

The Frontier Programming Environment at OLCF

David E. Bernholdt

Programming Environment and Tools Lead, OLCF Oak Ridge Leadership Computing Facility

Oak Ridge National Laboratory







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 Epyc CPU and Instinct GPU. It will support: C, C++, and Fortran and have GPU offload support. HIP for converting CUDA codes to run on AMD GPUs.

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 (GCC)
 - OpenMP (all)
 - HIP (Cray, AMD) New: Cray has added HIP support to CPE
 - 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)
 - 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

2.6 substantially complete, 2.7 planned



Programming Tools

Debuggers and Correctness Tools

System-Level Tools Arm DDT Cray CCDB Cray ATP STAT Node-Level Tools ROCgdb Cray GDB4HPC

Items in green are also available on Summit

Performance Tools

Tool				
System-Level Tools				
Arm MAP/Performance Reports				
CrayPat/Apprentice2 (Cray)				
Reveal (Cray)				
TAU				
HPCToolkit				
Score-P / VAMPIR				
Node-Level Tools				
gprof				
PAPI				
ROCprof				
ROC-profiler & ROC-tracer libraries				





Scientific Libraries and Tools

Functionality	CPU	GPU	Notes
BLAS	Cray LibSci, AMD BLIS, PLASMA	Cray LibSci_ACC, AMD roc/hipBLAS, AMD rocAMD ROCm Tensile, MAGMA	MAGMA and PLASMA are open source software led by the UTK Innovative Computing Laboratory
LAPACK	Cray LibSci, AMD libFlame, PLASMA	Cray LibSci_ACC, AMD roc/hipSolver, MAGMA	
ScaLAPACK	Cray LibSci	ECP SLATE, Cray LibSci_ACC	
Sparse		AMD roc/hipSparse, AMD rocALUTION	
Mixed-precision iterative refinement	Cray IRT, MAGMA	MAGMA	
FFTW or similar	Cray, AMD, ECP FFTX, FFT-ECP	AMD rocFFT, ECP FFTX, FFT-ECP	FFT-ECP focuses on 3D FFTs
PETSc, Trilinos, HYPRE, SUNDIALS, SuperLU			Spack recipes from ECP xSDK

Functionality in **green** is also available on Summit



Timeline...

- Early Access System (spock) now available
 - "n-1" hardware (processors, network, etc.)
 - With the evolving Cray and AMD programming environments
- Frontier will be delivered in 2021, with acceptance expected in first half of 2022
 - ECP expected to gain access in June 2022
 - INCITE access will ramp up from Jan 2023 to full allocation starting Jan 2024
 - ALCC access will ramp up from Jul 2023 to full allocation starting Jul 2024

In the mean time

- Summit provides many of the same tools and a similar architecture
 - Especially useful if you're new to GPU programming
- Early Access systems will provide the (evolving) software stack on near-Frontier hardware



