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

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PART 1: Integrating Kokkos with CASTLES

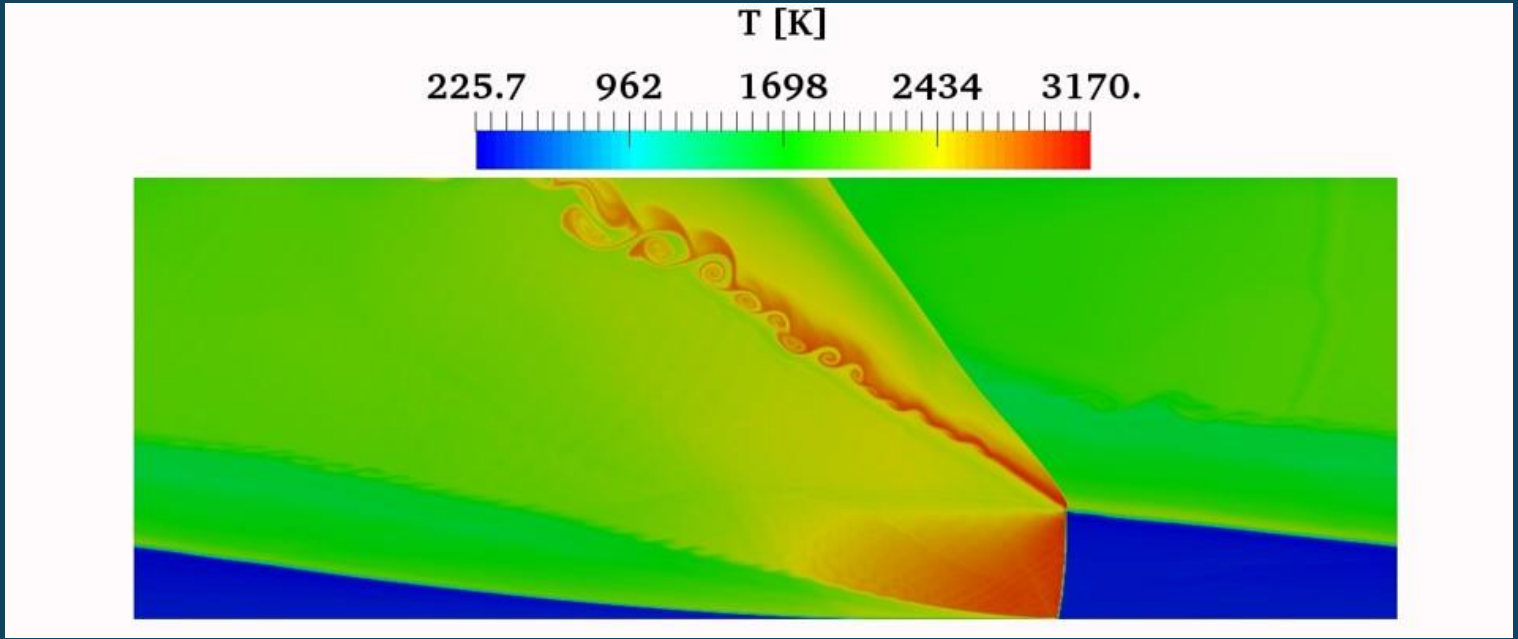
What do you do when someone hands you 100,000 lines of Fortran and says "make this run on anything?"

PART 2: GPU-specific kernel optimizations

How do I make per-grid-point inner loops blazing fast?
Highly general/easily transferrable to other applications.

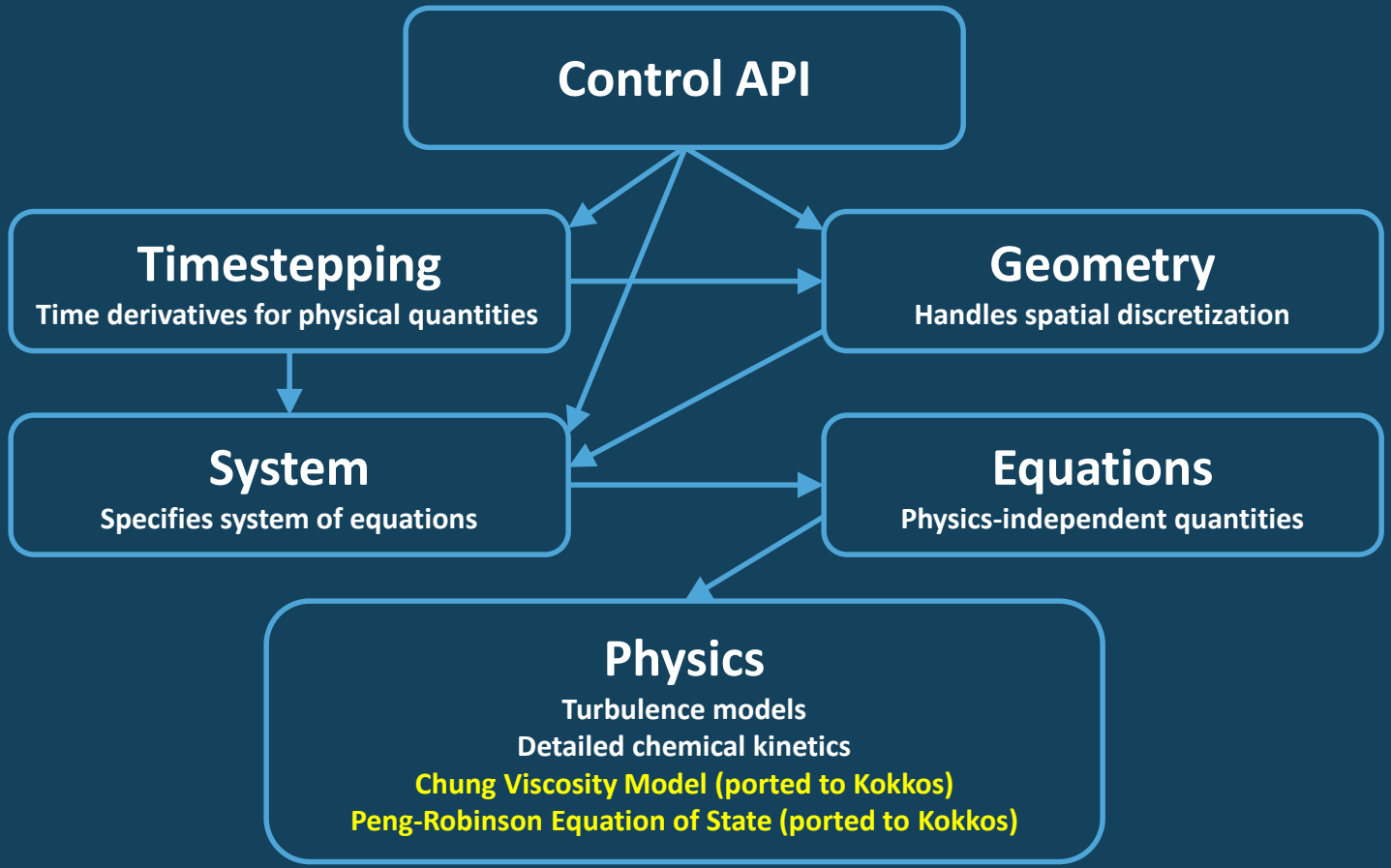
CASTLES: Cartesian Adaptive Solver Technology for Large Eddy Simulations

- A high-order Navier-Stokes solver for turbulent combustion
- Written in Fortran
- MPI parallelism, but no intra-node parallelism



CASTLES simulation of rotating detonation engine
(courtesy of Dr. Christopher Lietz)

Structure of CASTLES



What is Kokkos?

C++ Framework. Claims "Performant cross platform parallelism": write once, compile for many architectures.

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 structures provide 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:
https://github.com/kokkos/kokkos/blob/master/doc/Kokkos_PG.pdf

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

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```

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Easy to see global structure and call chains.

Can also do bottom up profile (default)

Looks like those “preos” and “chung” routines are burning a lot of 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_rhstimessp34_
| |   29.77% interfacegeom_mp_rhsgeomrescalc_
| |   | 15.46% interfacegeom_mp_rhsgeom3dresad1lr_
| |   | | 15.35% interfacesysexternal_mp_rhssysupdiss_
| |   | | | 15.35% interfacesysinternal_mp_rhssysscalarupdiss_
| |   | | |   9.85% eosmodule_mp_eoscalcrhoh0fromtp_
| |   | | |   | 9.64% eosmodule_mp_eosrhohfromtpprop_
| |   | | |   |   9.64% preosmodule_mp_preosrhohfromtpprop_
...
| |   | | |   5.18% eosmodule_mp_eosgammajacobianproperties_
| |   | | |     5.10% preosmodule_mp_preosgammajacobianproperties_
...
| |   | 13.90% interfacegeom_mp_rhsgeom3dviscres2_
| |   | | 13.84% interfacesysexternal_mp_rhssysviscflux_
| |   | |   13.32% preosmodule_mp_preosviscousfluxproperties_
| |   | |   | 7.85% chungtransmodule_mp_chungcalctransprop_
...
| |   | |   | 3.27% preosmodule_mp_preoscriticalstate_
...
| |   18.33% interfacegeom_mp_bcgeomrescalc_
| |   | 14.77% interfacegeom_mp_bcgeomsubin_
| |   | | 14.77% interfaceeqnfluids_mp_bcfluidseqnsubin_velocity_
| |   | |   14.77% preosmodule_mp_preoscalctfromhp_
...
| |   | 3.56% interfacesysexternal_mp_stepsys3dcalcqadd_
| |   |   3.53% eosmodule_mp_eosthermalproperties_
| |   |   | 3.50% 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.

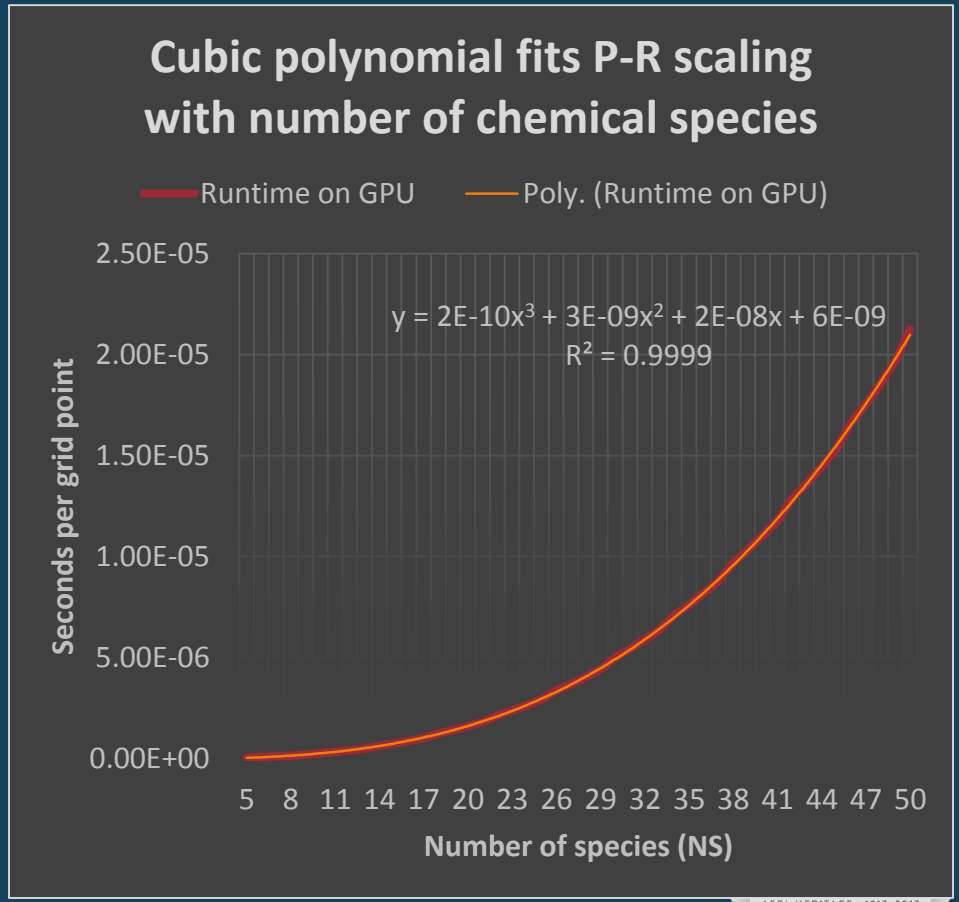
Properties are computed individually per cell
(or interpolated points at cell interfaces),
so **trivially parallel**

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 $a*NS + b*NS^2 + c*NS^3$

Occupies majority of CASTLES runtime for ns >= 4ish



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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TVProperties* gettvproperties();
```

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(…);
…
```

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…

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

TVImpl

```
// Contains members of TVProperties that don't need
// external visibility (pimpl idiom)
// Owns and allocates Kokkos Views
View1DType T;
View1DType P;
View1DType Yi;
…(several dozen of these)

// Owns std::unordered_maps to launch kernels
// and communicate data by name
unordered_map<string,View1DType>
      select1DViewByName;
unordered_map<string,View2DType>
      select2DViewByName;
// Owns Launcher for each kernel
// (lightweight wrapper with string identifier,
// inherits common timing routines from
// LauncherBase)
unordered_map<string,LauncherBase*> launchers;
```

```
void safeLaunch(…);
```

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

Kernel launches and data comms are referred to TVProperties* owned by Frame.

For modularity and consistency: one subroutine->one kernel

Fortran subroutine:
Operates on a single grid point at a time

```
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:
Operates on `nActivePoints` grid points in parallel

Parallel pattern

Parallel work index `t`

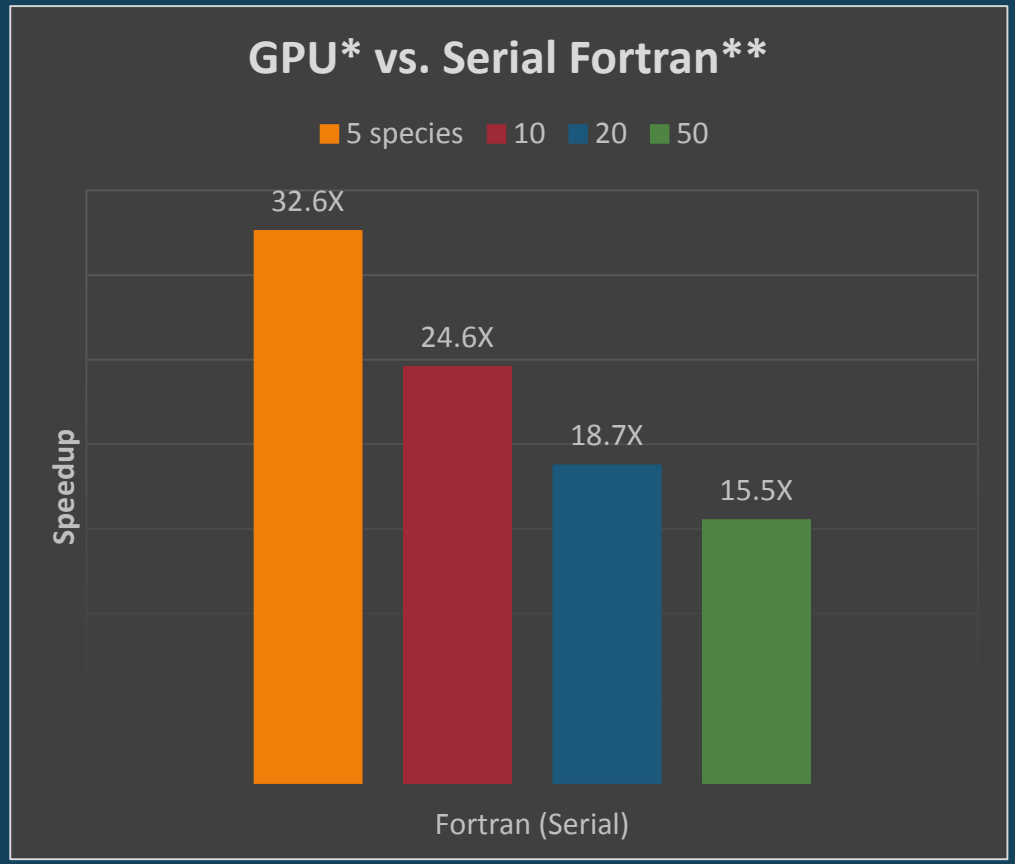
```
parallel_for( tvimpl->nActivePoints,
    KOKKOS_LAMBDA( const int& t )
    {
        c(t) = sqrt( rho(t)*hT(t)/
            ( rho(t)*rhoP(t)*hT(t)
            + rhoT(t)*( 1.0-rho(t)*hP(t) ) ) )
    } );
```

User-defined functor (lambda)

Kokkos Views,
captured by value from members of `TVImpl`)
(View copy constructor is a lightweight shallow copy)

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

GPU Speedups for Standalone Peng-Robinson



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)

*** Nvidia Kepler K40**

**** Intel Xeon E5-2620 v3 CPU**

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.

Interface function to initialize Kokkos and allocate storage

```
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

```
! 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

```
extern "C" void
frame_tvproperties_eosthermalandviscousproperties_(
    int nActivePoints )
{
    frame.gettvproperties()->eosThermalAndViscousProperties(
        nActivePoints );
}
```

Corresponding Fortran call

```
call
frame_tvproperties_eosthermalandviscousproperties&
    ( %VAL( NumThisStripe ) )
```

Integrating Kokkos with CASTLES: Interface Functions

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Interface function to initialize Kokkos and allocate storage

Disallow name mangling by C++ compiler

Trailing _ expected by Fortran linker

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extern "C" void frame_initialize_( int device_id,
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    int iTurb )
{
    frame.initialize( device_id, // GPU device to select
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Corresponding Fortran call

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call frame_initialize( %VAL( KokkosDeviceID,&
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    %VAL( nspe ),&
    %VAL( nq ),&
    %VAL( iTurbType ) )
```

Pass integers by value

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

```
extern "C" void
frame_tvproperties_eosthermalandviscousproperties_(
    int nActivePoints )
{
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        nActivePoints );
}
```

Corresponding Fortran call

```
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

```
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

```
! 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. Extracts volume of data to Views, 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. No free lunch here. Annoying indexing.

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

Standalone Kokkos application:

Within code:

```
Kokkos::initialize( int& argc, char* argv[] );
```

To run:

```
$ mpirun -n numprocs ./myKokkosApp \
>        --kokkos-ndevices=2
```

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

My application (embedded within a big Fortran code):

Pass num GPU devices per node in Fortran input file:

```
&KokkosInputs
  KokkosNumDevices = 2
  ...
/
```

Within Fortran, compute device to use as (MPI rank%num devices):

```
call MPI_COMM_RANK( MPI_COMM_WORLD, rank, ierror )
KokkosDeviceID = mod( rank, KokkosNumDevices )
```

…and call the interface function to initialize Kokkos:

```
call frame_initialize( %VAL( KokkosDeviceID ), ... )
```

Finally, within C++ frame.initialize():

```
Kokkos::InitArguments args;
args.device_id = KokkosDeviceID;
Kokkos::initialize( args );
```

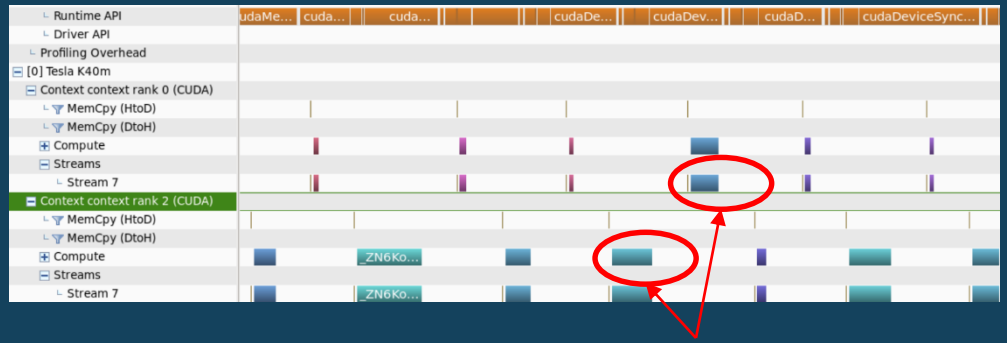
No need for arguments to executable.

** 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).

Cluster-level concerns: Nvidia Multi-Process Service (MPS)

Without MPS:

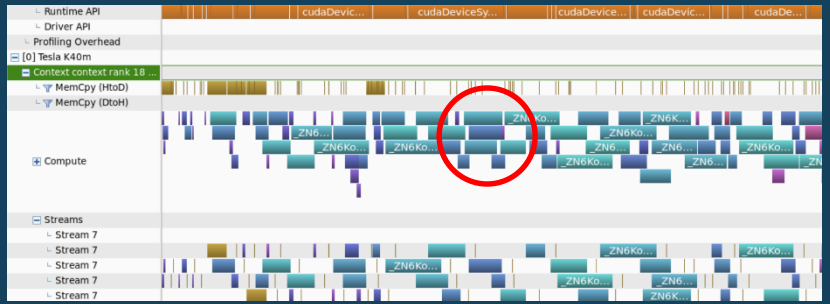
Each MPI process has its own CUDA context.
Multi-process profile shows one process at a time using a given GPU.



Kernels from different processes do not overlap

With MPS:

Multiple processes can share a given GPU simultaneously.

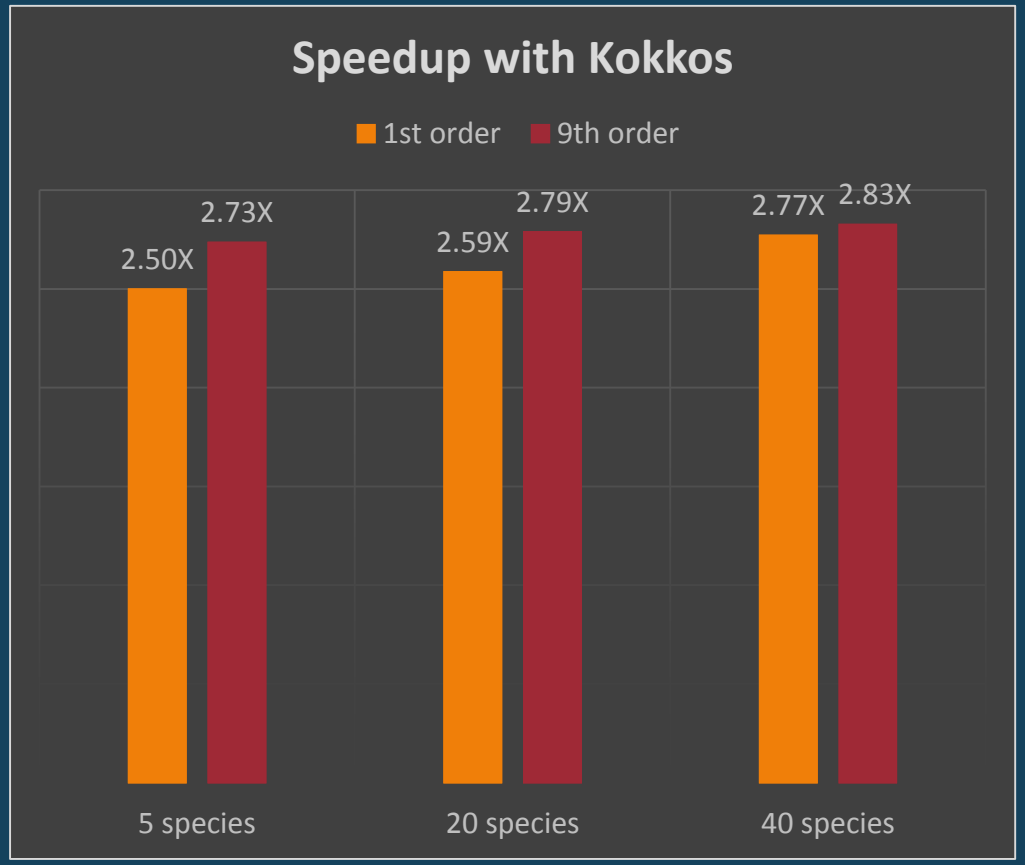


Kernels from different processes overlap
For small NS, turning on MPS makes overall application up to **3X faster**

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).

See http://on-demand.gputechconf.com/gtc/2016/presentation/s6142-jiri-kraus-multi-gpu-programming-mpi.pdf

GPU Speedup of Overall CASTLES+Kokkos



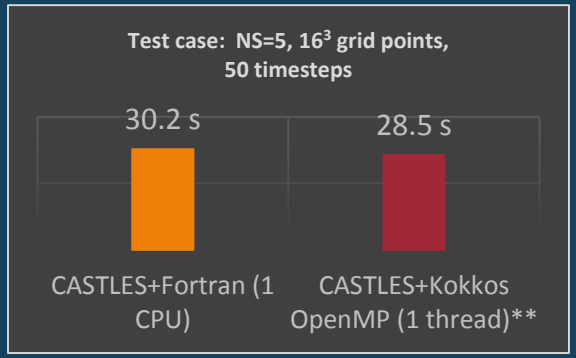
Production-style runs:
40 MPI ranks on 2 nodes.

- 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?



**KMP_AFFINITY=compact,1,granularity=core

Often, naively porting Fortran to C++ results 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.**

To compile for CPU, just change arguments to makefile (see Kokkos documentation).

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
}
```

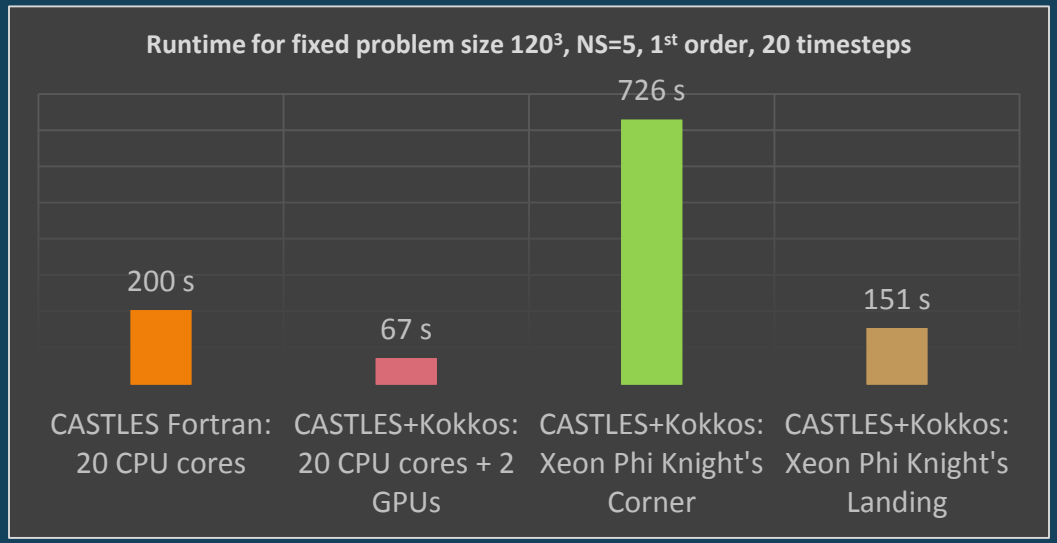
Kokkos promise of "performant cross-platform parallelism" more or less fulfilled.

Node level performance + comparison with Xeon Phi

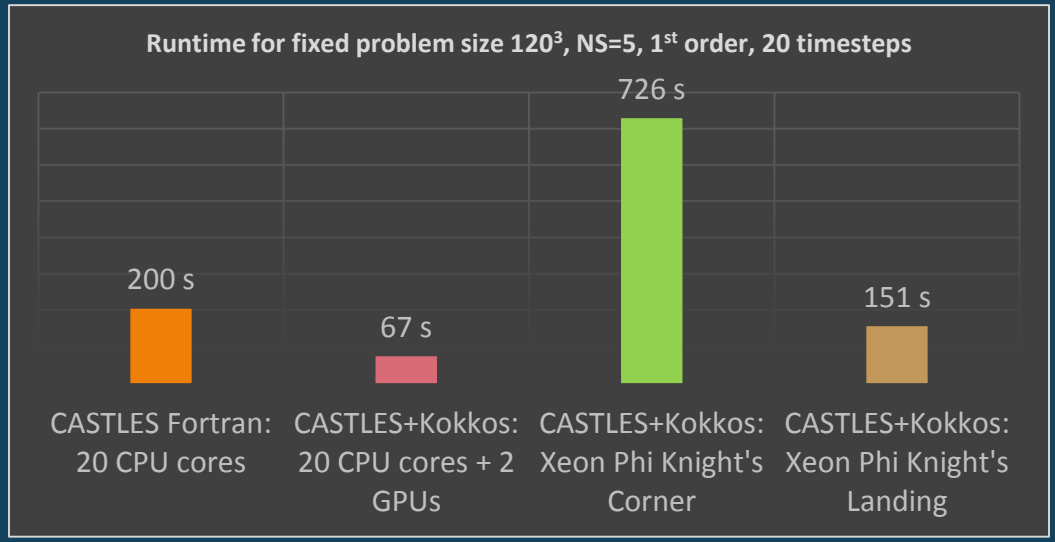
Kokkos runs on Xeon Phis in native mode.

- 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.



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 significantly.

2x10 core Intel Xeon E5-2650 v3
+ 2 Kepler K40 GPUs.
KokkosMaxBlock = 12288
Same MPI config as CASTLES Fortran.

One Knight's Corner 5110P (60 cores, 240 logical processors).
KokkosMaxBlock = 1024
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), flat memory mode, SNC-4 cluster mode
KokkosMaxBlock = 1024
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 enforces 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.

PART 1: Integrating Kokkos with CASTLES

What do you do when someone hands you 100,000 lines of Fortran and says "make this run on anything?"

PART 2: GPU-specific kernel optimizations

How do I make per-grid-point inner loops blazing fast?
Highly general/easily transferrable to other applications.

Bandwidth-Bound 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 serial loop over grid points):

```
// Loop over N grid points (trivially parallel)
for( int t = 0; t < N; t++ )
    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];
```

Arrays of size NS*N that store per-grid-point input data

"Embarrassingly parallel," and inner loops are simple…
but achieving high performance is an interesting problem!

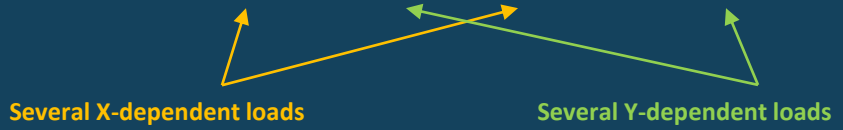
Bandwidth-Bound Per-Grid-Point Inner Loops

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 serial loop over grid points):

```
// Loop over N grid points (trivially parallel)
for( int t = 0; t < N; t++ )
    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!

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 100 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

```
__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.

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```

Grid point index "t" is fast index for coalescing

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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.

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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.

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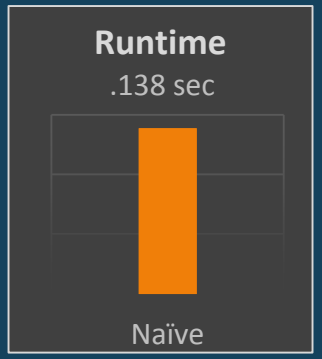

Kernel "naïve" is strongly bandwidth-bound, and accesses are already coalesced. What should we do?

Standard CPU-informed strategy: tile the loop?

Recall why loop tiling helps on CPU:

```
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];
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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 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

```
__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]
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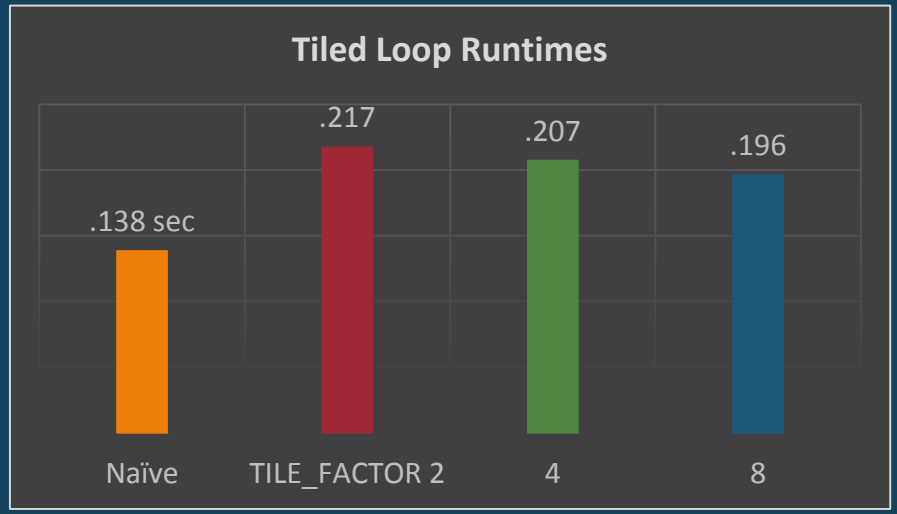

Tiling is worse than naïve. Cache per grid point (thread) is just too small.

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.**

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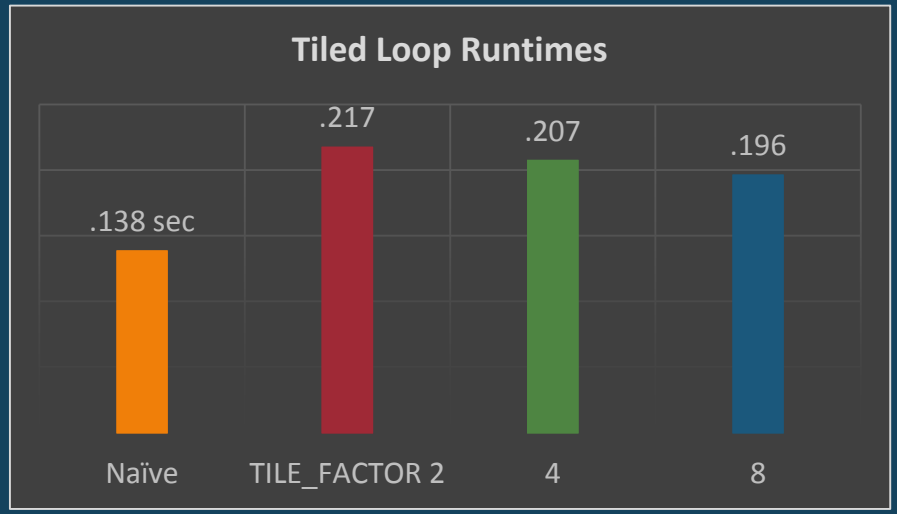

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nvprof confirms poor hit rates (results for TILE_FACTOR 2 shown):**

```
nvprof --kernels ::tiled:1 -metrics \
nc_cache_global_hit_rate,tex_cache_hit_rate ./a.out
. . .                                          Min         Max
. . . Non-Coherent Global Hit Rate        0.85%       0.85%
. . .       Texture Cache Hit Rate        0.65%       0.65%
```

** 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.

```
__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]
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}
```

** 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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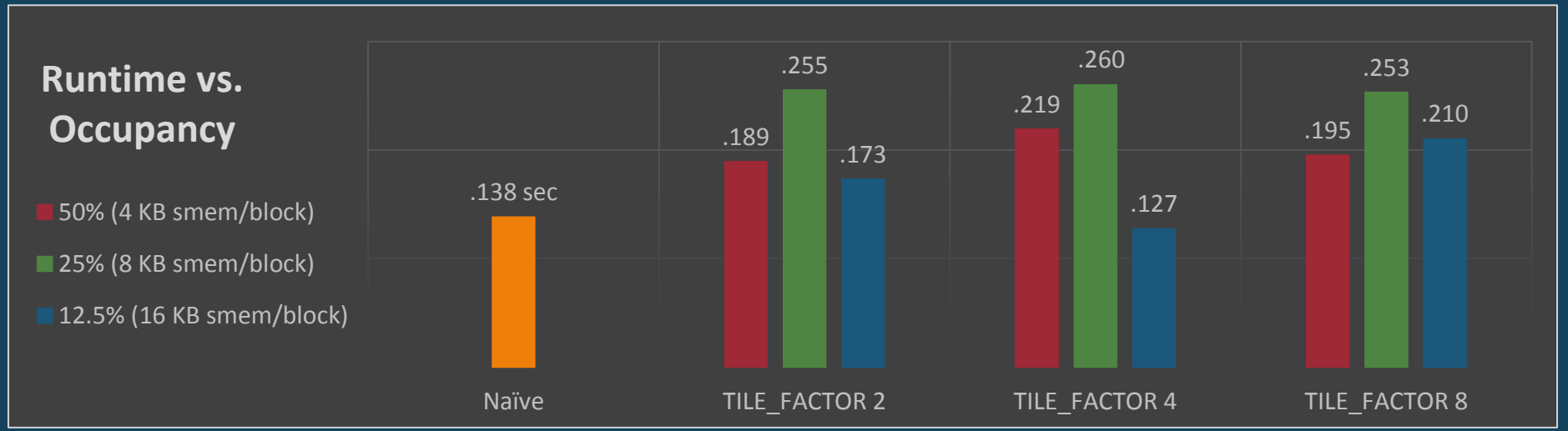

Mostly worse than naïve.

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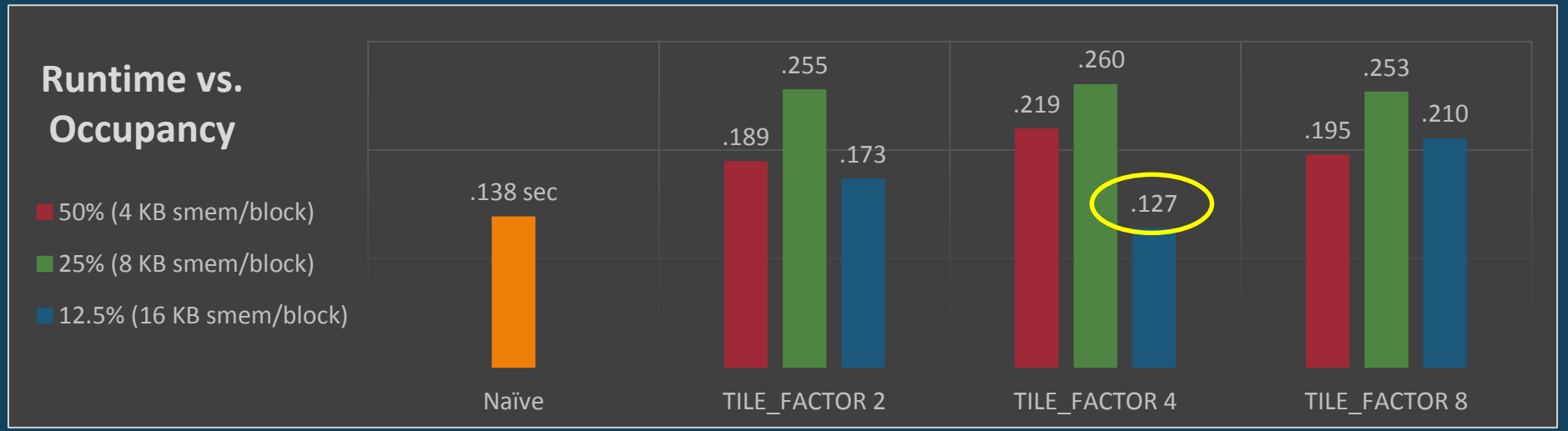

Mostly worse than naïve. **Sweet spot at TILE_FACTOR 4, 12.5% occupancy can be explained by cache hits:**

```
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)**

```
__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];
    }
}
```

** On Kepler, local loads are cached in L1. On Maxwell, L1/tex is a single unified cache, and local loads are cached in L2 only. Therefore, I expect tiling with local memory to be helpful on Kepler only. Maxwell has separate hardware for shared memory, so you could try using thread-local smem arrays instead.
See https://devblogs.nvidia.com/parallelforall/fast-dynamic-indexing-private-arrays-cuda/ for an in-depth discussion of where the compiler places thread-local arrays.
See http://docs.nvidia.com/cuda/kepler-tuning-guide/#l1-cache and http://docs.nvidia.com/cuda/maxwell-tuning-guide/#l1-cache for microarchitecture details.

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    {
        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]
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    {
        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++ )
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    }
}
```

Thread-local arrays for Y-dependent loads (cached in L1)

X-dependent loads cached in read-only

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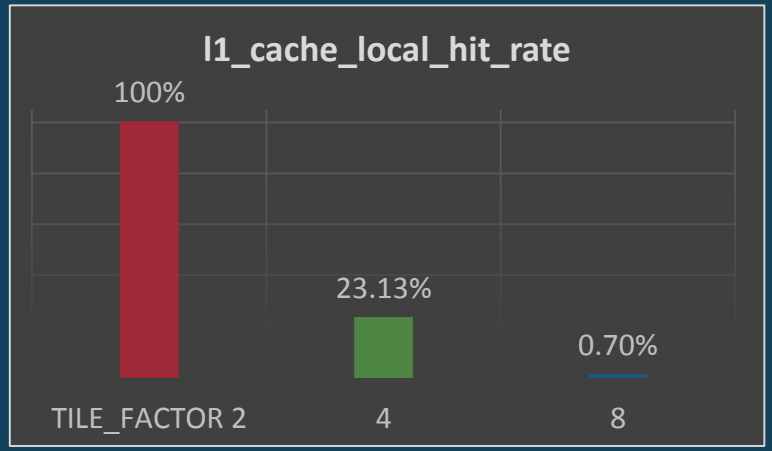
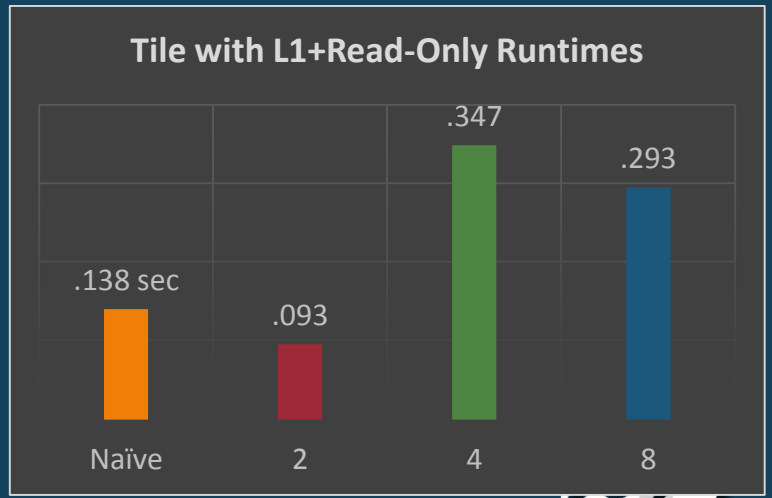
                                     + bx[x*N+t]*by_local[y-yy];
    }
}
```

X-dependent loads cached in read-only

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.

```
__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

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.

```
__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;
        }
    }
}
```

Y-dependent loads reused x times in x-loop

X-dependent loads used twice

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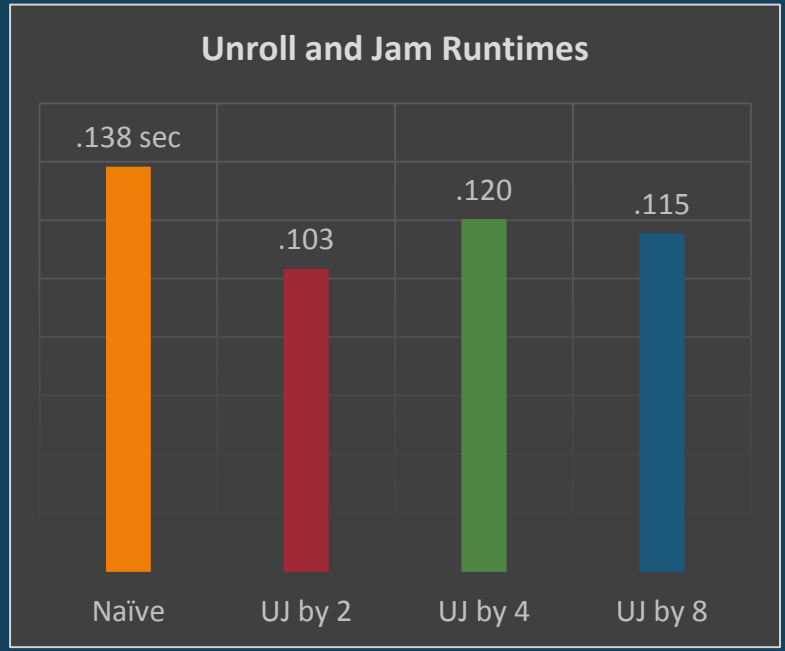
    {   ay_local0 = ay[(yy+0)*N+t];
        by_local0 = by[(yy+0)*N+t];
        ay_local1 = ay[(yy+1)*N+t];
        by_local1 = by[(yy+1)*N+t];
        #pragma unroll 1
        for( int x = 0; x < NS; x++ )
        {
            output[N*(NS*(yy+0)+x)+t] = ax[x*N+t]*ay_local0
                                      + 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



In practice I like this approach. Helpful on Kepler, Maxwell, and Pascal.

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”

Cooperative pattern

Each grid point handled by ~~a single thread~~ a warp.

```
__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.

Cooperative pattern

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    int t = warpid;
    #pragma unroll 1
    for( int y = laneid; y < NS; y += 32 )
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        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-dependent loads broadcast a value across the warp. Uncoalesced.

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 next x-load will hit?

Cooperative pattern best so far!

Each grid point handled by ~~a single thread~~ a warp.

```
__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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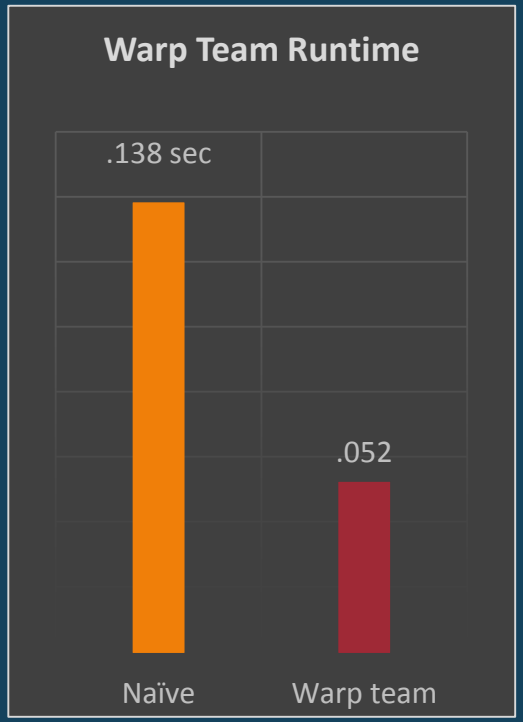
X-dependent loads broadcast a value across the warp. Uncoalesced.



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 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%
```

Downside to cooperative: need different memory layout.

Kernel with each thread handling a grid point

```
__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`

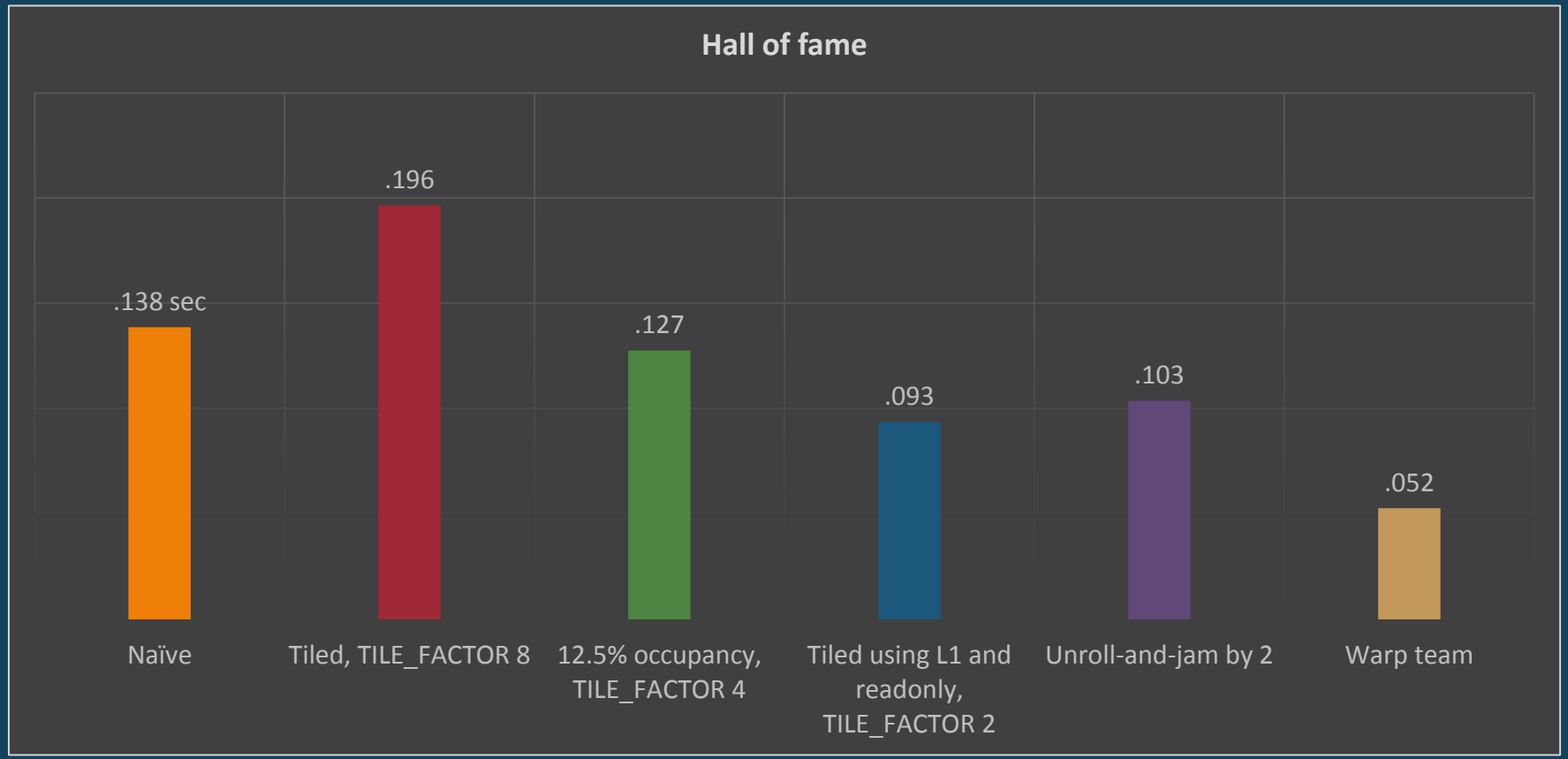
Cooperative kernel

```
__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. For `output`, `y` is chosen to be fastest, so that writes are coalesced.

Corresponds to `Kokkos::LayoutRight`



Kokkos versions

Naïve kernel

```
parallel_for( N,
    KOKKOS_LAMBDA( const int& t )
    {
        #pragma unroll 1
        for( int y = 0; y < NY; y++ )
            #pragma unroll 1
            for( int x = 0; x < NX; x++ )
                output(t,y,x)  = ax(t,x)*ay(t,y)  +
                                 bx(t,x)*by(t,y);
    } );
```

On GPU, Views are Kokkos::LayoutLeft (t is fastest index)

Unroll and jam by 2 kernel

```
parallel_for( N,
    KOKKOS_LAMBDA( const int& t )
    {
        double ay_local0, ay_local1;
        double by_local0, by_local1;
        #pragma unroll 1
        for( int yy = 0; yy < NY; yy += 2 )
        {
            ay_local0 = ay(t,yy+0); ay_local1 = ay(t,yy+1);
            by_local0 = by(t,yy+0); by_local1 = by(t,yy+1);
            #pragma unroll 1
            for( int x = 0; x < NX; x++ )
            {
                output(t,yy+0,x)  = ax(t,x)*ay_local0
                                  + bx(t,x)*by_local0;
                output(t,yy+1,x)  = ax(t,x)*ay_local1
                                  + bx(t,x)*by_local1;
            }
        }
    } );
```

Order of x, y doesn't matter much on GPU. Writes are coalesced either way.
Noticeable (but minor) effect on performance: y before x makes naïve kernel slightly slower and unroll+jam slightly faster. I'm not sure why…TLB issues?
I choose innermost loop index x as rightmost for later portability to CPU. On CPU, Views become LayoutRight, rightmost index becomes fastest, and innermost loop can then vectorize with stride-1 writes.

Kokkos versions

Warp team kernel**

becomes `blockDim.y`
becomes `blockDim.x`

```
int team_size = 8;
int vectorlen = 32;
parallel_for( TeamPolicy<>( N/team_size, team_size, vectorlen ),
    KOKKOS_LAMBDA( const TeamPolicy<>::member_type& team_member
)
    {
        int team_rank = team_member.team_rank();
        int league_rank = team_member.league_rank();
        int t = league_rank*team_member.team_size() + team_rank;
        parallel_for( ThreadVectorRange( team_member, NY ),
            [&]( const int& y )
            {
                double ayy = ay(t,y);
                double byy = by(t,y);
                #pragma unroll 1
                for( int x = 0; x < NX; x++ )
                    output(t,x,y) = ax(t,x)*ayy + bx(t,x)*byy;
            } );
    } );
```

Ranges from 0 to `team_size-1`.
For `vectorlen = 32`,
`team_rank` = warp id within block.

For `vectorlen = 32`,
`t` = global warp id.

Global block index

Hierarchical parallelism

Consecutive vector indices `y` map to consecutive threads in the warp, so `y` must be rightmost here for coalesced writes

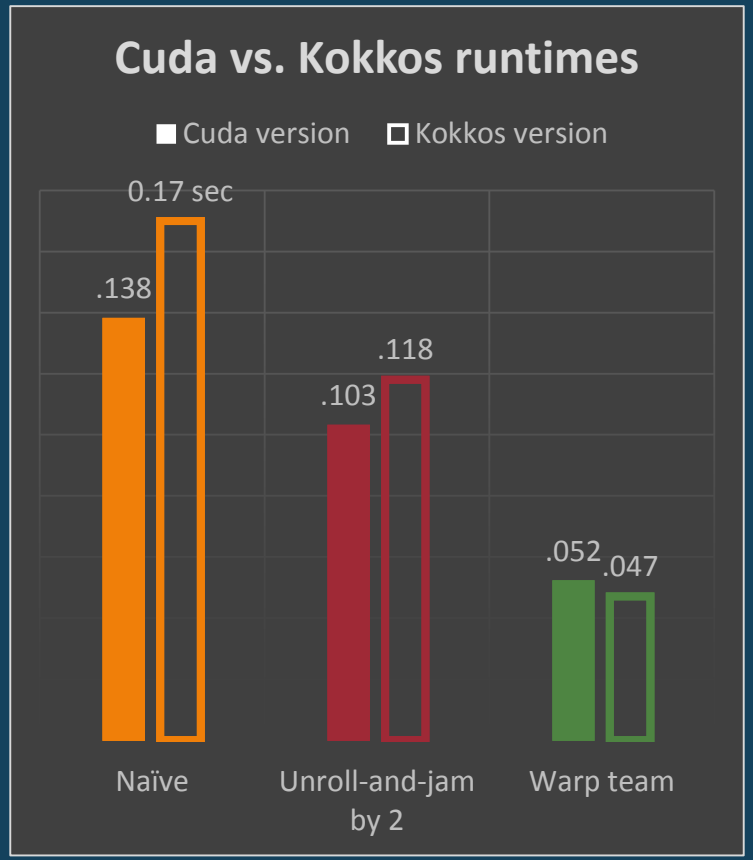
Views should now be Kokkos::LayoutRight, even on GPU (rightmost index fastest)

** See the Kokkos Programming Guide (https://github.com/kokkos/kokkos/blob/master/doc/Kokkos_PG.pdf) for details on team policies and hierarchical parallelism.

Kokkos is slower.
Could be reduced occupancy
due to register pressure.

Kokkos version uses 38 registers/thread.
38*256 = 9728 registers/block,
65,536/9728 = 6.74 => only 6 blocks of 256
threads can be live on each Kepler SM.

Theoretical occupancy = 6*256/2048 = 75%.
`achieved_occupancy = 0.735`



Register pressure?

I don't know why Kokkos is faster!

I know Kokkos version uses L1 instead of
readonly cache though.
`l1_cache_global_hit_rate = 91.65%,`
`nc_cache_global_hit_rate = 0.00%`

Questions?

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https://www.linkedin.com/in/mfcarilli/
https://github.com/mcarilli
(I'll post runnable example code if/when it gets cleared for public release)