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Porting the RTE+RRTMGP radiative transfer package for next-generation supercomputers

EXASCALE COMPUTING PROJECT

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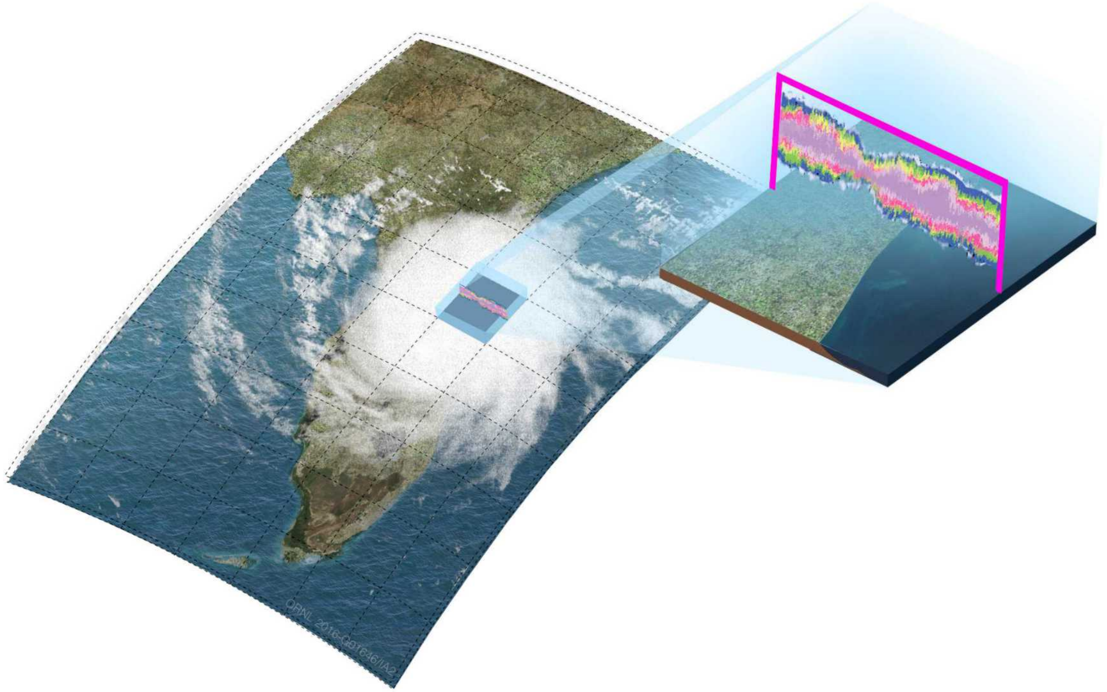
Two paths toward a DOE global cloud-permitting model

- Simple Cloud-Resolving E3SM Atmosphere Model (SCREAM)
  - Rewrite our existing atmosphere in C++/kokkos for *performance portable* GPU support with simplified physics
  - Scale up to 3km resolution
  - Target simulations in 2021
- E3SM using the Multi-scale Modeling Framework (E3SM-MMF)
  - Multiscale modeling approach, “superparameterization”
  - Cloud resolving convection
  - Very high computational intensity – ideal for GPUs
  - Fortran with OpenACC for GPU support



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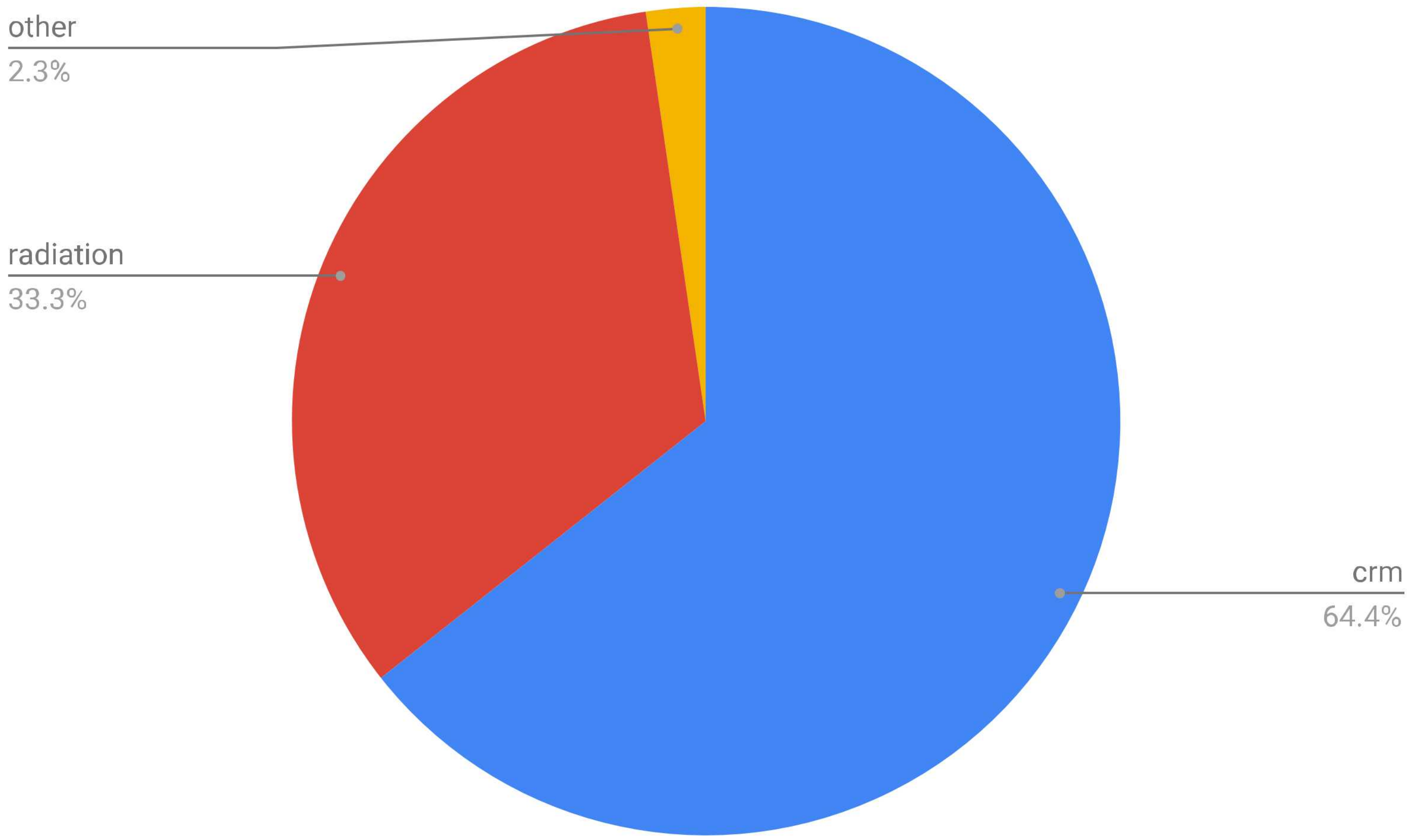
E3SM-MMF Highlights

- Complete port of the CRM superparameterization to GPUs
  - refactored 30K lines of code to enable openACC acceleration
  - represents about 50% of the cost of the model
  - Port of remaining 40% (RRTMGP package) recently completed
- Summit Early Science Simulation
  - 1024 Summit nodes, running at 0.62 SYPD
  - 6 year simulation, 300K node-hours
  - Running a weather resolving global model (25km) with a cloud resolving 2D CRM (1km superparameterization)
- Gordon Bell Submission SC2019
  - 4600 Summit nodes, ~5.4PF
  - 1.8 SYPD with 2km resolution
  - 0.22 SYPD at 500m resolution

Radiative transfer cost

- Radiative transfer is expensive: ~1/3 the cost of the atmospheric physics
- CRM has already been ported to GPU on Summit: ~15x speed-up
- This talk: efforts to port the radiative transfer package to GPU

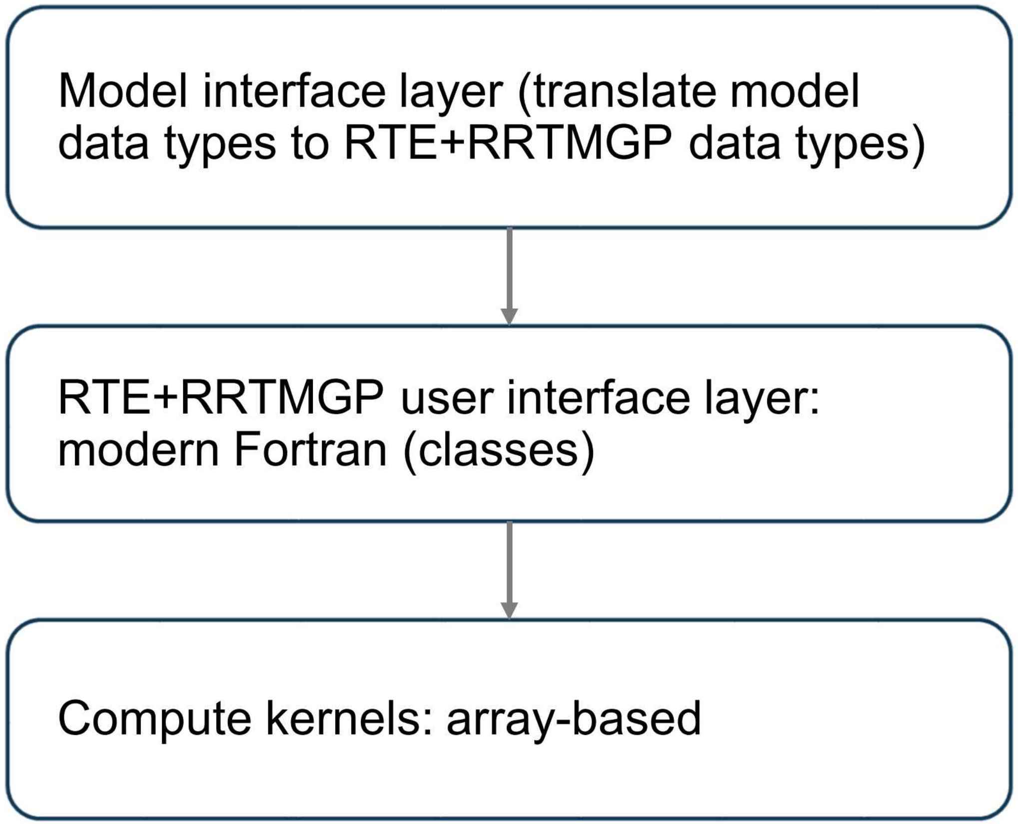


Relative cost of physics packages on Intel Sandy Bridge

Radiative transfer package: RTE+RRTMGP

- Rewrite of popular RRTMG radiation package
- Expose parallelism
- Modern software practices

Implementation: levels of abstraction



Goal: port *kernels* for performance portability, leaving *interface* largely untouched

Porting RTE+RRTMGP using OpenACC

- Goal: RTE+RRTMGP fully running on Summit GPU
- Steps:
  - Expose parallelism
  - Wrap with OpenACC directives *without* explicit data management
  - Compile with ptxinfo flag to highlight generation of implicit data copying code
  - Add explicit data management to directives

Porting: example

Tightly-nested loops (expose parallelism)

```fortran
!$acc parallel loop gang vector collapse(2)
do ilev = 1, nlev
  do icol = 1, ncol
    broadband_flux_net(icol,ilev) = 0
  end do
end do

!$acc parallel loop gang vector collapse(3)
do ilev = 1, nlev
  do icol = 1, ncol
    do igpt = 1, ngpt
      tmp = spectral_flux_dn(icol, ilev, igpt) - spectral_flux_up(icol, ilev, igpt)
      !$acc atomic update
      broadband_flux_net(icol,ilev) = broadband_flux_net(icol,ilev) + tmp
    end do
  end do
end do
```

```fortran
+ !$acc enter data copyin(spectral_flux_dn, spectral_flux_up) create(broadband_flux_net)
+
  !$acc parallel loop gang vector collapse(2)
  do ilev = 1, nlev
    do icol = 1, ncol
      broadband_flux_net(icol,ilev) = 0
    end do
  end do

  !$acc parallel loop gang vector collapse(3)
  do ilev = 1, nlev
    do icol = 1, ncol
      do igpt = 1, ngpt
        tmp = spectral_flux_dn(icol, ilev, igpt) - spectral_flux_up(icol, ilev, igpt)
        !$acc atomic update
        broadband_flux_net(icol,ilev) = broadband_flux_net(icol,ilev) + tmp
      end do
    end do
  end do
+
+ !$acc exit data copyout(broadband_flux_net) delete(spectral_flux_dn, spectral_flux_up)
+
```

Structured data statements keep data on the device

Testing

- How do we know we have the right answer (and didn't screw anything up)?
- Need to test after each code addition!
  - Rapid, easy to launch regression tests
- Testing framework based on RTE+RRTMGP RFMIP example code (provided in RTE+RRTMGP Git repo)
  - End-to-end, stand-alone test
  - Code: reads in example atmosphere data, computes radiative fluxes due to gaseous absorption
  - Test: compare outputs from a test run with outputs from a baseline (before the code modification)
  - Challenge: answers are *not* bit-for-bit due to floating point differences arising from atomic updates on the GPU (cannot guarantee order of updates)

Testing: example

Diffs between CPU and reference:

```
Variable rlu: No diffs
Variable rld differs (max abs difference: 3.814697e-06; max frac. difference: 1.178709e-05%)
Variable rsu differs (max abs difference: 3.051758e-05; max frac. difference: 1.185221e-05%)
Variable rsd differs (max abs difference: 6.103516e-05; max frac. difference: 1.087066e-05%)
```

Diffs between GPU and reference:

```
Variable rlu: No diffs
Variable rld differs (max abs difference: 1.490116e-08; max frac. difference: 1.173428e-05%)
Variable rsu differs (max abs difference: 3.051758e-05; max frac. difference: 1.184619e-05%)
Variable rsd differs (max abs difference: 6.103516e-05; max frac. difference: 1.087066e-05%)
```

Diffs between CPU and GPU:

```
Variable rlu: No diffs
Variable rld differs (max abs difference: 3.814697e-06; max frac. difference: 1.178709e-05%)
Variable rsu differs (max abs difference: 3.051758e-05; max frac. difference: 1.185221e-05%)
Variable rsd differs (max abs difference: 3.051758e-05; max frac. difference: 9.782132e-06%)
```

Subjectively, differences order 1e-5 are "tolerable"

When things go bad…

```
call zero_array(block_size, def_tsi)
!$acc parallel loop collapse(2) copy(def_tsi) copyin(toa_flux)
do igpt = 1, ngpt
  do icol = 1, block_size
    !$acc atomic update
    def_tsi(icol) = def_tsi(icol) + toa_flux(icol, igpt)
  end do
end do
```

```
call zero_array(block_size, def_tsi)
!$acc parallel loop collapse(2) copy(def_tsi) copyin(toa_flux)
do igpt = 1, ngpt
  do icol = 1, block_size
    !!$acc atomic update
    def_tsi(icol) = def_tsi(icol) + toa_flux(icol, igpt)
  end do
end do
```

Missing atomic update in reduction operation leads to wrong answers!

```
Variable rlu: No diffs
Variable rld differs (max abs difference: 1.490116e-08; max frac. difference: 1.173428e-05%)
Variable rsu differs (max abs difference: 4.540662e+06; max frac. difference: 1.999758e+02%)
Variable rsd differs (max abs difference: 2.117698e+07; max frac. difference: 1.999758e+02%)
```

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Debugging tools

- Cuda-memcheck
- Valgrind (on CPU)
- Bounds checking (on CPU)
- Simplifying data movement

Profiling tools

- PGI_ACC_TIME=1: quick timing info for compute vs data movement

```
/autofs/nccs-svm1_home1/brhillman/codes/rte-rrtmgp/branches/master/build/../rte/kernels-openacc/mo_rte_solver_kernels.F90
  lw_source_noscat  NVIDIA  devicenum=0
    time(us): 10,078
    495: compute region reached 1 time
        495: kernel launched 1 time
            grid: [65535]  block: [128]
             device time(us): total=10,078 max=10,078 min=10,078 avg=10,078
            elapsed time(us): total=10,113 max=10,113 min=10,113 avg=10,113
    495: data region reached 2 times
```

- NVPROF: visual representation of profiling data
  - Run code on compute node, save nvprof output
  - View using nvvp
  - Useful for identifying bottlenecks and excessive data movement

PGI_ACC_TIME=1 example

```
/autofs/nccs-svm1_home1/brhillman/codes/rte-rrtmgp/branches/master/examples/rfmip-clear-sky/rrtmgp_rfmip_lw.F90
  rrtmgp_rfmip_lw  NVIDIA  devicenum=0
    time(us): 131
    228: data region reached 1 time
        228: data copyin transfers: 1
             device time(us): total=20 max=20 min=20 avg=20
    229: data region reached 1 time
        229: data copyin transfers: 1
             device time(us): total=13 max=13 min=13 avg=13
    230: data region reached 1 time
        230: data copyin transfers: 4
             device time(us): total=32 max=8 min=8 avg=8
    253: compute region reached 1 time
        253: kernel launched 1 time
            grid: [225]  block: [128]
             device time(us): total=14 max=14 min=14 avg=14
            elapsed time(us): total=159 max=159 min=159 avg=159
    253: data region reached 4 times
        253: data copyin transfers: 1
             device time(us): total=9 max=9 min=9 avg=9
    301: data region reached 1 time
    302: data region reached 1 time
        302: data copyin transfers: 1
             device time(us): total=11 max=11 min=11 avg=11
    303: data region reached 1 time
        303: data copyin transfers: 4
             device time(us): total=32 max=8 min=8 avg=8
    304: data region reached 1 time
```

This is a high-level routine doing a lot of data movement

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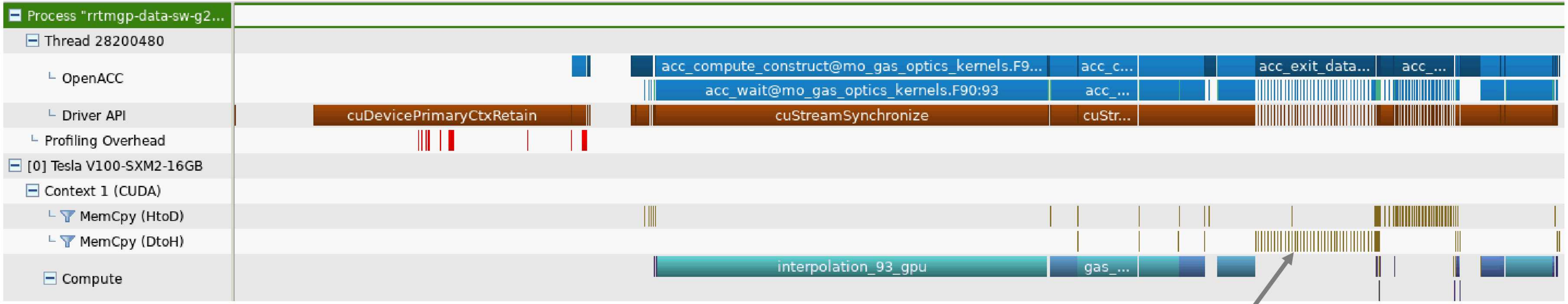
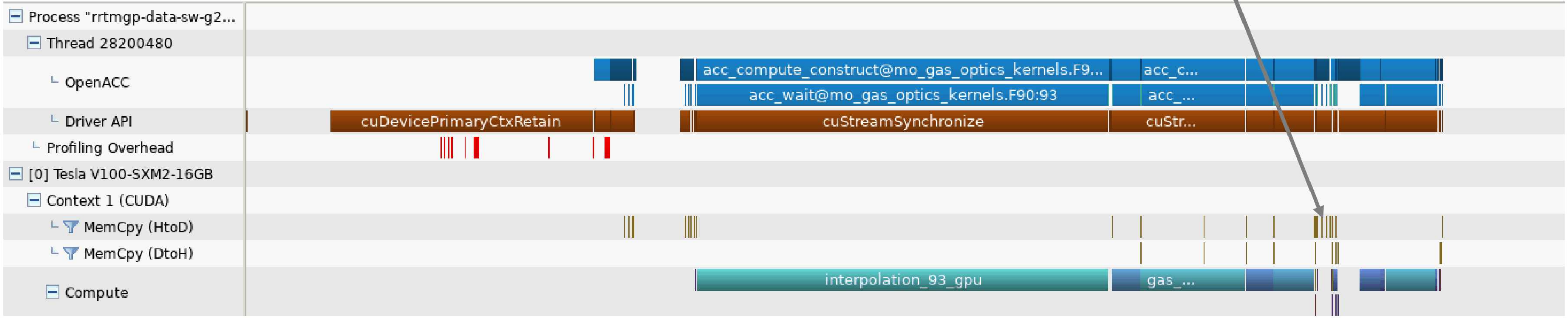
NVPROF example



After explicit data movement: much less device to host transfers



Future directions: transition to OpenMP Offload, and managed memory

- For enhanced portability, we are creating an OpenMP 4.5+ version of the code
  - OpenMP 4.5+ includes a kernel offload for accelerators
  - OpenMP4.5 and OpenACC have a nearly 1:1 correspondence
    - !$acc copyin() --> !$omp map(to:)
    - !$acc update host() --> !$omp target update(from:)
    - !$acc parallel loop --> !$omp target teams distribute parallel for
  - Deep copy issues get a little more hairy, but we plan to sidestep that
- We plan to use managed memory
  - Automatically pages data to/from GPU (no more data statements!)
  - -ta=nvidia,managed for PGI for now (currently there are bugs, though)
  - We will replace "allocate()" with custom cudaMallocManaged() routine using the LLNL Umpire pool allocator

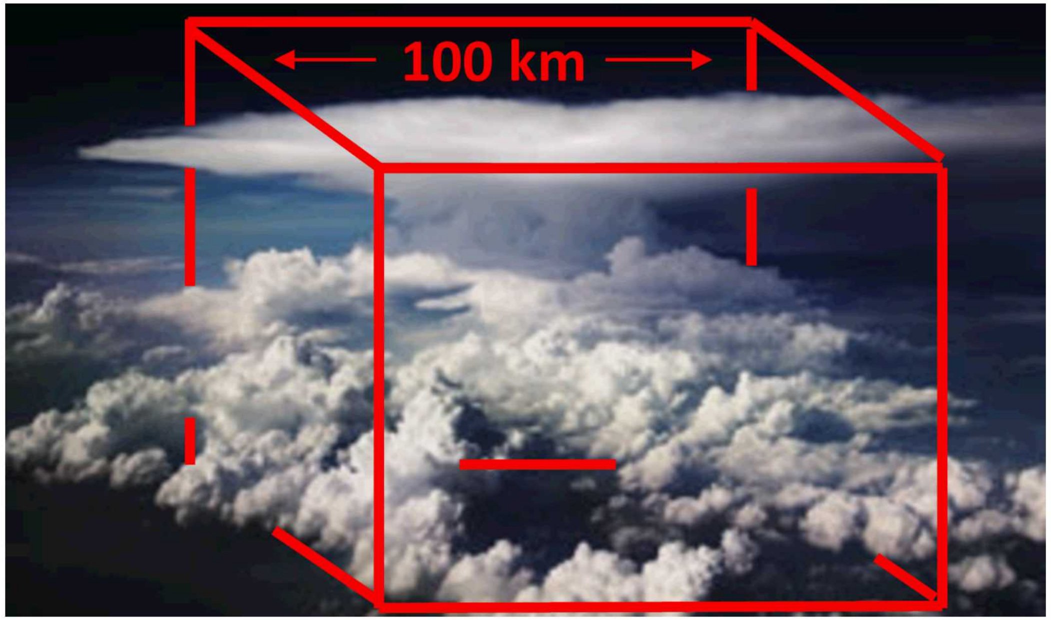
Summary and challenges

- RTE+RRTMGP radiative transfer code ported to GPU using OpenACC directives
- The need to minimize data movement between device and host requires adding directives pretty high up in the code – impossible to confine to kernels
- A number of compiler bug work-arounds needed
- Next step: evaluating performance in the full model

Extra slides

Context: Developing a cloud-permitting climate model for DOE exascale achitectures

- Cloud-resolving simulations (with $\Delta x < 3$ km) avoid the need for convection parameterizations, which are the main source of climate change uncertainty (Sherwood et al., Nature 2014)
- Resolved convection will substantially reduce major systematic errors in precipitation because of its more realistic and explicit treatment of convective storms.
- Improve our ability to assess regional impacts of climate change on the water cycle that directly affect multiple sectors of the US and global economies, especially agriculture and energy production.



How do we parameterize this sub-grid variability?

Radiative transfer package: RTE+RRTMGP

- Separation of concerns

RRTMGP
- Optical properties
- Source functions
- Spectral discretization: correlated k-distribution

RTE: solvers
- One-dimensional plane-parallel RT equations
- Absorption/emission or two-stream
- Adding for transport
- Extensible to multi-stream methods