OAK RIDGE National Laboratory

OpenMP Offloading Code on Frontier : Hands on

Wael R. Elwasif, Reuben Budiardja,
Swaroop Pophale

Oak Ridge Leadership Computing Facility
Oak Ridge National Laboratory

Frontier Compilers : Summary Table

Programming Environment	Compilers C	C++	Fortran	Compiler Modules	OpenMP Flags	Offloading Support
PrgEnv-cray	cc *(craycc*	CC *craycxx*	ftn *crayftn)*	cce craype-accel-amd-gfx90a rocm	-fopenmp	Yes
PrgEnv-amd	cc *(amdclang*	CC *amdclang++*	ftn *amdflang)*	amd rocm	-fopenmp	Yes
PrgEnv-gnu	cc *(gcc*	CC *g++*	ftn *gfortran)*	gcc	-fopenmp	**No**

- craycc and craycxx are based on the LLVM clang compiler suite
- *crayftn front end **NOT** based on LLVM/ backend LLVM based*
- *craycc/craycxx/crayftn backend uses proprietary Cray/HPE code.*
- amdclang and amdclang++ are based on the LLVM clang compiler
- amdflang is based on the "old" flang compiler, ***not advisable for use in production***
- *MI250X offloading support for GCC under development, performance ??*

GPU PARALLELISM MAPPING POLICIES : **CCE**

Curtsey : Jeff Sandoval, HPE

NVIDIA	AMD	CCE Fortran OpenACC	Old CCE 15 Fortran OpenMP	Old CCE 15 C/C++ OpenMP	New CCE 16 OpenMP
Threadblock	Work group	`acc gang`	`omp teams`	`omp teams`	`omp teams`
Warp	Wavefront	`acc worker`	`omp parallel`	`omp parallel`	`omp parallel`
Thread	Work item	`acc vector`	`omp simd`	`omp simd`	`omp simd`

- New/improved "omp parallel" support in CCE 16
  - More consistent across C/C++/Fortran within CCE
  - More consistent with upstream Clang and other vendor implementations
- Current best practice:
  - Use "omp teams" to express GPU threadblock/work group parallelism
  - Use "omp parallel do/for simd" to express GPU thread/work item parallelism
- Future possibilities:
  - Improve CCE performance for "omp loop"
  - Leverage multi-dimensional grids or blocks
  - Support three levels of parallelism in OpenMP

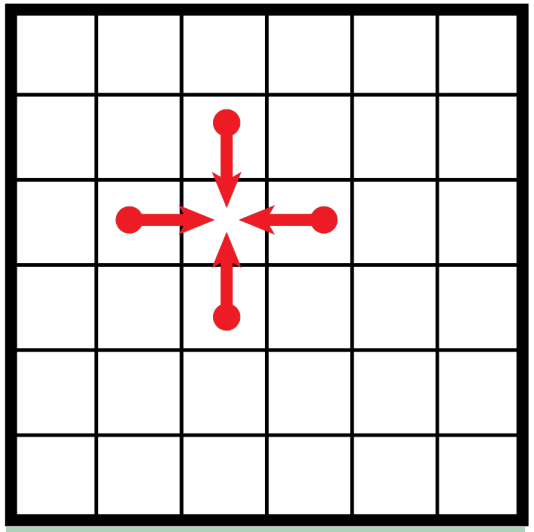
Goal: let users express parallelism with any construct they think makes sense, and CCE will map to available hardware parallelism

Compilers & Modules on Frontier

- `module reset`
- CCE (15.0.0) (default)
  - `module load PrgEnv-cray rocm craype-accel-amd-gfx90a`
    `[module load **cpe/22.12**]  #-- Only needed if going back from CCE/16.0.1 below`
- CCE 16.0.1
  - `module load PrgEnv-cray rocm craype-accel-amd-gfx90`
    `module load **cpe/23.09**  #-- this automatically loads cce/16.0.1`
- ROCm
  - `module load PrgEnv-amd amd`
- GCC (Experimental offloading)
  - `module use /sw/crusher/ums/compilers/modulefiles`
    `module load  module load gcc/13.2.1-dev-latests`

Tutorial Code

- Repo : https://github.com/olcf/openmp-offload.git
- Simple Jacobi iterations with random initial conditions
  - C & Fortran versions of each variant
- Makefiles for the different compilers available
  - Pass **COMPILER=XYZ** flag to control which compiler to use
  - Make sure the right modules are loaded for each compiler
- Example: Compile using CCE



Simple 2D Jacobi Iteration

```
[elwasif@login07.frontier openmp-offload]$ module load PrgEnv-cray cce rocm craype-accel-amd-gfx90a
[elwasif@login07.frontier openmp-offload]$ cd C/0-serial/
[elwasif@login07.frontier 0-serial]$ make COMPILER=cce
Make sure the following modules are loaded: PrgEnv-cray cce craype-accel-amd-gfx90a
cc -Ofast -fopenmp  -lm jacobi.c -o jacobi.C.cce.exe
```

- Command line arguments : `num_cells max_iterations`
  - Except for code in **5-openmp-gpu-implicit/**

Jacobi iterations : Initialization

- Random seed generated and saved
- Regenerate the same problem for validation, or for runs using different configurations

```
void init(double* T){

  static int first_time = 1;
  static int seed = 0;
  if (first_time == 1) {
    seed = time(0);
    first_time = 0;
  }
  srand(seed);

  for (unsigned i = 0; i <= n_cells + 1; i++) {
    for (unsigned j = 0; j <= n_cells + 1; j++) {
      T(i, j) = (double)rand() / (double)RAND_MAX;
    }
  }
}
```

Jacobi iterations : Serial version

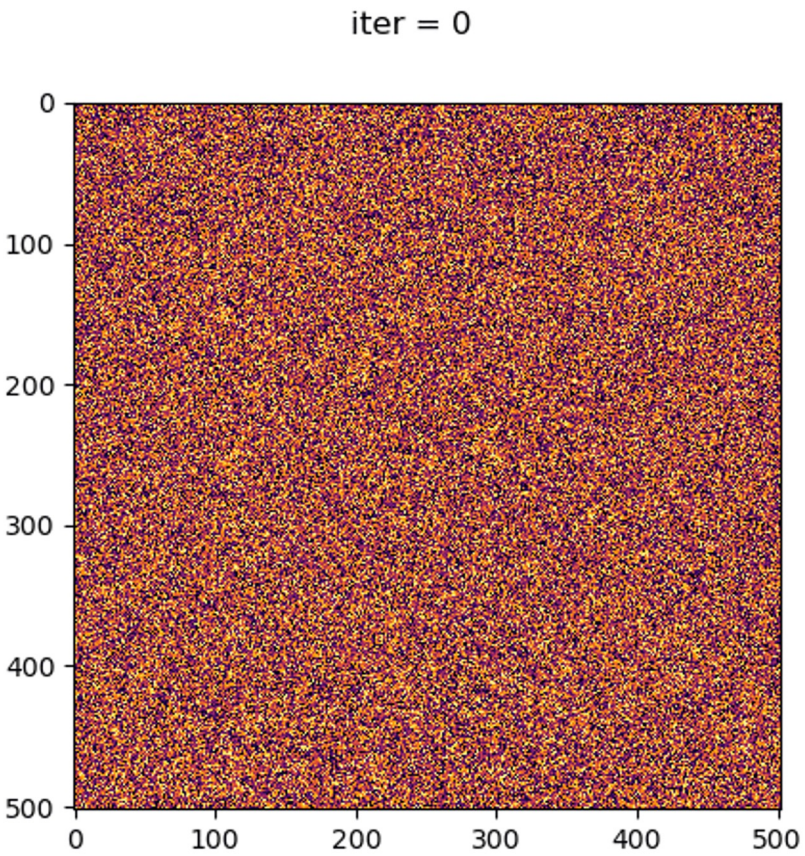
```
// simulation iterations
 while (residual > MAX_RESIDUAL && iteration <= max_iterations) {

   // main computational kernel, average over neighbors in the grid
   for (unsigned i = 1; i <= n_cells; i++)
     for (unsigned j = 1; j <= n_cells; j++)
       T_new(i, j) = 0.25 * (T(i + 1, j) + T(i - 1, j) + T(i, j + 1) + T(i, j - 1));

   // reset dt
   residual = 0.0;

   // compute the largest change and copy T_new to T
   for (unsigned int i = 1; i <= n_cells; i++) {
     for (unsigned int j = 1; j <= n_cells; j++) {
       residual = MAX(fabs(T_new(i, j) - T(i, j)), residual);
       T(i, j) = T_new(i, j);
     }
   }
   iteration++;
 }
 printf("Serial Residual = %.9lf\n", residual);
```

Jacobi iterations : Serial version

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           T_new(i, j) = 0.25 * (T(i+1, j) + T(i-1, j) + T(i, j+1) + T(i, j-1));

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     for (unsigned int i = 1; i <= n_cells; i++) {
        for (unsigned int j = 1; j <= n_cells; j++) {
            residual = MAX(fabs(T_new(i, j) - T(i, j)), residual);
            T(i, j) = T_new(i, j);
        }
     }
     iteration++;
  }
  printf("Serial Residual = %.9lf\n", residual);
```

The C/C++ & Fortran OpenMP Variants

Directory	Description	Comments
`0-serial/`	Base serial version	
`1-openmp-cpu/`	OpenMP CPU only	
`2-openmp-gpu-teams/`	GPU: Teams only	Day 1
`3-openmp-gpu-parallel/`	GPU: Teams + Threads	Day 1
`4-openmp-gpu-data/`	GPU: Manage data movement	Day 2
`5-openmp-gpu-implicit/`	GPU: Implicit data movement	Day 2 – C++
`6-openmp-combined/`	All variants	
`7-loop-combined/`	Using loop construct (amd >= 5.5.1, gcc only)	

Similar Directory Structure for Fortran code

Submitting Jobs On Frontier

- Use your own project ID
- Reservations from 11:45 – 3:30
  - **`--reservation=openmp`**
- Sample batch script for 7 CPU threads
- Template in code repo
- ***Match compile and execution modules***

```
#!/bin/bash
#SBATCH -A ABC123
#SBATCH -J omptutorial
#SBATCH -o %x-%j.out
#SBATCH -t 00:10:00
#SBATCH -p batch
#SBATCH -N 1
#SBATCH --reservation=openmp
ulimit -s unlimited # Needed for implicit mapping example

#For CCE
module load PrgEnv-cray cpe/23.09 cce/16.0.1 rocm craype-
accel-amd-gfx90a

cd /PATH/TO/TUTORIAL/openmp-offload/C/1-openmp-cpu/
export OMP_NUM_THREADS=7    # for CPU OpenMP
./jacobi.C.cce.exe <args>
```

Experiments

Please post questions here: Google doc for OpenMP Offload Part 1

- Compile and run the (GPU) code for the different compilers
  - Performance difference across compilers ??
  - Profile : https://docs.olcf.ornl.gov/systems/frontier_user_guide.html#profiling-applications
- When is it profitable to offload to the GPU ?
  - Does it depend on the compiler ?
- Frontier GPU's have 64 GB each: What's the biggest problem you can solve?
  - Does the maximum problem size depend on the compiler?
- What's the impact of changing **`num_teams`** and **`thread_limit`** on performance
  - Can you figure out the default values used by the different compilers?