<td>17</td>
<td>2.00E-05</td>
</tr>
<tr>
<td>20</td>
<td>2.50E-05</td>
</tr>
<tr>
<td>23</td>
<td>5.00E-03</td>
</tr>
<tr>
<td>26</td>
<td>1.00E-02</td>
</tr>
<tr>
<td>29</td>
<td>2.00E-02</td>
</tr>
<tr>
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</tr>
<tr>
<td>35</td>
<td>5.00E-02</td>
</tr>
<tr>
<td>38</td>
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<tr>
<td>41</td>
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</tr>
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<tr>
<td>47</td>
<td>5.00E-01</td>
</tr>
<tr>
<td>50</td>
<td>1.00E+00</td>
</tr>
</tbody>
</table>

---

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Architecture of my Kokkos framework

Designed for minimally-invasive operation alongside large Fortran code.

| Frame |
|---|---|
| // Owns and allocates TVProperties object |
| TVProperties* tvproperties; |
| // Controls Kokkos initialization/finalization |
| void initialize(...); |
| void finalize(...); |
| TVProperties* gettvproperties(); |

Everything is controlled from Fortran through a single lightweight global Frame object.

Kernel launches and data comms are referred to TVProperties* owned by Frame.
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<table>
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// Controls Kokkos initialization/finalization  
void initialize(...);  
void finalize(...);  
TVProperties* gettvproperties();  

| Architectures of my Kokkos framework  
TVProperties  
// Owns and allocates TVImpl object  
TVImpl* impl;  

// Public member functions to communicate data  
// to/from Views in TVImpl  
void populateInputStripe(...);  
void populateOutputStripe(...);  
void populateprEOSSharedData(...);  
void populatechungSharedData(...);  
...  

// Public member functions to launch collections of  
// kernels  
void prEOSThermalProperties(...);  
void prEOSViscousProperties(...);  
void eosGammaJacobianProperties(...);  
... |

Everything is controlled from Fortran through a single lightweight global Frame object.

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</tr>
</thead>
<tbody>
<tr>
<td>// Owns and allocates TVProperties object</td>
<td>// Owns and allocates TVImpl object</td>
<td>// Contains members of TVProperties that don’t need</td>
</tr>
<tr>
<td>TVProperties* tvproperties;</td>
<td>TVImpl* impl;</td>
<td>// external visibility (pimpl idiom)</td>
</tr>
<tr>
<td>// Controls Kokkos initialization/finalization</td>
<td>// Public member functions to communicate data</td>
<td>// Owns and allocates Kokkos Views</td>
</tr>
</tbody>
</table>
| void initialize(...); | // to/from Views in TVImpl | View1DType T;
| void finalize(...); | void populateInputStripe(...); | View1DType P;
| TVProperties* gettvproperties(); | void populateOutputStripe(...); | View1DType Yi;
|                                | void populateprEOSSharedData(...); | ...(several dozen of these) |
|                                | void populatechungSharedData(...); | |
|                                | ... | // Owns std::unordered_maps to launch kernels |
|                                | // Public member functions to launch collections of | // and communicate data by name |
|                                | // kernels | unordered_map<string,View1DType> |
|                                | void prEOSThermalProperties(...); | select1DViewByName;
|                                | void prEOSViscousProperties(...); | unordered_map<string,View2DType> |
|                                | void eosGammaJacobianProperties(...); | select2DViewByName;
|                                | ... | // Owns Launcher for each kernel |
|                                |                                | (lightweight wrapper with string identifier, |
|                                |                                | // inherits common timing routines from |
|                                |                                | // LauncherBase) |
|                                |                                | unordered_map<string,LauncherBase*> launchers; |
|                                |                                | void safeLaunch(...); |
For modularity and consistency: one subroutine->one kernel

Fortran subroutine

```fortran
pure subroutine prEOSCalcSoundSpeed(&
   rho, rhop, rhoT, hp, hT, c)
use useGENKindDefs, only: dp
implicit none
real(dp), intent(in) :: rho, rhop, rhoT, hp, hT
real(dp), intent(out) :: c

  c = sqrt( rho*ht/
    ( rho*rhop*ht + rhoT*( 1.0_dp-rho*hp ) ) )

end subroutine prEOSCalcSoundSpeed
```

Kokkos kernel launch

```fortran
parallel_for( tvimpl->nActivePoints,
   KOKKOS_LAMBDA(const int& t)
   {
   c(t) = sqrt( rho(t)*hT(t)/
     ( rho(t)*rhop(t)*hT(t)
     + rhoT(t) *( 1.0_dp-rho(t)*hp(t) ) ) )
   });
```

Operates on nActivePoints grid points in parallel

- `c, rho, hT, etc. are Kokkos Views, captured by value from members of TVImpl`
- `(View copy constructor is a lightweight shallow copy)`
- `t is the parallel work index`

There are roughly 50 of these that serve as building blocks.
Good speedups overall.

GPU speedup is better for fewer species (NS)
- smaller per-thread data set => improved cache hit rates on GPU
- Smaller inner loops => vectorization less efficient on CPU

(a combination of GPU doing better and CPU doing a bit worse)
Integrating Kokkos with CASTLES: Interface Functions

C++ Interface functions (callable from Fortran) tell Frame object to initialize/finalize Kokkos, launch collections of kernels, or communicate data.

Decorated with ‘extern “C”’ to disallow name mangling, added trailing underscore_ expected by Fortran linker.

Interface function to initialize Kokkos and allocate internal storage

```c++
extern “C” void frame_initialize_( int device_id,
    int nGridPoints
    int ns
    int nq
    int iTurb )
{
    frame.initialize( device_id, // GPU device to select
        nGridPoints, // Chunk size for Kokkos launches
        ns, // Num chemical species
        nq, // Utility values
        iTurb );
}
```

Corresponding Fortran call

```fortran
! Compute KokkosDeviceID as MPI rank%num devices
! Num devices is supplied by input file
call frame_initialize( %VAL(KokkosDeviceID),&
    %VAL(KokkosMaxBlock),&
    %VAL(nspe),&
    %VAL(nq),&
    %VAL(iTurbType) )
```

Interface function to launch collection of kernels for thermal and viscous properties

```c++
extern “C” void
frame_tvproperties_eosthermalandviscousproperties_(
    int nActivePoints )
{
    frame.gettvproperties()->eosThermalAndViscousProperties(
        nActivePoints );
}
```

Corresponding Fortran call

```fortran
call
frame_tvproperties_eosthermalandviscousproperties&
( %VAL(NumThisStripe) )
```
Communicating Data

Data communication must translate between 4D Fortran pointers (x,y,z,dataindx) and Kokkos Views. For some computations, a halo of fringe points must be ignored.

C++ interface function

```cpp
extern "C" void frame_castles_populateinputstripe_(
  const char name[8], // Name tag of destination View
double* data, // Source pointer (from Fortran)
int nx, int ny, int nz, // Dims of block (including fringes)
int SptX, int EptX, // Fringe boundaries in x-direction
int SptY, int EptY, // " y-direction
int SptZ, int EptZ, // " z-direction
int SptData, // Start of data region (slowest index)
int EptData, // End of data region
int stripeStart, // Start and end of selected x,y,z
int stripeEnd) // stripe; used when looping over block
// in chunks (stripes) of fixed size
{
  frame.gettvproperties()->populateInputStripe(name,
      data, nx, ny, nz, SptX, EptX, SptY, EptY,
      SptZ, EptZ, SptData, EptData, stripeStart, stripeEnd);
}
```

Corresponding Fortran call

```fortran
! Name tag of destination View
tag = "Q"//char(0)
call frame_castles_populateinputstripe(tag,&
  Q,& ! 4D Fortran pointer, source of copy
  %VAL(NumX), %VAL(NumY), %VAL(NumZ),&
  %VAL(SptX), %VAL(EptX),&
  %VAL(SptY), %VAL(EptY),&
  %VAL(SptZ), %VAL(EptZ),&
  %VAL(SptData), %VAL(EptData),&
  %VAL(SptStripe), %VAL(EptStripe) )
```

Fortran <-> C++ communication works as follows:

1. C++ framework receives double* from Fortran
2. Iterates linearly through x,y,z values, copying data to Views and skipping fringe points.
3. In Views, x,y,z indices are flattened into a single parallel-work index, t.
4. After computation, reverse the process, copying data from Views back into double* storage with data layout expected by Fortran.

C++ framework must know xdim, ydim, zdim, and fringe boundaries to unpack and repack data. Annoying indexing math...
Data marshalling challenges

Challenge #1:
Kokkos launches need enough parallel work (enough grid points) to saturate GPU.

Solution:
Ensure availability of this process’ entire block of data where Kokkos interface functions are called. Restructuring some Fortran calling functions was required, but minimal impact to code overall.

Challenge #2:
Block size handled by each process may change between timesteps, due to adaptive mesh refinement. Prefer not to reallocate Kokkos data structures, or worse, exhaust GPU memory.

Solution:
Launch Kokkos computations via a loop over this process’ block in chunks of largeish but fixed size “KokkosMaxBlock.”

KokkosMaxBlock is a tuning parameter in input file, large enough that one chunk’s launch should saturate GPU when 10-20 processes are sharing the GPU via Nvidia Multi-Process Service.

KokkosMaxBlock = 8192 or 12288 usually gives good performance.
Cluster-level concerns: Multiple GPUs per node

Kokkos can handle multiple GPUs.

Standalone Kokkos application:

Pass
  --kokkos-ndevices=2
on the command line and call
Kokkos::initialize(int& argc, char* argv[])
within code.

Kokkos will detect available GPUs and assign MPI ranks to GPUs round robin.

Minor Caveat:
If MPI process is bound to a specific set of cores, Kokkos does not try to select the optimally hardware co-located GPU (this may have changed since last I checked).

My application (embedded deep within a big Fortran code):

Pass number of available GPU devices in input file.

Manually compute which device to use as (MPI rank%num devices).

Tell this process’ Kokkos kernels to use that device as follows:
Kokkos::InitArguments args;
args.device_id = device_id;
Kokkos::initialize( args );
Cluster-level concerns: Nvidia Multi-Process Service (MPS)

Without MPS:
Each MPI process has its own CUDA context.
Multi-process profile shows one process at a time using a given GPU.

With MPS:
Multiple processes can share a given GPU simultaneously.

Kernels from different processes do not overlap
Kernels from different processes overlap

For small NS, turning on MPS makes overall application up to 3X faster

Better utilization and dramatic speedup for my application, and easy to use
(just run `nvidia-cuda-mps-control -d` on each compute node to start the daemons).

GPU Speedup of Overall CASTLES+Kokkos

Production-style runs: 40 MPI ranks on 2 nodes.

- CASTLES Fortran uses 20 CPUs/node only.
- CASTLES+Kokkos uses 20 CPUs + 2 GPUs/node.
- Speedup computed as (CASTLES Fortran runtime)/(Castles+Kokkos runtime)

2.5-3.0X consistently observed across range of desirable problem parameters.
Kokkos on CPU matches Fortran on CPU

Can the Kokkos-enabled codebase compile for CPU as well as GPU, with good performance?

Often, naively porting Fortran to C++ can result in a slowdown (e.g. compiler has a harder time optimizing/vectorizing loops). Need to use hardware-specific (Intel) compiler and manually tweak vector pragmas for some in-kernel loops, but in the end **Kokkos C++ is as fast as original Fortran.**

![Table showing performance comparison between Castles+Fortran and Castles+Kokkos OpenMP](image)

**Test case: NS=5, 16^3 grid points, 50 timesteps**

<table>
<thead>
<tr>
<th></th>
<th>30.2 s</th>
<th>28.5 s</th>
</tr>
</thead>
<tbody>
<tr>
<td>CASTLES+Fortran (1 CPU)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CASTLES+Kokkos OpenMP (1 thread)**</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**KMP_AFFINITY=compact,1,granularity=core**

To compile for CPU, just change arguments to makefile.

nvcc ignores Intel pragmas. Kokkos-enabled source code is (almost entirely) same as used for GPU.

Only two kernels needed moderately divergent code for good performance on both CPU and GPU. Kokkos build system provides pragmas to select different code when compiling for different hardware:

```
KOKKOS_LAMBDA( const int& t )
{
    #ifdef KOKKOS_HAVE_CUDA
        ...GPU-optimal code goes here...
    #else
        ...CPU-optimal code goes here...
    #endif
}
```

**Kokkos promise of “performant cross-platform parallelism” more or less fulfilled.**
Node level performance + comparison with Xeon Phi

Kokkos runs on Xeon Phis in **native mode**:
- MPI+Kokkos processes see Phi cores as additional CPU cores.
- Kokkos computations are not offloaded GPU-style.
- Entire process runs on a set of Phi cores just like on a multicore CPU.

GPUs are offload coprocessors, so can’t compare Phi vs. GPU apples-to-apples. But we can get an idea at node level.

### Runtime for fixed problem size $120^3$, $NS=5$, 1st order, 20 timesteps

<table>
<thead>
<tr>
<th>Configuration</th>
<th>Runtime (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CASTLES Fortran: 20 CPU cores</td>
<td>200</td>
</tr>
<tr>
<td>CASTLES+Kokkos: 20 CPU cores + 2 GPUs</td>
<td>67</td>
</tr>
<tr>
<td>CASTLES+Kokkos: Xeon Phi Knight's Corner</td>
<td>726</td>
</tr>
<tr>
<td>CASTLES+Kokkos: Xeon Phi Knight's Landing</td>
<td>151</td>
</tr>
</tbody>
</table>
System details

2x10 core Intel Xeon E5-2650 v3
Config file for Intel MPI:
-genv I_MPI_PIN_DOMAIN=auto:compact
-n 20 ./CASTLES.kokkos
Although cores are hyperthreaded (40 logical cores available),
adding more processes does not improve performance noticeably.

2x10 core Intel Xeon E5-2650 v3
+ 2 Kepler K40 GPUs.
Same MPI config as CASTLES Fortran.

One Knight's Corner 5110P
(60 cores, 240 logical processors).
Config file for Intel MPI:
-genv I_MPI_PIN_DOMAIN=4:compact -genv OMP_NUM_THREADS 4
-host mic0 -n 60 -env KMP_AFFINITY=compact,granularity=core ./CASTLES.knc

One Knight's Landing 7230 (64 cores, 256 logical processors), using SNC4 clustering
Config file for Intel MPI:
-genv I_MPI_PIN_DOMAIN=1:compact -genv OMP_NUM_THREADS 1
-n 256 -env KMP_AFFINITY=compact,granularity=core numactl -m 4,5,6,7 ./CASTLES.knl
Numactl -m 4,5,6,7 encourages first-touch allocation in onboard high-bandwidth memory.
I experimented with fewer MPI processes, bigger domains, and more OpenMP threads,
and found 256 procs with 1 thread/proc best.
Bandwidth Optimizations for Per-Grid-Point Inner Loops

P-R and Chung involve nested inner loops over chemical species NS (can be 50 or more).

Independent calculations for each grid point.

Toy example (shown as CPU-style serial loop over grid points):

```c
// Loop over N grid points (trivially parallel)
for( int t = 0; t < N; t++ )
  // ax[], ay[], bx[], and by[]:
  // arrays of size NS*N that store per-grid-point input data.
  for( int y = 0; y < NS; y++ ) // NS ~ up to 50ish
    for( int x = 0; x < NS; x++ )
      output[N*(NS*y+x)+t] = ax[x*N+t]*ay[y*N+t] + bx[x*N+t]*by[y*N+t];
```

“Embarrassingly parallel,” and inner loops are simple... but achieving high performance is an interesting problem!
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```

“Embarrassingly parallel,” and inner loops are simple... but achieving high performance is an interesting problem!
Testing Parameters

Tesla K40 GPU
- 12 GB device memory
- 15 Kepler SMs

Kepler architecture:
- 192 single-precision cores and 64 double-precision cores per SM
- 100% occupancy = 2048 active threads per SM
- 65,536 registers available per SM
- 64KB L1 cache/shared memory per SM, configurable as either 48 KB L1 + 16 KB shared, 32 KB L1 + 32 KB shared, or 16 KB L1 + 32 KB shared
- 48 KB read-only cache (declare pointers with const __restrict__ to use this**)

Compiled with nvcc version 7.5, opt-in L1 caching, verbose to see register/local mem use, targeting compute capability 3.5
nvcc -Xptxas="-dlcm=ca" -Xptxas="-v" -arch=sm_35 kernels.cu

Runtime call to cudaDeviceSetCacheConfig(cudaFuncCachePreferL1) to set the 48 KB L1 + 16 KB shared option in case the compiler chooses to load via L1

For timing purposes, I use N=2048*120, NS=64, 960 blocks, 256 threads/block. On a K40 with 15 SMs, this is 8 full waves.

Kernel wall times averaged over 10 trials.

**In subsequent examples, I do not write “const.” Although the Kepler Tuning Guide is pretty adamant that writing “const” is necessary to trigger loads via the 48 KB read-only cache, I found that for toy kernels presented here, the compiler uses read-only cache even if “const” is omitted.
Naïve Cuda Kernel – one thread per grid point

```c
__global__ void naive( double* __restrict__ ax, double* __restrict__ bx,
                        double* __restrict__ ay, double* __restrict__ by, double* __restrict__ output )
{
    // Ordinarily we might wrap this in a grid stride loop...omitted to save space.
    int t = threadIdx.x + blockIdx.x*blockDim.x;
    #pragma unroll 1 // Disallow compiler unrolling so we know what’s happening.
    for( int y = 0; y < NS; y++ )
        #pragma unroll 1
        for( int x = 0; x < NS; x++ )
            output[N*(NS*y+x)+t] = ax[x*N+t]*ay[y*N+t] + bx[x*N+t]*by[y*N+t];
}
```

**If we omit the “#pragma unroll 1”s and let the compiler unroll as it wishes, register use goes up (as expected), occupancy falls, and the “naïve” kernel’s performance worsens. 100% occupancy is not always essential, but in this case, explicitly including the pragmas is better than relying on compiler heuristics.
Naïve Cuda Kernel – one thread per grid point

```c
__global__ void naive( double* __restrict__ ax, double* __restrict__ bx,
                      double* __restrict__ ay, double* __restrict__ by, double* __restrict__ output )
{
    // Ordinarily we might wrap this in a grid stride loop...omitted to save space.
    int t = threadIdx.x + blockIdx.x*blockDim.x;
    #pragma unroll 1 // Disallow compiler unrolling so we know what’s happening.
    for( int y = 0; y < NS; y++ )
        # pragma unroll 1
            for( int x = 0; x < NS; x++ )
                output[N*(NS*y+x)+t] = ax[x*N+t]*ay[y*N+t] + bx[x*N+t]*by[y*N+t];
}
```

Grid point index “t” is the fast index for coalescing
(corresponds to Kokkos::LayoutLeft)
__global__ void naive( double* __restrict__ ax, double* __restrict__ bx,
            double* __restrict__ ay, double* __restrict__ by, double* __restrict__ output )
{
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        for( int x = 0; x < NS; x++ )
            output[N*(NS*y+x)+t] = ax[x*N+t]*ay[y*N+t] + bx[x*N+t]*by[y*N+t];
}

Grid point index “t” is the fast index for coalescing
(corresponds to Kokkos::LayoutLeft)

y-dependent loads should hit in cache (or be promoted to registers) during loop over x.
I find that manually hoisting y-loads to a register does not affect performance.
__global__ void naive( double* __restrict__ ax, double* __restrict__ bx,
                     double* __restrict__ ay, double* __restrict__ by, double* __restrict__ output )
{
    int t = threadIdx.x + blockIdx.x*blockDim.x;
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    for( int y = 0; y < NS; y++ )
        #pragma unroll 1
        for( int x = 0; x < NS; x++ )
            output[ N*(NS*y+x)+t ] = ax[ x*N+t ]*ay[ y*N+t ] + bx[ x*N+t ]*by[ y*N+t ];
}

Grid point index “t” is the fast index for coalescing (corresponds to Kokkos::LayoutLeft)

y-dependent loads should hit in cache (or be promoted to registers) during loop over x. I find that manually hoisting y-loads to a register does not affect performance.

Each x-load is used only once per outer y-loop iteration. Probably won’t hit in cache on the next outer y-loop iteration.
Kernel “naïve” is strongly bandwidth-bound, and accesses are already coalesced. What should we do?

```c
__global__ void naive( double* __restrict__ ax, double* __restrict__ bx,
                     double* __restrict__ ay, double* __restrict__ by, double* __restrict__ output )
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    for( int y = 0; y < NS; y++ )
        for( int x = 0; x < NS; x++ )
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Kernel “naïve” is strongly bandwidth-bound, and accesses are already coalesced. What should we do?
Standard CPU-informed strategy: tile the loop?

Recall why loop tiling helps on CPU:

```c
for( int yy = 0; yy < NS; yy += TILE_FACTOR )
    for( int x = 0; x < NS; x++ )
        for( int y = yy; y < yy + TILE_FACTOR; y++ )
            output[N*(NS*y+x)+t] = ax[x*N+t]*ay[y*N+t] + bx[x*N+t]*by[y*N+t];
```
Standard CPU-informed strategy: tile the loop?

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```

X-dependent loads should hit in cache for the inner y-loop, and be reused TILE_FACTOR times
Recall why loop tiling helps on CPU:

\[
\begin{align*}
\text{for( int } & \ y = 0; \ y < \text{NS}; \ y += \text{TILE}\_\text{FACTOR } ) \\
\text{for( int } & \ x = 0; \ x < \text{NS}; \ x++ \\
\text{for( int } & \ y = \text{yy}; \ y < \text{yy} + \text{TILE}\_\text{FACTOR}; \ y++ \\
\text{output[} & \text{N*(NS*y+x)+t] = ax[x*N+t]*ay[y*N+t] + bx[x*N+t]*by[y*N+t]} \\
\end{align*}
\]

X-dependent loads should hit in cache for the inner y-loop, and be reused TILE\_FACTOR times.

Each x-iteration now treats TILE\_FACTOR y-iterations instead of just one.

TILE\_FACTOR y-dependent loads should hit in cache on each iteration of the x-loop.

(in fact, for a typical CPU cache and modest values of NS like 64, the entire working set should easily fit in cache, and it’s not necessary to tile the loop at all.)

Pretty standard stuff...but do we expect this to work on a Kepler GPU?
Loop tiling on GPU

```c
__global__ void tiled(...same args as naïve...)
{
    int t = threadIdx.x + blockIdx.x*blockDim.x;
    for( int yy = 0; yy < NS; yy += TILE_FACTOR )
        for( int x = 0; x < NS; x++ )
            for( int y = yy; y < yy + TILE_FACTOR; y++ )
                output[N*(NS*y+x)+t] = ax[x*N+t]*ay[y*N+t] + bx[x*N+t]*by[y*N+t];
}
```
Loop tiling on GPU

Tiling is worse than naïve. Cache per grid point (thread) is just too small.

Read-only cache and L1 cache are only 48 KB each.
Whichever compiler chooses to use:

100% occupancy = 2048 threads
48 KB/2048 threads = only 3 doubles’ worth of cache per thread.
Loop tiling on GPU

Tiling is worse than naïve. Cache per grid point (thread) is just too small.

Read-only cache and L1 cache are only 48 KB each. Whichever compiler chooses to use:

100% occupancy = 2048 threads
48 KB/2048 threads = only 3 doubles’ worth of cache per thread.

nvprof confirms poor hit rates (results for TILE_FACTOR 2 shown):**

```
nvprof --kernels ::tiled:1 -metrics \
nc_cache_global_hit_rate,tex_cache_hit_rate ./a.out
```

<table>
<thead>
<tr>
<th>.135 s</th>
<th>.234 s</th>
<th>.230 s</th>
<th>.209 s</th>
</tr>
</thead>
<tbody>
<tr>
<td>Naïve</td>
<td>TILE_FACTOR 2</td>
<td>4</td>
<td>8</td>
</tr>
</tbody>
</table>

**As mentioned previously, the compiler appears to use read-only/texture cache for loads. I’m not sure why there are separate metrics to describe “read-only cache accesses” and “texture cache accesses” (it’s the same hardware). Perhaps some Cuda ninja can explain?
Tile with reduced occupancy

100% occupancy is not a strict requirement for peak performance. Lower occupancy = more cache per grid point.**

Manually suppress occupancy by giving each block “dummy” shared memory. For example: 16 KB shared memory is available on each SM. If we assign each block 4096 B smem, only 4 blocks can fit on each SM. 4*256 = 1024 threads. 1024/2048 = 50% occupancy.

```c
__global__ void tiled_reduced_occupancy(...) {
    extern __shared__ int smem[];
    int t = threadIdx.x + blockIdx.x*blockDim.x;
    for( int yy = 0; yy < NS; yy += TILE_FACTOR )
        for( int x = 0; x < NS; x++ )
            for(int y = yy; y < yy + TILE_FACTOR; y++)
                output[N*(NS*y+x)+t] = ax[x*N+t]*ay[y*N+t]
                                  + bx[x*N+t]*by[y*N+t];
}
```

**See “GPU Memory Bootcamp II: Beyond Best Practices” from GTC 2015 (http://on-demand.gputechconf.com/gtc/2015/presentation/S5376-Tony-Scudiero.pdf) for a more detailed discussion of occupancy vs. hit rate.
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    for( int yy = 0; yy < NS; yy += TILE_FACTOR )
        for( int x = 0; x < NS; x++ )
            for( int y = yy; y < yy + TILE_FACTOR; y++ )
                output[N*(NS*y+x)+t] = ax[x*N+t]*ay[y*N+t]
                                + bx[x*N+t]*by[y*N+t];
}
```

---

**Runtime vs. Occupancy**

<table>
<thead>
<tr>
<th>Occupancy</th>
<th>Naïve</th>
<th>TILE_FACTOR 2</th>
<th>TILE_FACTOR 4</th>
<th>TILE_FACTOR 8</th>
</tr>
</thead>
<tbody>
<tr>
<td>50% (4 KB smem/block)</td>
<td>.135 s</td>
<td>.193 s</td>
<td>.228 s</td>
<td>.254 s</td>
</tr>
<tr>
<td>25% (8 KB smem/block)</td>
<td>.176 s</td>
<td>.248 s</td>
<td>.254 s</td>
<td>.254 s</td>
</tr>
<tr>
<td>12.5% (16 KB smem/block)</td>
<td>.242 s</td>
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Mostly worse than naïve.
Tile with reduced occupancy

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For example: 16 KB shared memory is available on each SM.
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Runway vs. Occupancy

<table>
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</table>

Mostly worse than naïve. **Sweet spot at TILE_FACTOR 4, 12.5% occupancy can be explained by cache hits:**

nvprof --kernels tiled_reduced_occupancy:4 --metrics achieved_occupancy nc_cache_global_hit_rate, tex_cache_hit_rate ./a.out

... Achieved Occupancy 0.124771 0.124771
... Non-Coherent Global Hit Rate 75.81% 75.81%
Tile using both L1 and read-only cache

On Kepler, 48 KB read-only cache and 64 KB L1+shared cache are independent. Use both!

Tile using thread-local arrays:
(placed in a local memory stack frame. Allocated in device global memory, but cached in L1)**

```c
__global__ void tiled_local_arrays(...)
{
    double ay_local[TILE_FACTOR]; // Thread-local arrays
    double by_local[TILE_FACTOR]; // (placed in local memory)
    int t = threadIdx.x + blockIdx.x*blockDim.x;
    for( int yy = 0; yy < NS; yy += TILE_FACTOR )
    {
        for( int y = yy; y < yy + TILE_FACTOR; y++ )
        {
            ay_local[y-yy] = ay[y*N+t];
            by_local[y-yy] = by[y*N+t];
        }
        for( int x = 0; x < NS; x++ )
        {
            for( int y = yy; y < yy + TILE_FACTOR; y++ )
            {
                output[N*(NS*y+x)+t] = ax[x*N+t]*ay_local[y-yy]
                + bx[x*N+t]*by_local[y-yy];
            }
        }
    }
}
```

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```c
__global__ void tiled_local_arrays(...)
{
    double ay_local[TILE_FACTOR]; // Thread-local arrays
    double by_local[TILE_FACTOR]; // (placed in local memory)
    int t = threadIdx.x + blockIdx.x*blockDim.x;
    for( int yy = 0; yy < NS; yy += TILE_FACTOR )
    {
        for( int y = yy; y < yy + TILE_FACTOR; y++ )
        {
            ay_local[y-yy] = ay[y*N+t];
            by_local[y-yy] = by[y*N+t]; // Thread-local arrays for Y-dependent loads (cached in L1)
        }
        for( int x = 0; x < NS; x++ )
        {
            for( int y = yy; y < yy + TILE_FACTOR; y++ )
            {
                output[N*(NS*y+x)+t] = ax[x*N+t]*ay_local[y-yy] + bx[x*N+t]*by_local[y-yy];
            }
        }
    }
}
```
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    for( int yy = 0; yy < NS; yy += TILE_FACTOR )
    {
        for( int y = yy; y < yy + TILE_FACTOR; y++ )
        {
            ay_local[y-yy] = ay[y*N+t]; // Thread-local arrays for Y-dependent loads (cached in L1)
            by_local[y-yy] = by[y*N+t];
        }
        for( int x = 0; x < NS; x++ )
        {
            for( int y = yy; y < yy + TILE_FACTOR; y++ )
            {
                output[N*(NS*y+x)+t] = ax[x*N+t]*ay_local[y-yy] + bx[x*N+t]*by_local[y-yy];
            }
        }
    }
}
```

X-dependent loads cached in read-only
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{
    double ay_local[TILE_FACTOR]; // Thread-local arrays
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    int t = threadIdx.x + blockIdx.x*blockDim.x;
    for( int yy = 0; yy < NS; yy += TILE_FACTOR )
    {
        for( int y = yy; y < yy + TILE_FACTOR; y++ )
        {
            ay_local[y-yy] = ay[y*N+t]; // Thread-local arrays for
            by_local[y-yy] = by[y*N+t]; // Y-dependent loads (cached in L1)
        }
        for( int x = 0; x < NS; x++ )
            for( int y = yy; y < yy + TILE_FACTOR; y++ )
                output[N*(NS*y+x)+t] = ax[x*N+t]*ay_local[y-yy] + bx[x*N+t]*by_local[y-yy];
    }
}
```

Fast for TILE_FACTOR = 2! L1 cache fields all y-dependent loads (100% hit rate)

Slower for TILE_FACTOR = 4 and 8. Hit rate decreases.
Tile with explicit register use ("unroll-and-jam")

Kepler SM has 65,536 4B registers = 262 KB of near-core memory available as registers.

>2.5X more than read-only and L1 caches combined.

```c
__global__ void unroll_and_jam_by2_registers(...) {
    // Encourage these to be placed in registers
    double ay_local0, by_local0, ay_local1, by_local1;
    int t = threadIdx.x + blockIdx.x*blockDim.x;
    #pragma unroll 1
    for( int yy = 0; yy < NS; yy += 2 )
    {
        ay_local0 = ay[(yy+0)*N+t];
        by_local0 = by[(yy+0)*N+t];
        ay_local1 = ay[(yy+1)*N+t];
        by_local1 = by[(yy+1)*N+t];
        #pragma unroll 1
        for( int x = 0; x < NS; x++ )
        {
            output[N*(NS*(yy+0)+x)+t] = ax[x*N+t]*ay_local0
                                        + bx[x*N+t]*by_local0;
            output[N*(NS*(yy+1)+x)+t] = ax[x*N+t]*ay_local1
                                        + bx[x*N+t]*by_local1;
        }
    }
}
```
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    int t = threadIdx.x + blockIdx.x*blockDim.x;
    #pragma unroll 1
    for( int yy = 0; yy < NS; yy += 2 )
    {
        ay_local0 = ay[(yy+0)*N+t];
        by_local0 = by[(yy+0)*N+t];
        ay_local1 = ay[(yy+1)*N+t];
        by_local1 = by[(yy+1)*N+t];
        # pragma unroll 1
        for( int x = 0; x < NS; x++ )
        {
            output[N*(NS*(yy+0)+x)+t] = ax[x*N+t]*ay_local0
                + bx[x*N+t]*by_local0;
            output[N*(NS*(yy+1)+x)+t] = ax[x*N+t]*ay_local1
                + bx[x*N+t]*by_local1;
        }
    }
}
```

Y-dependent loads reused x times in x-loop
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    int t = threadIdx.x + blockIdx.x*blockDim.x;
    #pragma unroll 1
    for( int yy = 0; yy < NS; yy += 2 )
    {
        ay_local0 = ay[(yy+0)*N+t];
        by_local0 = by[(yy+0)*N+t];
        ay_local1 = ay[(yy+1)*N+t];
        by_local1 = by[(yy+1)*N+t];
        # pragma unroll 1
        for( int x = 0; x < NS; x++ )
        {
            output[N*(NS*(yy+0)+x)+t] = ax[x*N+t]*ay_local0
            + bx[x*N+t]*by_local0;
            output[N*(NS*(yy+1)+x)+t] = ax[x*N+t]*ay_local1
            + bx[x*N+t]*by_local1;
        }
    }
}
```

Y-dependent loads reused
x times in x-loop

X-dependent loads used twice
Tile with explicit register use ("unroll-and-jam")

Kepler SM has 65,536 4B registers = 262 KB of near-core memory available as registers.

>2.5X more than read-only and L1 caches combined.

In practice I like this approach. At 50% occupancy you can use up to 64 registers (32 DP values) for tiling. Unrolling by 2 or 4 is not too annoying for a few performance-limiting kernels.

…but don’t do it for all your kernels.

"Premature optimization is the root of all evil"

__global__ void unroll_and_jam_by2_registers(...)
{
    // Encourage these to be placed in registers
    double ay_local0, by_local0, ay_local1, by_local1;
    int t = threadIdx.x + blockIdx.x*blockDim.x;
    #pragma unroll 1
    for( int yy = 0; yy < NS; yy += 2 )
    {   ay_local0 = ay[(yy+0)*N+t];
        by_local0 = by[(yy+0)*N+t];
        ay_local1 = ay[(yy+1)*N+t];
        by_local1 = by[(yy+1)*N+t];
        # pragma unroll 1
        for( int x = 0; x < NS; x++ )
        {
            output[N*(NS*(yy+0)+x)+t] = ax[x*N+t]*ay_local0 + bx[x*N+t]*by_local0;
            output[N*(NS*(yy+1)+x)+t] = ax[x*N+t]*ay_local1 + bx[x*N+t]*by_local1;
        }
    }
}

Unroll and Jam Runtimes

<table>
<thead>
<tr>
<th></th>
<th>Naïve</th>
<th>UJ by 2</th>
<th>UJ by 4</th>
<th>UJ by 8</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>.135s</td>
<td>.106s</td>
<td>.126s</td>
<td>.114s</td>
</tr>
</tbody>
</table>

Y-dependent loads reused \(x\) times in \(x\)-loop

X-dependent loads used twice

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At 50% occupancy you can use up to 64 registers (32 DP values) for tiling. Unrolling by 2 or 4 is not too annoying for a few performance-limiting kernels.

“Premature optimization is the root of all evil”
Cooperative pattern

Each grid point handled by a single thread a warp.

```cpp
__global__ void warp_team(...) {
    int warpid = ( threadIdx.x + blockIdx.x*blockDim.x )/32;
    int laneid = threadIdx.x%32;
    int t = warpid;
    #pragma unroll 1
    for( int y = laneid; y < NS; y += 32 )
    {
        double ayy = ay[NS*t+y];
        double byy = by[NS*t+y];
        #pragma unroll 1
        for( int x = 0; x < NS; x++ )
        {
            output[NS*NS*t+NS*x+y] = ax[NS*t+x]*ayy + bx[NS*t+x]*byy;
        }
    }
}
```
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    int laneid = threadIdx.x%32;
    int t = warpid;
    #pragma unroll 1
    for( int y = laneid; y < NS; y += 32 )
    {
        double ayy = ay[NS*t+y];
        double byy = by[NS*t+y];
        # pragma unroll 1
        for( int x = 0; x < NS; x++ )
        {
            output[NS*NS*t+NS*x+y] = ax[NS*t+x]*ayy + bx[NS*t+x]*byy;
        }
    }
}
```

Y-dependent loads are coalesced.
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    {
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        double byy = by[NS*t+y];
        #pragma unroll 1
        for( int x = 0; x < NS; x++ )
            output[NS*NS*t+NS*x+y] = ax[NS*t+x]*ayy + bx[NS*t+x]*byy;
    }
}
```

Y-dependent loads are coalesced.

X-loads are uncoalesced...BUT next x-iteration accesses next contiguous location in memory...
AND **effective cache per grid point is now 32X higher**...perhaps the next x-load will hit?
Cooperative pattern is fastest!

Each grid point handled by a single thread a warp.

```c
__global__ void warp_team(...) {
    int warpid = ( threadIdx.x + blockIdx.x*blockDim.x )/32;
    int laneid = threadIdx.x%32;
    int t = warpid;
    #pragma unroll 1
    for( int y = laneid; y < NS; y += 32 )
    {
        double ayy = ay[NS*t+y];
        double byy = by[NS*t+y];
        # pragma unroll 1
        for( int x = 0; x < NS; x++ )
            output[NS*NS*t+NS*x+y] = ax[NS*t+x]*ayy + bx[NS*t+x]*byy;
    }
}
```

Y-dependent loads are coalesced.

X-loads are uncoalesced…BUT next x-iteration accesses next contiguous location in memory…AND effective cache per grid point is now 32X higher…perhaps the next x-load will hit?

Nvprof confirms: high hit rates => fast kernel!!

nc_cache_global_hit_rate = 95.39%, tex_cache_hit_rate = 95.39%

Warp Team Runtime

<table>
<thead>
<tr>
<th>Naive</th>
<th>Warp team</th>
</tr>
</thead>
<tbody>
<tr>
<td>.135 s</td>
<td>.052 s</td>
</tr>
</tbody>
</table>
Downside to cooperative: need different memory layout.

Kernel with each thread handling a grid point

```c
__global__ void naive(...) {
    int t = threadIdx.x + blockIdx.x*blockDim.x;
    #pragma unroll 1
    for( int y = 0; y < NS; y++ )
        # pragma unroll 1
        for( int x = 0; x < NS; x++ )
            output[N*(NS*y+x)+t] =
                ax[x*N+t]*ay[y*N+t] +
                bx[x*N+t]*by[y*N+t];
}
```

**Grid point index t is fast index** for output, ax, ay, bx, by.

Consecutive threads handle consecutive grid points => coalesced access.

**Corresponds to** Kokkos::LayoutLeft

Cooperative kernel

```c
__global__ void warp_team(...) {
    int warpid = (threadIdx.x + blockIdx.x*blockDim.x)/32;
    int laneid = threadIdx.x%32;
    int t = warpid;
    #pragma unroll 1
    for( int y = laneid; y < Ns; y += 32 )
        {
            double ayy = ay[NS*t+y];
            double byy = by[NS*t+y];
            # pragma unroll 1
            for( int x = 0; x < NS; x++ )
                output[NS*NS*t+NS*x+y] =
                    ax[NS*t+x]*ayy +
                    bx[NS*t+x]*byy;
        }
}
```

Each warp handles one grid point.

**Fast index must be species index x or y** (they are symmetric) for spatially local accesses by warps.

**Corresponds to** Kokkos::LayoutRight
Hall of fame

<table>
<thead>
<tr>
<th>Method</th>
<th>Time</th>
<th>Improvement</th>
</tr>
</thead>
<tbody>
<tr>
<td>Naïve</td>
<td>0.135s</td>
<td></td>
</tr>
<tr>
<td>Tiled, TILE_FACTOR 8</td>
<td>0.209s</td>
<td>54%</td>
</tr>
<tr>
<td>12.5% occupancy, TILE_FACTOR 4</td>
<td>0.127s</td>
<td>42%</td>
</tr>
<tr>
<td>Tiled using L1 and readonly,</td>
<td>0.096s</td>
<td>27%</td>
</tr>
<tr>
<td>TILE_FACTOR 2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Unroll-and-jam by 2</td>
<td>0.106s</td>
<td>23%</td>
</tr>
<tr>
<td>Warp team</td>
<td>0.052s</td>
<td></td>
</tr>
</tbody>
</table>
Questions?