Use case: Optimizing the Weather Research and Forecasting Model (WRF) with OpenMP Offload and Codee

NERSC Codee Training, September 6, 2024

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The Weather Research & Forecasting Model

- An atmospheric model written in Fortran written in the 1990's by a number of organizations such as the National Center for Atmospheric Research (NCAR) and the National Centers for Environmental Prediction (NCEP)
- Solves the 3D Euler equations using finite differences and explicit timestepping
- Used in both research and operational, real-time forecasting worldwide
- NERSC development branch: https://github.com/NERSC/WRF

Optimization goals

- Current parallelism: domain decomposition (MPI) into patches (`ims:ime, kms:kme, jms:jme`) and shared memory (OpenMP) among tiles (`its:ite, kts:kte, jts:jte`)
- MPI + GPU approach: offloading work from each patch to a GPU
- Programming workflow
  - Profilers (gprof, perftools, Nsight)
  - Static code inspection (Codee)

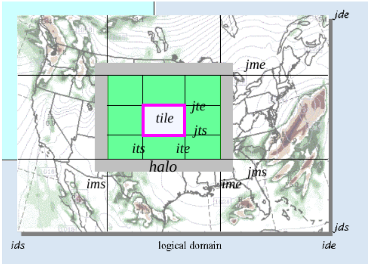


Figure 1: WRF decomposition layer. Image from Dudhia, J. "WRF Modeling System Overview".

Fast Spectral-Bin Microphysics (FSBM)

- Particle size spectrum divided into 33 intervals (bins)
- Computations required for each particle type and size at each grid point
- Require small timesteps (5-10 s)
- Universal; can be used for different atmospheric phenomena
- Current version in WRF: FSBM-2 (Shpund et al., 2019)

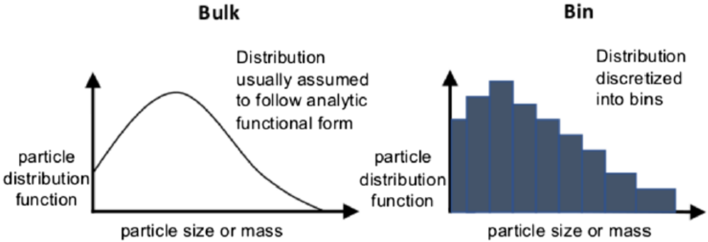
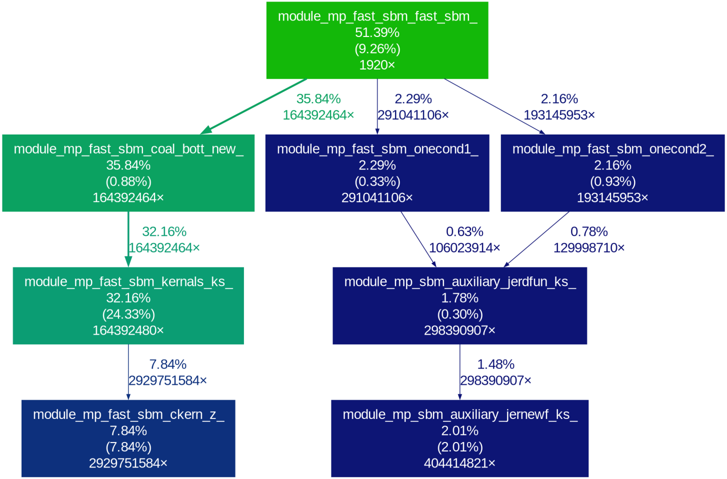


Figure 2: Image from Morrison et al., 2020.

Test case setup on Perlmutter

- Conus-12km test case
  - 425 x 300 x 50 grid
  - One-day restart
  - Time step: 5s
- Compilers: PrgEnv-nvidia/8.5.0 (NVHPC 23.9)
  - nvfortran, nvc, nvc++
  - Good GPU support for OpenMP, OpenACC, CUDA
  - GPU flags: `-mp=gpu -target-accel=nvidia80`
- WRF configure option: 4 (dm+sm) PGI (pgf90/gcc)

Finding time-consuming routines with Gprof



Inside the FSBM routine

- Subroutine Fast_SBM() in phys/module_mp_fast_sbm.F coal_bott_new()

```fortran
    do j = jts:jte
      do k = kts:kte
        do i = its:ite
          ! Collision-Coalescence process
          call COAL_BOTT_NEW(...)

          ! do stuff
        enddo
      enddo
    enddo


```

OpenMP GPU offloading

- A set of directives for C and Fortran that let the compiler generate GPU code
- Can manage parallelism and data transfer like CUDA API
- Directive-based: more portable and easier to port existing code to GPU, but less control

```
#pragma omp target teams
distribute parallel for
num_teams(3)
for (int i = 0; i < 12; ++i)
{
    C[i] = A[i] + B[i];
}
```

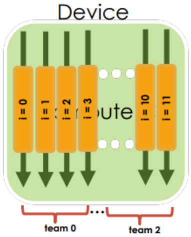


Figure 3: Image from https://www.olcf.ornl.gov/wp-content/uploads/2021/08/ITOpenMP_Day1.pdf

Inside the FSBM routine

- Subroutine `Fast_SBM()` in `phys/module_mp_fast_sbm.F`
- Parallelization granularity: number of grid points, assuming no race conditions inside `coal_bott_new()`

```fortran
do j = jts:jte
  do k = kts:kte
    do i = its:ite
      ! Collision-Coalesence process
      call COAL_BOTT_NEW(...)

      ! do stuff
    enddo
  enddo
enddo
```

Inside the Kernals_KS subroutine

- Global collision tables, e.g. cwlg,cwls are being modified at each grid point (i,k,j)

```
do n = 1,33
  do m = 1,33
    ckern_1 = ...
    ckern_2 = ...
    ! water - graupel
    cwlg(m,n) = (ckern_2 + (ckern1-ckern_2* ..)) * ...

    ckern_1 = ...
    ckern_2 = ...
    ! water - snow
    cwls(m,n) = (ckern_2 + (ckern1-ckern_2* ..)) * ...

    ! 18 more arrays

  enddo
enddo

```

Setting up Codee for WRF

```
# Capture compilation flags in JSON file
bear -- ./compile -j 8 wrf

# Initial screening report
codee screening --config compile_commands.json

# Checks report
codee checks --config compile_commands.json

# Example: in-place OpenMP offload insertion
codee rewrite --offload omp --in-place \
  module_mp_fast_sbm.f90:6293:4 \
  --config compile_commands.json
```

Codee analysis of Kernals_KS

- Codee implies there are no loop-carried dependencies, so the individual entries can be computed independently

```fortran
! Codee: Loop modified
!$omp target teams distribute parallel do &
!$omp private(n) map(from: cwlg, cwls, ...) ...
do n = 1,33
  ! Codee: Loop modified
  !$omp simd
  do m = 1,33
    ckern_1 = ...
    ckern_2 = ...
    cwlg(m,n) = (ckern_2 + (ckern1-ckern_2* ..)) * ...

    ckern_1 = ...
    ckern_2 = ...
    cwls(m,n) = (ckern_2 + (ckern1-ckern_2* ..)) * ...

    ! 18 more arrays
  enddo
enddo
```

Removing the global arrays

- Replace looking up m, n entry with computing as needed

```
    pure real function get_cwlg(..., m, n)
    pure real function get_cwls(..., m, n)

```

- No more shared arrays between grid points
- Speedup: around 1.4x
  - A lot of collision types are not used in FSBM
  - Not every entry m,n are used

Offloading the main loop

- Each grid point can now be assigned to a thread
- Further memory optimization allows a full collapse(3)

```
!$omp target teams distribute parallel do collapse(3)
do j = jts:jte
  do k = kts:kte
    do i = its:ite
      ! Collision - Coalescence
      call COAL_BOTT_NEW(...)

      ! do stuff
    enddo
  enddo
enddo
```

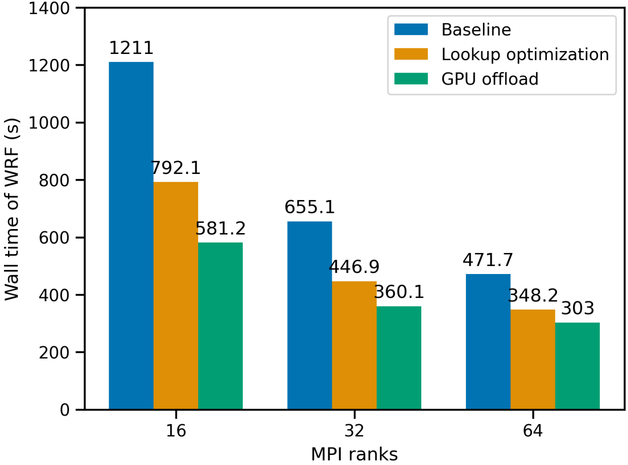
Speedup results

- 10-minute runs
- 1 OpenMP thread per MPI rank
- 1 GPU per MPI rank

Routine	Total speedup
coal_bott_new loop	66.6x
fast_sbm	2.99x
Overall	2.20x

Strong scaling

- No. of GPUs is fixed to 16, and no. of MPI ranks is varied from 16 to 64



Summary

- Accelerated a big part of the FSBM routine to GPUs through loop restructuring and OpenMP device offload
  - Codee's dependency analysis functionality exposed independence between computations among different grid points
- Achived an overall speedup of 2.2x for the 1 GPU per rank case for the CONUS-12km case
- A combination of runtime profiling and static code analysis is a very helpful aid in optimization efforts, especially for those not fully familiar with the context of the code

QUESTIONS