The Frontier Programming Environment at OLCF

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Overview
Contributors to Frontier Programming Environment

Vendor-Provided

- Cray Programming Environment (CPE)
  - Includes Cray compiler for C, C++, and Fortran plus GCC compiler. All the Cray profiling, tuning, and debugging tools. OpenMP and Cray MPI optimized for AMD GPU direct.
- AMD ROCm programming environment
  - Includes LLVM compiler to generate optimized code for both the AMD Trento CPU and MI250X GPU.
  - Support: C, C++, and Fortran and have GPU offload support. HIP, a CUDA-like direct GPU programming model (with CUDA to HIP conversion utilities).

Other Sources

- ECP
  - LLVM enhancements: Flang (Fortran frontend), OpenMP, OpenACC
  - Kokkos and RAJA
  - HIP LZ (HIP support for Aurora)
  - MPI, HPCToolkit, PAPI enhancements
  - ...
- ALCF + OLCF
  - Pilot implementation of DPC++/SYCL for Frontier
- OLCF
  - GCC enhancements to better support OpenACC, OpenMP, Fortran on Summit and Frontier
Programming Environment

• Compilers Offered
  – Cray PE (C/C++ LLVM-based; Cray Fortran)
  – AMD ROCm (LLVM-based)
  – GCC

• Programming Languages & Models Supported (in which compilers)
  – C, C++, Fortran (all)
  – OpenACC (Cray Fortran OpenACC 2.0+ & GCC 2.6 substantially complete, 2.7 planned)
  – OpenMP (all) 5.0-5.2 in progress – most priority features complete, details vary
  – HIP (Cray, AMD)
  – Kokkos/RAJA (all)
  – UPC (Cray, GCC)

• Transition Paths
  – CUDA: semi-automatic translation to HIP
  – CUDA Fortran: HIP kernels called from Fortran (a more portable approach)
    o CUDA Fortran kernels need to be translated to C++/HIP (manual process)
    o Fortran bindings to HIP and ROCm libraries and HIP runtime available through AMD’s hipfort project

Items in green are also available on Summit
# Programming Tools

## Debuggers and Correctness Tools

<table>
<thead>
<tr>
<th>Tool</th>
<th>System-Level Tools</th>
<th>Node-Level Tools</th>
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<tbody>
<tr>
<td>Arm DDT</td>
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<td>Cray CCDB</td>
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<td>Cray ATP</td>
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<td>STAT</td>
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## Performance Tools

<table>
<thead>
<tr>
<th>Tool</th>
<th>System-Level Tools</th>
<th>Node-Level Tools</th>
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<tbody>
<tr>
<td>Arm MAP/Performance Reports</td>
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<tr>
<td>CrayPat/Apprentice2 (Cray)</td>
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<td>Reveal (Cray)</td>
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<td>TAU</td>
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<td>HPCToolkit</td>
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<td>Score-P / VAMPIR</td>
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Items in green are also available on Summit.
## Scientific Libraries and Tools

<table>
<thead>
<tr>
<th>Functionality</th>
<th>CPU</th>
<th>GPU</th>
<th>Notes</th>
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<tbody>
<tr>
<td>BLAS</td>
<td>Cray LibSci, AMD BLIS, PLASMA</td>
<td>Cray LibSci_ACC, AMD roc/hipBLAS, AMD rocAMD ROCm Tensile, MAGMA</td>
<td>MAGMA and PLASMA are open source software led by the UTK Innovative Computing Laboratory</td>
</tr>
<tr>
<td>LAPACK</td>
<td>Cray LibSci, AMD libFlame, PLASMA</td>
<td>Cray LibSci_ACC, AMD roc/hipSolver, MAGMA</td>
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<tr>
<td>ScaLAPACK</td>
<td>Cray LibSci</td>
<td>ECP SLATE, Cray LibSci_ACC</td>
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<tr>
<td>Sparse</td>
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<td>AMD roc/hipSparse, AMD rocALUTION</td>
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<tr>
<td>Mixed-precision</td>
<td>Cray IRT, MAGMA</td>
<td>MAGMA</td>
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<tr>
<td>iterative refinement</td>
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<tr>
<td>FFTW or similar</td>
<td>Cray, AMD, ECP FFTX, FFT-ECP</td>
<td>AMD rocFFT, ECP FFTX, FFT-ECP</td>
<td>FFT-ECP focuses on 3D FFTs</td>
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<tr>
<td>PETSc, Trilinos,</td>
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<td>HYPRE, SUNDIALS,</td>
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<td>SuperLU</td>
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<tr>
<td></td>
<td><strong>Functionality in green is also available on Summit</strong></td>
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Digging a Little Deeper
For C/C++ Codes

• Multiple compilers available
  – AMD
  – Cray
  – LLVM

• But they’re all based on LLVM
  – HPE and AMD are among the many organizations contributing to the development of LLVM
  – Most work is “upstreamed” (contributed to the core LLVM source)
    o But not everything is accepted (immediately), or may be held back as proprietary
  – Capabilities (and bugs) are likely to be generally similar at any point in time…
  – But not identical!

• LLVM is also available on Summit
Upstream LLVM @ OLCF

• Summit:
  – OLCF deployed modules (with offloading): latest llvm/14.0.0
  – Periodic main snapshots:
    module use /sw/summit/modulefiles/ums/stf010/Core
    module load llvm/17.0.0-latest  # Also from specific dates

• Crusher:
  – Periodic main snapshots (maintained by the ECP SOLLVE project)
    module use /sw/crusher/ums/ums012/modules
    module load llvm/17.0.0-20230213  # Also from other dates

• Frontier:
  – TBD
For Fortran Codes

- One useful compiler available at present
  - Cray
    - *Not* based on LLVM

- AMD provides a Fortran implementation, but we don’t recommend it
  - It is based on “classic Flang”, in the LLVM ecosystem
  - Support for both the latest language standards and OpenMP offload are limited

- There is extensive work underway in the LLVM community on Flang, but it will be some time before it is production quality
But What About GCC?

• On this slide “GCC” refers to the whole suite, including gfortran
  – With support for offloading using OpenMP/OpenACC

• OLCF is working with Siemens to implement OpenMP in GCC

• OLCF will provide recent release and development versions of GCC on Frontier

• For various reasons, you should not expect gcc-generated executables to be performant for offload at this time
  – Results will vary
  – We are interested in improving the performance of gcc. If you have a troublesome case, reach out to me. (No guarantees, however)

• GCC is also available on Summit
GCC+offloading

• Summit:
  – OLCF deployed modules (with offloading): latest gcc/12.1.0
  – Periodic development snapshots:
    module use /sw/summit/modulefiles/ums/stf010/Core
    module load gcc/12.2.1-latest  # Also from specific dates

• Crusher:
  – Periodic development snapshots
    module use /sw/crusher/ums/compilers/modulefiles
    module load gcc/12.2.1-latest  # Also from specific dates

• Frontier:
  – TBD
For HIP (and CUDA) Codes

- HIP runs today on AMD and NVIDIA GPUs
- An ECP project is working on supporting HIP on Intel GPUs
- Recommend a one-time translation of CUDA codes to HIP and make the HIP version primary from then on
- Both Cray and AMD compilers support HIP
  - They both use the AMD runtime
- More on HIP available in the OLCF Training Archive
- HIP is also available on Summit

- AMD provides tools to translate CUDA to HIP
  - hipify-perl and hipify-clang
  - Not fully automatic
- hipfort
  - https://github.com/ROCmSoftwarePlatform/hipfort
  - Fortran bindings to HIP and ROCm libraries and HIP runtime
  - Build depends on ROCm version & Fortran compiler used
- Related: SYCLomatic - Intel tool to translate CUDA to Sycl
  - https://github.com/oneapi-src/SYCLomatic
  - Intel® DPC++ Compatibility Tool
  - Not fully automatic
For OpenMP Codes

• OpenMP is very much a work in progress in the LLVM community
  – Most of 5.0 is implemented
  – Parts of 5.1, 5.2 are implemented

• We (DOE labs, including ORNL/OLCF) are trying to help prioritize the order of implementation based on what users tell us they need/want
  – So if you could really use features that aren’t available yet, please let us know!

• Cray and AMD compilers use different OpenMP runtimes

• Remember that Cray Fortran is not based on LLVM

• OpenMP implementation in GCC is also a work in progress

• More on OpenMP available in the OLCF Training Archive

• OpenMP is available on Summit, but different progress on impl
For OpenACC Codes

- Cray Fortran supports OpenACC 2.0+
  - "CCE supports full OpenACC 2.0 and partial OpenACC 2.x/3.x for Fortran (OpenACC is not supported for C and C++)"
  - Work is underway to 3.2 (latest)
    - but no timeline has been given

- OLCF provides OpenACC support via GCC
  - 2.6 currently supported --- 2.7 planned
  - 3.x not currently planned – let us know if there are particular features that you could really use
  - Don’t expect this to be performant at present

- Work is also underway in the LLVM community on OpenACC
  - Unknown when these will be production

- OpenACC is also available on Summit

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**CCE OpenACC 2.x/3.x features – CCE/15:**

- `attach/detach` behavior and clauses
- `default(present)` clause
- Implied present-or behavior for `copy`, `copyin`, `copyout`, and `create` data clauses
- `if_present` clause on `acc update`
- `if` clause on `acc wait`
- `async` and `wait` clauses on `acc data`
- `acc_attach` and `acc_attach_async` APIs
- `finalize` clause on `exit data`
- `no_create` clause on structured data and compute constructs
- `if` clause on `host_data`
What about SYCL?

• OLCF and ALCF have partnered with Codeplay on a pilot implementation of the Intel DPC++ compiler for AMD GPUs
  – ALCF has also partnered with NERSC on NVIDIA support

• Pilot implementation is complete
  – ~“50%” level of support
  – Tested with a small set of benchmarks and mini-apps
  – Spock: `module load ums ums015 dpcpp`
  – Crusher: `module load dpcpp` #dpcpp/22.09

• Seeking interested users to try out the pilot implementation
  – Provide feedback
  – Shake out issues
  – Provide motivation to complete the port
Help Us Help You…

- If you have a liaison, work with them

*If you encounter an issue, file a ticket with OLCF* — otherwise the facility won’t (necessarily) know about it, and can’t track it
  - Summit, Spock, Crusher, Frontier…

- Take advantage of training events like this one
  - *Preparing for Frontier* series in the OLCF Training Archive
  - If you have Crusher access: office hours, hackathons, additional trainings