Preparing for Frontier On Summit

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Summit OpenMP Offloading Compiler Support

• Vendor Provided & Supported:
  – XL
  – NVHPC Toolkit

• Community (Open Source):
  – LLVM
  – GCC
## Summit Compilers: Summary Table

<table>
<thead>
<tr>
<th>C</th>
<th>Compiler</th>
<th>C++</th>
<th>Fortran</th>
<th>Module</th>
<th>Offloading Flags</th>
<th>Useful Flags</th>
<th>Useful Environment variables (verbose)</th>
</tr>
</thead>
<tbody>
<tr>
<td>xlC</td>
<td>xlC</td>
<td>xlf</td>
<td></td>
<td>x1/16.1.1-10</td>
<td>-qsmp=omp -qoffload</td>
<td></td>
<td></td>
</tr>
<tr>
<td>nvc</td>
<td>nvc++</td>
<td>nvfortran</td>
<td></td>
<td>nvhpc/22.5</td>
<td>-mp=gpu -gpu=cc70</td>
<td>-Minfo=accel -Minfo=mp -Minfo=loop</td>
<td>NVCOMPILER_ACC_NOTIFY</td>
</tr>
<tr>
<td>clang</td>
<td>clang++</td>
<td>flang</td>
<td></td>
<td>llvm/14.0.0</td>
<td>-fopenmp \</td>
<td></td>
<td>LIBOMPTARGET_INFO=-1</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>-fopenmptargets=nvptx64-nvidia-cuda \</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>-Xopenmp-target \</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>-march=sm_70</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>gcc</td>
<td>g++</td>
<td>gfortran</td>
<td></td>
<td>gcc/12.1.0</td>
<td>-fopenmp</td>
<td>-foffload=“-lm -latomic”</td>
<td>GOMP_DEBUG=1</td>
</tr>
</tbody>
</table>

*Note: The cuda module needs to be loaded for the LLVM clang compiler to target GPU offloading*
Crusher/Frontier Compilers : Summary Table

<table>
<thead>
<tr>
<th>Programming Environment</th>
<th>C</th>
<th>Compilers</th>
<th>Compiler Modules</th>
<th>OpenMP Flags</th>
<th>Offloading Support</th>
</tr>
</thead>
<tbody>
<tr>
<td>PrgEnv-cray</td>
<td>cc</td>
<td>C (craycc</td>
<td>cce</td>
<td>-fopenmp</td>
<td>Yes</td>
</tr>
<tr>
<td></td>
<td></td>
<td>craycxx</td>
<td>craype-accel-amd-gfx90a</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>ftn</td>
<td>rocm</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>crayftn</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>PrgEnv-amd</td>
<td>cc</td>
<td>C (amdclang</td>
<td>amd</td>
<td>-fopenmp</td>
<td>Yes</td>
</tr>
<tr>
<td></td>
<td></td>
<td>amdclang++</td>
<td>rocm</td>
<td></td>
<td></td>
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<tr>
<td></td>
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<td>ftn</td>
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<tr>
<td></td>
<td></td>
<td>amdflang</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>PrgEnv-gnu</td>
<td>cc</td>
<td>C (gcc</td>
<td>gcc</td>
<td>-fopenmp</td>
<td>No</td>
</tr>
<tr>
<td></td>
<td></td>
<td>g++</td>
<td></td>
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<tr>
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<td>ftn</td>
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<tr>
<td></td>
<td></td>
<td>gfortran</td>
<td></td>
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<td></td>
</tr>
</tbody>
</table>

- craycc and craycxx are based on the LLVM clang compiler suite
- crayftn **NOT** based on LLVM/flang (proprietary Cray compiler)
- 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, may be made available when ready
Preparing for Frontier On Summit: Compiler Strategy

• C/C++
  – LLVM clang/clang++ provides best path for testing functionality
    o XL may also be an option, especially for mixed C/C++/Fortran codes
  – Performance tweaks will be needed
    o Different backends, and different optimizations (especially on the GPU).

• Fortran:
  – XL compiler on Summit gives best route for transitioning to Frontier
  – CCE Fortran compiler on Frontier will have support for more recent versions of the OpenMP specification
    o OpenMP `simd` clause needed for crayftn for thread parallelism on the GPU (see next slide)
  – Upstream gfortran with offloading to MI250X *may* be made available on Frontier
    o Performance lags vendor provided compilers on both V100 and MI250X cards
### OPENACC/OPENMP CONSTRUCT MAPPING TO GPU

<table>
<thead>
<tr>
<th>NVIDIA</th>
<th>AMD</th>
<th>CCE Fortran OpenACC</th>
<th>CCE Fortran OpenMP</th>
<th>CCE C/C++ OpenMP</th>
<th>Clang C/C++ OpenMP</th>
</tr>
</thead>
<tbody>
<tr>
<td>Threadblock</td>
<td>Work group</td>
<td>acc gang</td>
<td>omp teams</td>
<td>omp teams</td>
<td>omp teams</td>
</tr>
<tr>
<td>Warp</td>
<td>Wavefront</td>
<td>acc worker</td>
<td>omp parallel</td>
<td>omp parallel</td>
<td>omp parallel</td>
</tr>
<tr>
<td>Thread</td>
<td>Work item</td>
<td>acc vector</td>
<td>omp simd</td>
<td>omp simd</td>
<td>omp parallel</td>
</tr>
</tbody>
</table>

- Current best practice:
  - Use “teams” to express GPU threadblock/work group parallelism
  - Use “parallel for simd” to express GPU thread/work item parallelism
- Future direction:
  - Improve CCE support for “parallel” and “simd” in accelerator regions
  - Upstream Clang is expanding support for “simd” in accelerator regions

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

OpenMP Offloading Code on Summit (Hands On)

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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
  – Invoked based on the loaded compiler module at compile time

• Example: Compile using GCC

```
[elwasif@login1.summit openmp-offload]$ module load gcc/12.1.0
[elwasif@login1.summit openmp-offload]$ cd C/0-serial/
[elwasif@login1.summit 0-serial]$ make
gcc -Ofast -fopenmp -Wl,-rpath=/sw/summit/gcc/12.1.0-0/lib64 -lm \
    -foffload=nvptx-none="-Ofast -lm -latomic -misa=sm_35" jacobi.c -o jacobi.C.gcc.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

```c
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 neighbours 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 residual
    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 : 4-point filter

```c
// simulation iterations
while (residual > MAX_RESIDUAL && iteration <= max_iterations) {
    // main computational kernel, average over neighbours 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 residual
    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);
```
# The C/C++ Code variants

<table>
<thead>
<tr>
<th>Directory</th>
<th>Description</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>0-serial/</td>
<td>Base serial version</td>
<td></td>
</tr>
<tr>
<td>1-openmp-cpu/</td>
<td>OpenMP CPU only</td>
<td></td>
</tr>
<tr>
<td>2-openmp-gpu-teams/</td>
<td>GPU: Teams only</td>
<td>Day 1</td>
</tr>
<tr>
<td>3-openmp-gpu-parallel/</td>
<td>GPU: Teams + Threads</td>
<td>Day 1</td>
</tr>
<tr>
<td>4-openmp-gpu-data/</td>
<td>GPU: Manage data movement</td>
<td>Day 2</td>
</tr>
<tr>
<td>5-openmp-gpu-implicit/</td>
<td>GPU: Implicit data movement</td>
<td>Day 2 – C++</td>
</tr>
<tr>
<td>6-openmp-combined/</td>
<td>All variants</td>
<td></td>
</tr>
<tr>
<td>7-loop-combined/</td>
<td>Using loop construct (nvhpc, gcc only)</td>
<td>In development for Frontier - not imminent</td>
</tr>
</tbody>
</table>

*Similar Directory Structure for Fortran code*
Submitting Jobs On Summit

- Use your own project ID
- Reservations from 1:00 – 3:30
  - `#BSUB -U augomp`
- Sample batch script for 8 CPU threads
  - The `-c` and `-bind packed:<x>` argument needs to be (at least) the requested number of threads.

```bash
#!/bin/bash
# Begin LSF Directives
#BSUB -P PROJECT_ID
#BSUB -W 10:00
#BSUB -nnodes 1
#BSUB -U augomp
#BSUB -alloc_flags gpumps
#BSUB -J OMPtutorial
#BSUB -o OMPtutorial.%J
#BSUB -e OMPtutorial.%J

export OMP_NUM_THREADS=8
cd /PATH/TO/TUTORIAL/openmp-offload/C/1-openmp-cpu
date
cd /PATH/TO/TUTORIAL/openmp-offload/C/1-openmp-cpu
date
jsrun -n1 -c $OMP_NUM_THREADS -g1 -bind packed:$OMP_NUM_THREADS <EXECUTABLE>
```

See:
https://docs.olcf.ornl.gov/systems/summit_user_guide.html#single-task-multiple-gpus-multiple-threads-per-rs
Experiments

- Compile and run the (GPU) code for the different compilers
  - Performance difference across compilers ??
  - Profile using nsight : https://docs.olcf.ornl.gov/systems/summit_user_guide.html#optimizing-and-profiling

- When is it profitable to offload to the GPU ?
  - Does it depend on the compiler ?

- Summit GPU’s have 16 GB: 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?