OAK RIDGE National Laboratory

E3SM-MMF Experiences with AMD Hardware

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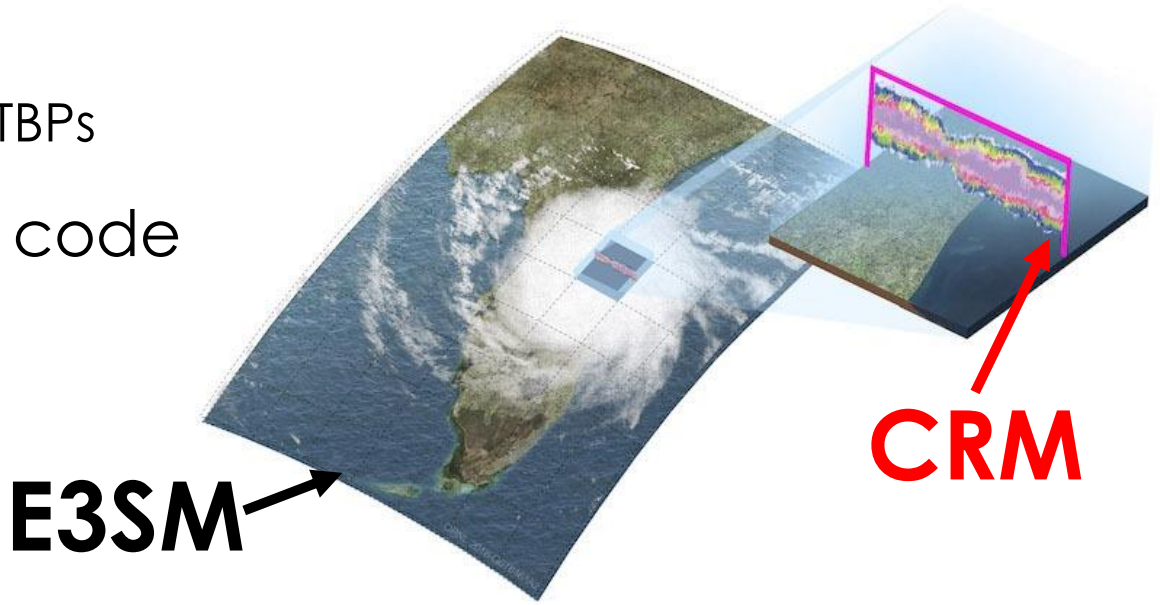
E3SM Multiscale Modeling Framework (E3SM-MMF)

- Energy Exascale Earth System Model: U.S. DOE hi-res climate model
  - Collection of atmosphere, ocean, land surface, sea ice, and land ice
- Multi-scale Modeling Framework (E3SM-MMF)
  - Embed hi-res (1km) Cloud Resolving Model (CRM) at each global model grid point
  - Explicit simulate moist convection on reduced domain
  - Improves upon heuristic "parameterization" for moist convection
  - 2 million lines of mostly Fortran 77, 90, 2003+
  - Threading is poorly exposed
  - Heavily reliant on Fortran classes, pointers, TBPs
- >90% of runtime concentrated in CRM code
  - Only 10-20K lines of code
  - Natural target for acceleration



Approach to AMD Hardware and Portability

- We chose to use C++ portability over Fortran + Directives

1. C++ can conveniently describe any code as an object (Lambdas)
   - We can then launch this code on CUDA, HIP, SYCL, OpenMP, etc. ourselves
   - Fortran cannot do this at this time
2. C is typically the first implementation a vendor develops
   - This is critical for efforts that must work on "day 1" for new architectures
3. C is the more reliable implementation
   - Fortran is less popular overall: fewer dedicated developers
   - C++ classes/templates better defined by standards than modern Fortran constructs

- However: Porting from Fortran to C++ is time consuming
  - Also, significant effort is needed to keep C++ user-level code **readable**
  - C++ Lambda capture semantics can be confusing to domain scientists
  - Have to put guardrails on C++ experts (reliance on std::, virtual inheritance, etc.)

What is Portable C++?

- A C++ library, not a separate language or a language extension
- Based on the "kernel" paradigm (e.g., CUDA, HIP, SYCL, …):
  - A kernel performs work on a single thread
  - Let the launcher know how many threads to launch
  - Requires no more work or information than you're already used to providing

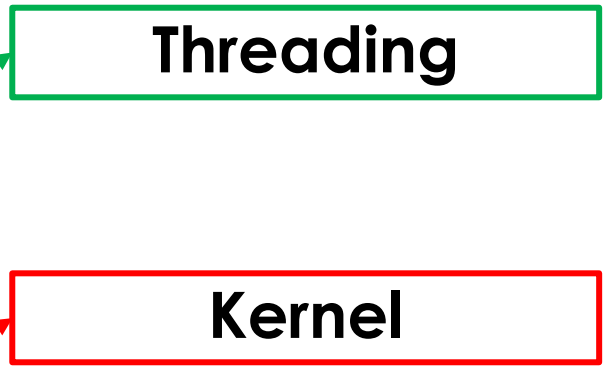
```
!$acc parallel loop collapse(4)
do l = 1 , numState
  do k = 1 , nz
    do j = 1 , ny
      do i = 1 , nx
        stateTend(i,j,k,l) = - ( stateFluxLimits(i+1,j,k,l) -
                                 stateFluxLimits(i  ,j,k,l) ) / dx;
      enddo
    enddo
  enddo
enddo
```

Loops define the threading

Kernel is the loop **body**

The Core of Portable C++

```
// for (int l=0; l < numState; l++) {
//   for (int k=0; k < nz; k++) {
//     for (int j=0; j < ny; j++) {
//       for (int i=0; i < nx; i++) {
parallel_for( Bounds<4>(numState,nz,ny,nx) ,
              YAKL_LAMBDA(int l, int k, int j, int i) {
  stateTend(l,k,j,i) = - ( stateFluxLimits(l,k,j,i+1) -
                           stateFluxLimits(l,k,j,i  ) ) / dx;
});
```



The Core of Portable C++

- C++ can pass code as an object

```
// for (int l=0; l < numState; l++) {
//   for (int k=0; k < nz; k++) {
//     for (int j=0; j < ny; j++) {
//       for (int i=0; i < nx; i++) {
parallel_for( Bounds<4>(numState,nz,ny,nx) ,
              YAKL_LAMBDA(int l, int k, int j, int i) {
  stateTend(l,k,j,i) = - ( stateFluxLimits(l,k,j,i+1) -
                           stateFluxLimits(l,k,j,i  ) ) / dx;
});
```

- C++ "lambdas" convert code into a class object for you
- You can then pass the code to whatever backend you want
  - "parallel_for" can launch with CUDA, HIP, OpenMP, OpenMP 4.5+, SYCL, etc.
- Just as flexible and generic as directives

Yet Another Kernel Launcher (YAKL)

- C++ Performance Portability Library for Fortran, simplicity, & readability
  - https://github.com/mrnorman/YAKL
- Syntax patterned after Kokkos & interoperates easily with Kokkos
- Focus on simplicity
  - Only one level of parallelism
    - Two levels of parallelism: already making statements about hardware
  - Only two memory spaces: host and device
- Allows Fortran-like behavior in multi-dimensional arrays
  - One-based indexing, column-major index ordering, basic slicing
  - Limited Fortran intrinsic library (size, shape, maxval, minloc, sum, etc.)
- Interacts with Fortran
  - Wrap existing Fortran allocations in YAKL Fortran-like Arrays
  - Pool allocator with CUDA Managed Memory hooks and Fortran hooks
  - Enables an incremental porting path with relatively little code change
- Convenient NetCDF, FFT, tridiagonal utilities for YAKL Arrays

YAKL Fortran-Like Multi-Dimensional Arrays

```
real stateTend      (nx  ,ny,nz,numState);
real stateFluxLimits(nx+1,ny,nz,numState);

!$acc parallel loop collapse(4)
do l = 1 , numState
  do k = 1 , nz
    do j = 1 , ny
      do i = 1 , nx
        stateTend(i,j,k,l) = - ( stateFluxLimits(i+1,j,k,l) -
                                 stateFluxLimits(i  ,j,k,l) ) / dx;
      enddo
    enddo
  enddo
enddo
```

Fortran code: Finite-Volume update from fluxes

Equivalent Portable C++

```
real4d stateTend      ("stateTend"      ,nx  ,ny,nz,numState);
real4d stateFluxLimits("stateFluxLimits",nx+1,ny,nz,numState);

// do l = 1 , numState
//   do k = 1 , nz
//     do j = 1 , ny
//       do i = 1 , nx
parallel_for( Bounds<4>(numState,nz,ny,nx) ,
              YAKL_LAMBDA(int l, int k, int j, int i) {
  stateTend(i,j,k,l) = - ( stateFluxLimits(i+1,j,k,l) -
                           stateFluxLimits(i  ,j,k,l) ) / dx;
});
```

YAKL Fortran-Like Multi-Dimensional Arrays

- YAKL Arrays inherently behave like Fortran assumed-shape arrays
  - They carry all metadata with them:

```
real3d transpose(real3d &a) {
  int nz = size(arr,3);
  int ny = size(arr,2);
  int nx = size(arr,1);
  real3d a_t("a_t",nz,ny,nx);
  parallel_for( Bounds<3>(nz,ny,nx) , YAKL_LAMBDA(int k, int j, int i) {
    a_t(k,j,i) = a(i,j,k);
  });
  return a_t;
}
```

- In practice, you would want to tile this loop

YAKL Reduction & Limited Fortran Intrinsics Library

- Computing the maximum stable time step for Shallow Water (**Portable C++**)

```
real max_stable_dt(real2d const &height, real2d const &u,
                   real2d const &v, real grav, real cfl,
                   real dx, real dy) {
  real2d dt2d("dt2d",nx,ny);
  parallel_for( Bounds<2>(ny,nx) , YAKL_LAMBDA (int j, int i) {
    real g_w = sqrt(grav * height(i,j));
    real dt_x = cfl * dx / ( abs(u(i,j)) + g_w );
    real dt_y = cfl * dy / ( abs(v(i,j)) + g_w );
    dt2d(i,j) = min( dt_x , dt_y );
  });
  return minval( dt2d );  // This is a device-wide reduction
}
```

Future Plans for YAKL

- YAKL currently works on CPU (serial), Nvidia GPUs, and AMD GPUs
- YAKL works on Intel GPUs with OpenMP Offload backend
  - Except for atomic min and max instructions (waiting on OpenMP 5.1 implementations)
- SYCL backend (Intel) is waiting on "is_memcpyable" implementation
- Coming soon to a YAKL near you:
  - CPU threading (OpenMP first, then pthreads for more efficiency if needed)
  - An approach to cache blocking and SIMD vectorizations
- Long term plan: create a version of YAKL that wraps Kokkos for as many components as possible

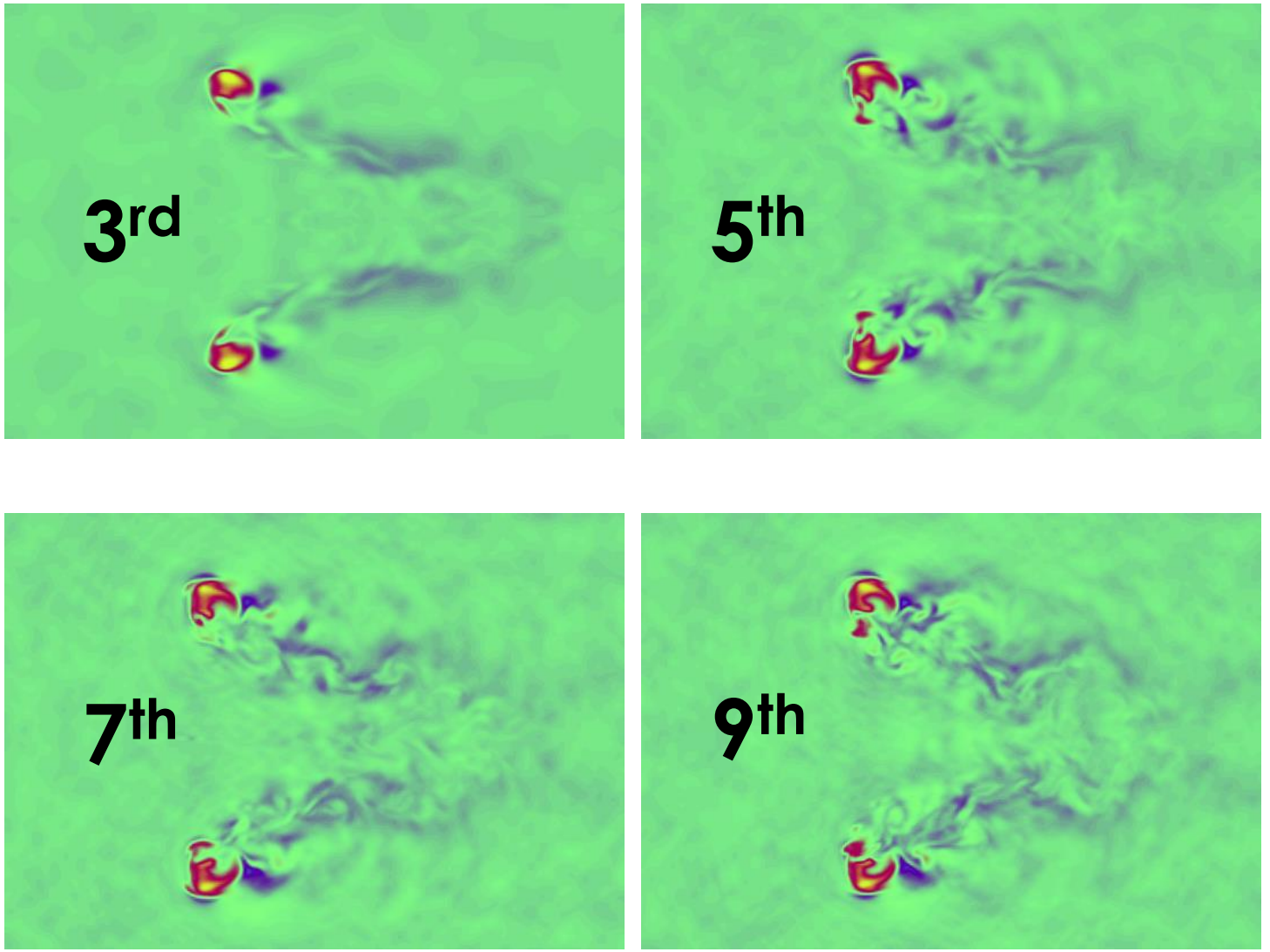
Algorithmic Advances for GPU Hardware

- Important to consider algorithms better suited for GPUs
- Arithmetically intense algorithms perform well on all architectures
- Increase computations while decreasing data movement

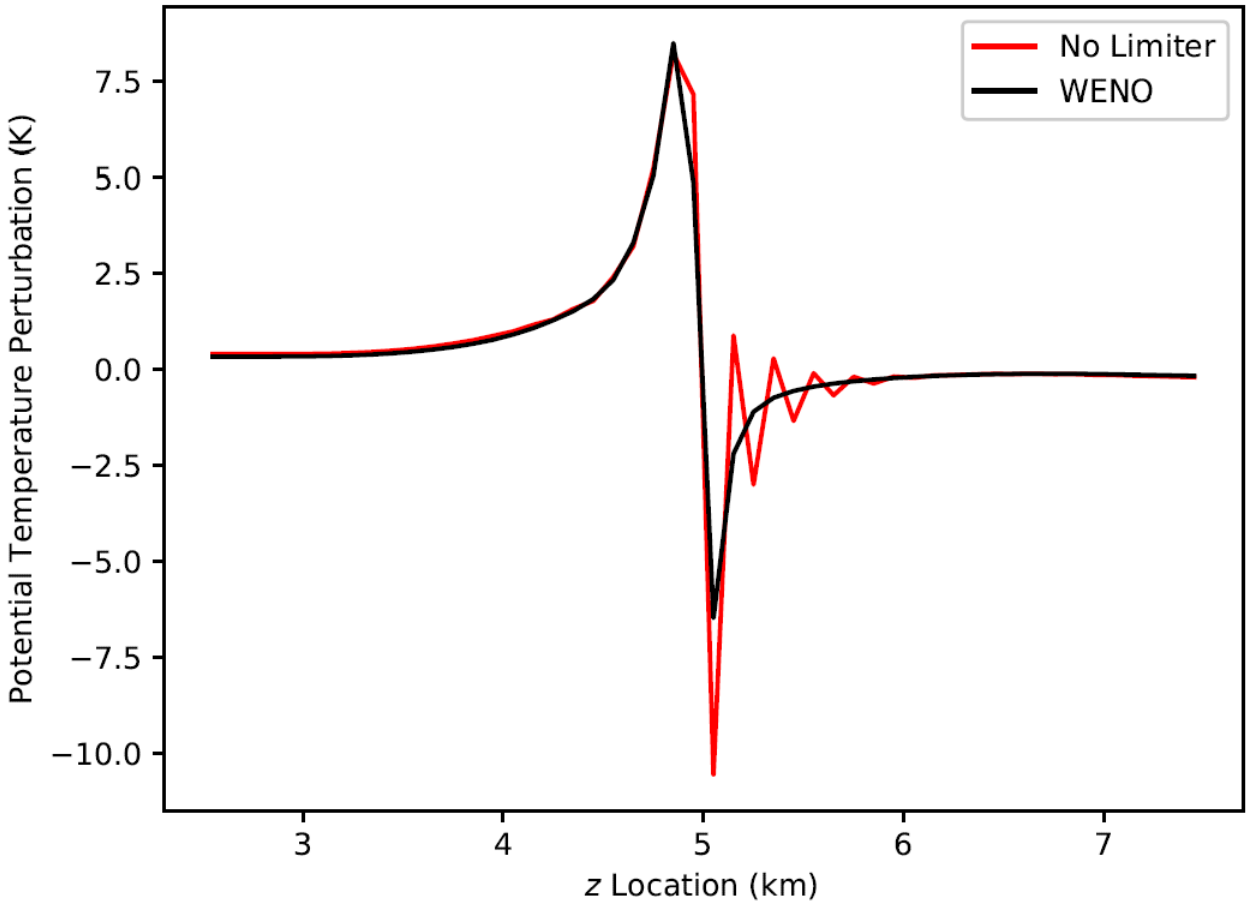
- E3SM-MMF Algorithmic Improvement Examples:
  - "A high-order WENO-limited finite-volume algorithm for atmospheric flow using the ADER-differential transform time discretization" https://rmets.onlinelibrary.wiley.com/doi/full/10.1002/qj.3989
  - "A Holistic Algorithmic Approach to Improving Accuracy, Robustness, and Computational Efficiency for Atmospheric Dynamics" https://epubs.siam.org/doi/abs/10.1137/19M128435X

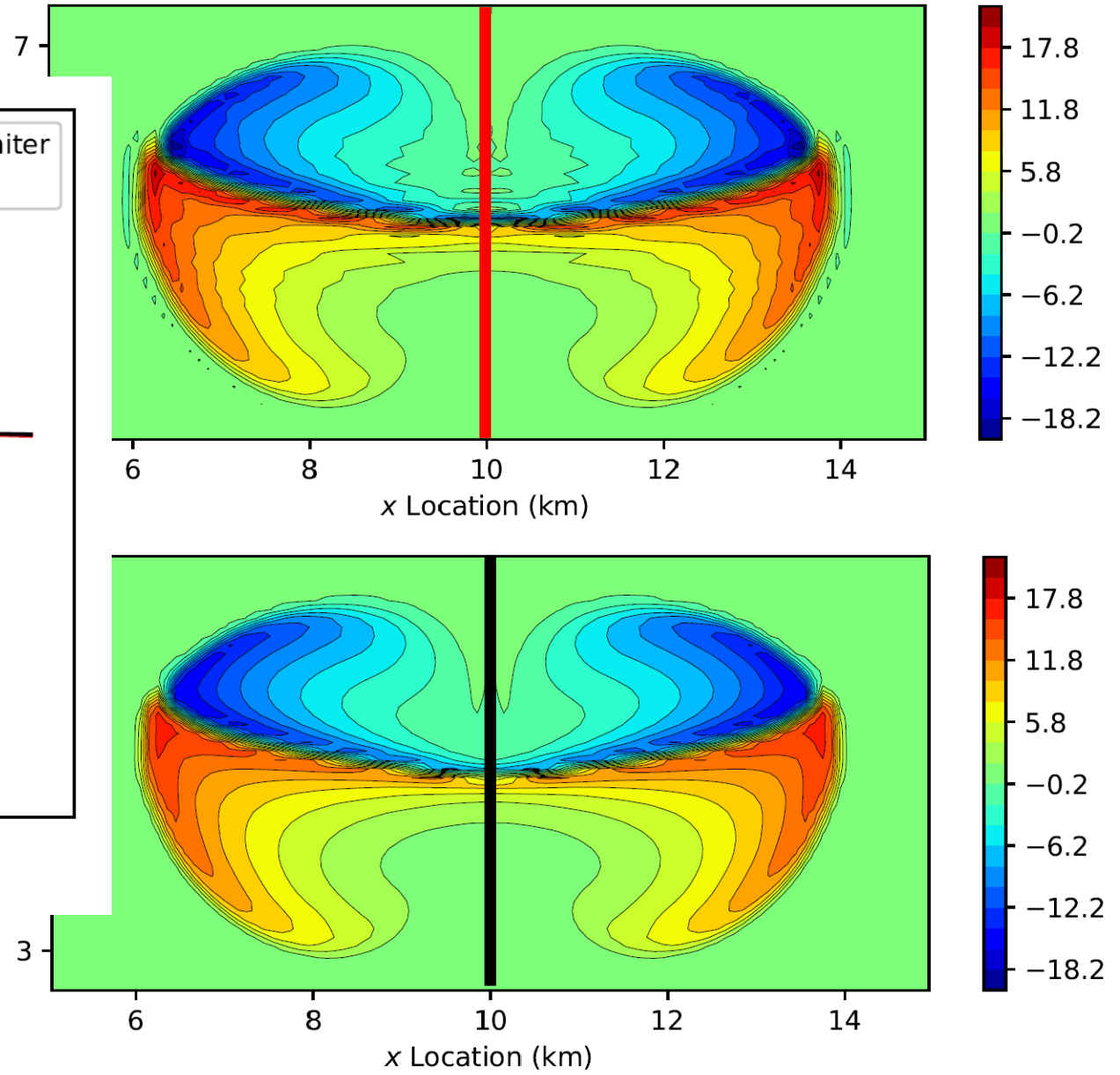
Algorithmic Advances for GPU Hardware: High-Order

- Splitting supercell test case
  - Cartesian grid
  - High CAPE, initial thermal
  - Splits into two cells
  - Doesn't use added viscosity from test case
- AWFL + P3 microphysics
- 20 second physics time step
  - Dycore sub-cycled
- 5km vertical velocity after 2 hrs plotted on right



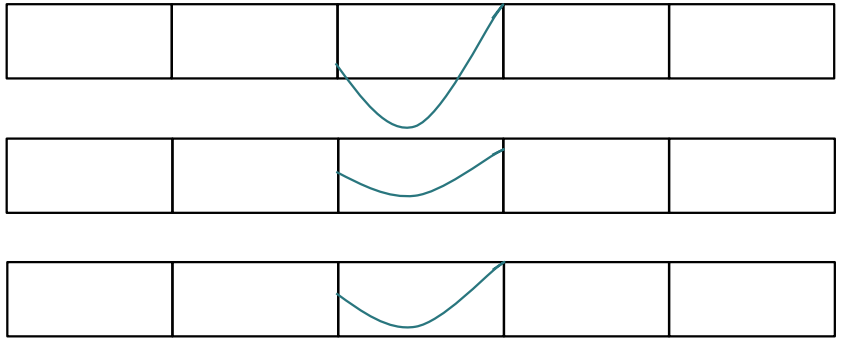
Algorithmic Advances for GPU Hardware: WENO Limiting





New Algorithm Increases Arithmetic Intensity

- Reconstruct variation from stencil
- Apply WENO limiting
- Compute high-order ADER time-average



- Compute upwind fluxes

- Update the cell average from fluxes

- Vast majority of computations use only a small stencil of data from DRAM
  - Significant compute intensity
  - Time stepping happens in the same loop as reconstruction / limiting

- Most expensive kernels: 80% peak flop/s on V100; "Quite good" on MI-60
- Currently working on MI-100 results

Further Resources & Questions

- YAKL Documentation: https://github.com/mrnorman/YAKL
- miniWeather parallel programming training app: https://github.com/mrnorman/miniWeather
- Readable C++: https://tinyurl.com/readable-cplusplus
- C++ Portability for Directives Folks: https://tinyurl.com/cplusplus-portability
- Other (more functional) C++ Portability Frameworks:
  - Kokkos: https://github.com/kokkos/kokkos/
  - RAJA: https://github.com/LLNL/RAJA
    - UMPIRE: https://github.com/LLNL/Umpire
  - SYCL: https://github.com/KhronosGroup/SYCL-Docs

Challenges with Portable C++

- Vectorization
  - C++ has less information than Fortran
  - C++ pointers need "restrict" keyword to allow the compiler to optimize more
- Staying away from non-portable C++ features
  - Most of the standard template library ("std::") is either invalid or non-portable for GPUs
  - Virtual functions in class inheritance is difficult on GPUs
- Unified shared memory helps with "std::" , **but**…
  - Unified memory often performs poorly
  - Unified memory isn't portable to all compilers and hardware
- C++ Lambdas behave strangely
  - They only "capture" needed data automatically if it's in the local scope
  - Global scope and class data are **not** captured automatically (more on this later)
- Portable C++ requires a rewrite of Fortran
  - However, YAKL significantly reduces this burden by allowing Fortran-like behavior

YAKL Scalar Live-Out

- Scalars written to in a device kernel and read from outside the kernel
  - Scalars are normally thread-private; here they must be allocated on the device
  - "Scalar Live-Out" is most common in error-checking routines

YAKL Scalar Live-Out

Fortran

```
logical :: data_is_bad
data_is_bad = .false.
!$acc parallel for collapse(3) copy(data_is_bad) async(id)
do k = 1 , nz
  do j = 1 , ny
    do i = 1 , nz
      if (density(i,j,k) <= 0) data_is_bad = .true.
    enddo
  enddo
enddo
!$acc wait(id)
if (data_is_bad) then
  ...
```

C++ Portability

```
ScalarLiveOut<bool> data_is_bad(false);
parallel_for( Bounds<3>(nz,ny,nx) , YAKL_LAMBDA (int k, int j, int i) {
  if (density(i,j,k) <= 0) data_is_bad = .true.
});
if (data_is_bad.hostRead()) { ...
```

YAKL Pool Allocator (Gator)

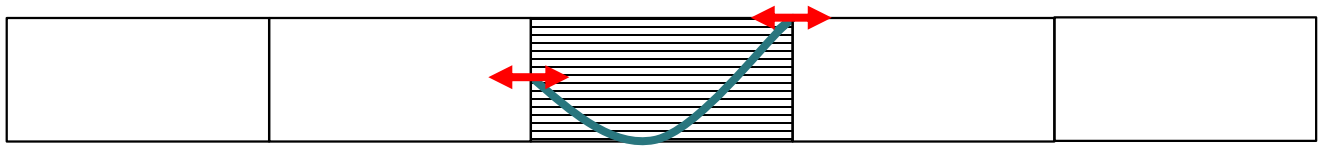
- The YAKL "pool alligator" (speech-to-text error)
- Allows cheap frequent allocations & free's
  - Optimized for "stack-like" allocation patterns
  - Most Fortran apps allocate in a stack-like fashion
  - Little to no segmentation and wasted memory
  - Does not behave well for random allocation patterns
- Fortran hooks for up to 7-D arrays
- Allows CUDA & HIP Managed Memory
  - Automatic hooks into OpenACC and OpenMP runtimes so data is handled by CUDA & HIP
- Controlled by environment variables

Readability

- Able to find the code
  - Need a **very** good reason for > 1 level of abstraction
  - Some code duplication is OK, it's a balance
  - Loops should live together, one after the other
- Comfortable syntax
  - The syntax should be familiar, Fortran-like, and clear
  - No "figuring out" what the code is doing (nothing "clever" or any such adjective)
  - Hide metaprogramming, SFINAE, complex template expressions from the user
  - Developer profanity should be minimized
- Looping should be clear
  - Typically no need for C++ iterators
- Data structures should be clear (Multi-dimensional Arrays)

Upwind Finite-Volume Spatial Discretization

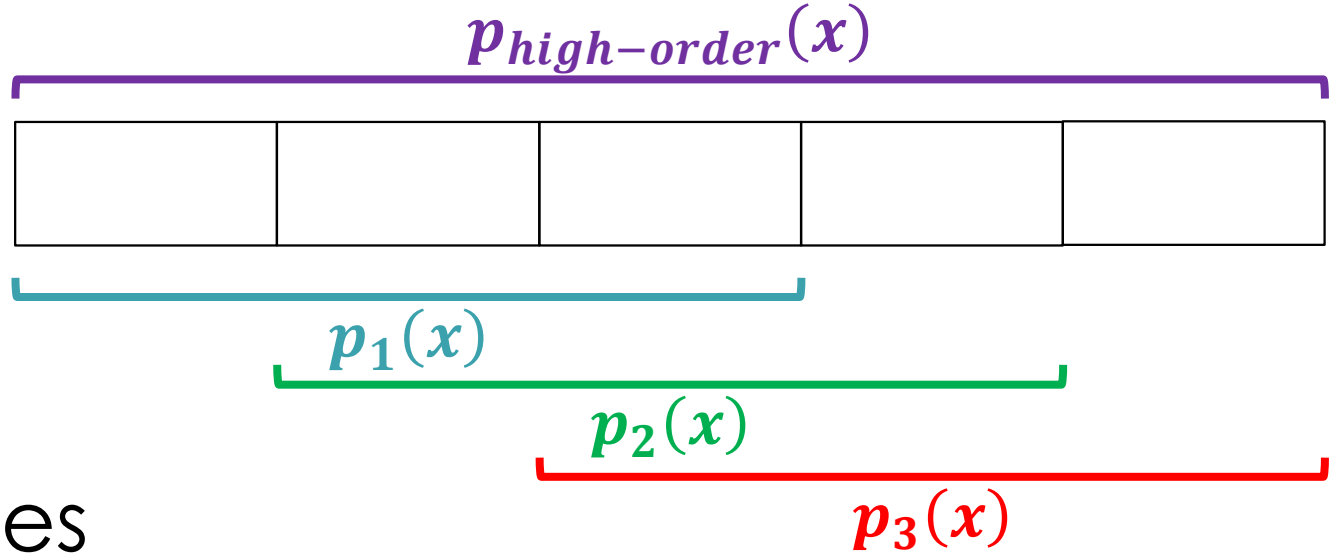
- Finite-Volume Algorithm
  - Solution is a set of non-overlapping cell averages
  - Cell average updates based on cell-edge fluxes
  - Use upwind Riemann solver to determine fluxes
  - Reconstruct intra-cell variation from surrounding "stencil" of cells



- Advantages
  - Conserves variables to machine precision
  - Large time step
  - Treats each Degree Of Freedom individually (accuracy)
  - Unconditionally stable for Euler eqns without added dissipation

Weighted Essentially Non-Oscillatory Limiting (WENO)

- WENO Algorithm
  - Compute multiple polynomials using multiple stencils
  - **Weight the most oscillatory polynomials the lowest**
  - Custom low-dissipation implementation



- Advantages
  - **Requires no additional data** when used with Finite-Volume
  - Very accurate and effective at limiting oscillations

Other Advantages of Portable C++

- Debugging
  - Fortran array metadata can change in routine interfaces (# of dimensions & sizes)
    - Thus, Fortran index checking can never fully be trusted
  - C++ Array class metadata is tied to the Array object and never changes
    - C++ index checking is far more reliable because of this
  - C++ exception throwing makes stack tracing more direct as well (e.g., in gdb)
- C++ compilers inline much better than Fortran compilers typically do
  - Rarely any need for an equivalent of "!$acc routine" or "!$omp declare target"
  - "!$acc routine" and OpenMP equivalent are typically quite buggy
- Simple C++ templating can significantly reduce code duplication
  - No more complex Fortran interface blocks for multiple data types

YAKL Fortran-Like Multi-Dimensional Arrays

- Use C++ “typedef” and “using” in a header to hide unsightly C++ namespace and template expressions

```
typedef yakl::Array<float,1,yakl::memDevice,yakl::styleFortran> real1d;
typedef yakl::Array<float,2,yakl::memDevice,yakl::styleFortran> real2d;
...
using yakl::fortran::parallel_for;
using yakl::fortran::Bounds;
```

YAKL Atomic

- Compute a column average:

Fortran

```
function col_average(var) rslt(avg)
  real, intent(in) :: var(:,:,:)
  real             :: avg(:)
  real tmp, factor
  factor = 1./(nx*ny)
  !$acc parallel loop
  do k = 1 , size(var,3)
    avg(k) = 0
  enddo
  !$acc parallel loop collapse(3)
  do k = 1 , size(var,3)
    do j = 1 , size(var,2)
      do i = 1 , size(var,1)
        tmp = var(i,j,k) / factor
        !$acc atomic update
        avg(k) = avg(k) + tmp
      enddo
    enddo
  enddo
end function max_stable_dt
```

C++ Portability

```
real1d col_average(real3d const &var) {
  real factor = 1./(nx*ny);
  real1d avg("avg",size(var,3));
  memset( avg , 0. );
  parallel_for( Bounds<3> (size(var,3),size(var,2),size(var,1)) ,
                YAKL_LAMBDA (int k, int j, int i) {
    // avg(k) = avg(k) + var(i,j,k) / factor
    yakl::atomicAdd( avg(k) , var(i,j,k) / factor );
  });
  return avg;
}
```