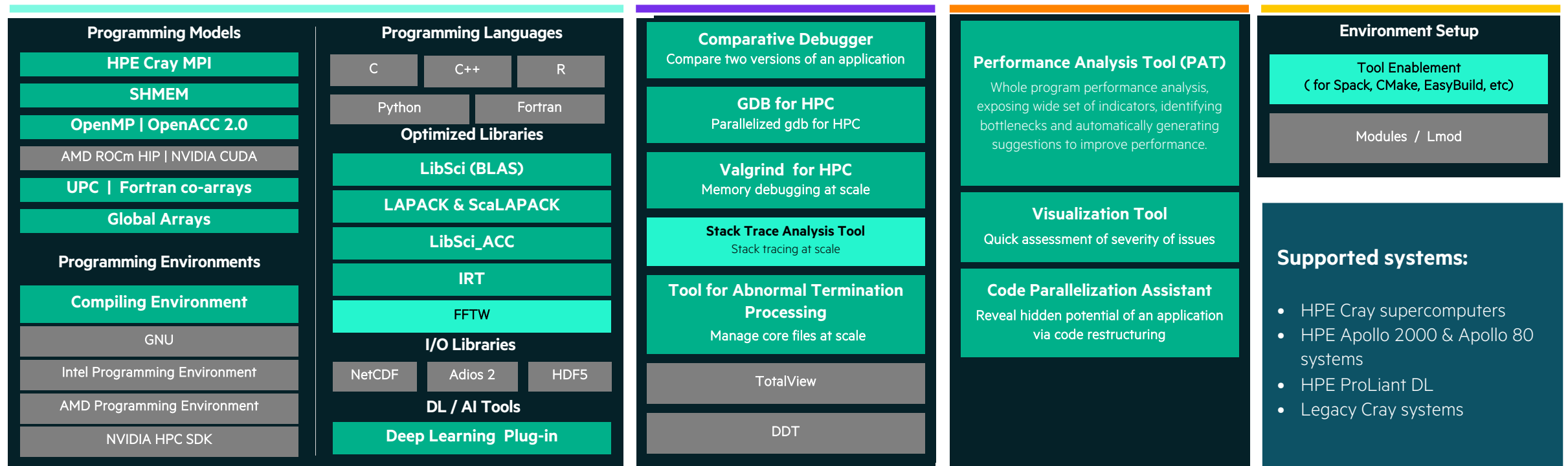# HPE CRAY PROGRAMMING ENVIRONMENT

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HPE CRAY PROGRAMMING ENVIRONMENT

Comprehensive set of tools for developing, porting, debugging, and tuning of HPC applications on HPE & HPE Cray systems

Programming Models
- **HPE Cray MPI**
- **SHMEM**
- **OpenMP | OpenACC 2.0**
- AMD ROCm HIP | NVIDIA CUDA
- **UPC | Fortran co-arrays**
- **Global Arrays**

Programming Environments
- **Compiling Environment**
- GNU
- Intel Programming Environment
- AMD Programming Environment
- NVIDIA HPC SDK

Programming Languages
C	C++	R
Python		Fortran

Optimized Libraries
- **LibSci (BLAS)**
- **LAPACK & ScaLAPACK**
- **LibSci_ACC**
- **IRT**
- FFTW

I/O Libraries
NetCDF	Adios 2	HDF5

DL / AI Tools
- **Deep Learning Plug-in**

Comparative Debugger
Compare two versions of an application

GDB for HPC
Parallelized gdb for HPC

Valgrind for HPC
Memory debugging at scale

Stack Trace Analysis Tool
Stack tracing at scale

Tool for Abnormal Termination Processing
Manage core files at scale

TotalView

DDT

Performance Analysis Tool (PAT)
Whole program performance analysis, exposing wide set of indicators, identifying bottlenecks and automatically generating suggestions to improve performance.

Visualization Tool
Quick assessment of severity of issues

Code Parallelization Assistant
Reveal hidden potential of an application via code restructuring

Environment Setup
Tool Enablement
(for Spack, CMake, EasyBuild, etc)

Modules / Lmod

Supported systems:
- HPE Cray supercomputers
- HPE Apollo 2000 & Apollo 80 systems
- HPE ProLiant DL
- Legacy Cray systems

HPE –authored | HPE Added-value to 3rd party | 3rd party

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HPE CRAY PROGRAMMING ENVIRONMENT COMPONENTS

- Cray Compiling Environment (CCE)
    - Cray Fortran Compiler
    - Cray Enhanced Clang/LLVM C/C++ Compiler
- Cray Scientific and Math Libraries (CSML)
    - BLAS, LAPACK, ScaLAPACK, and FFTW
- Cray Message Passing Toolkit (CMPT)
    - Cray MPI (mpich), Cray OpenSHMEMX
- Cray Environment Setup and Compiling Support (CENV)
    - Modules, compiler drivers
- Cray Performance Measurement & Analysis Tools (CPMAT)
    - Cray Perftools and the Performance API (PAPI)
- Cray Debugging Support Tools (CDST)
    - STAT, ATP, gdb4hpc, valgrind4hpc, and CCDB

COMPONENT VERSIONS FOR EX SYSTEMS WITH HPCM – BY RELEASE

- Monthly releases throughout 2021.

April release 21.04 installed on Spock today

HPE Cray Programming Environment Component	21.05	21.04
Cray Compiling Environment (CCE)	11.0.4	11.0.4
GNU Compiler Collection (GCC)	10.3.0	10.2.0
Cray Message Passing Toolkit - MPICH	8.1.5	8.1.4
Cray Message Passing Toolkit - OpenSHMEMX	11.2.1	11.2.0
Cray Scientific and Math Libraries – LibSci	21.04.1	21.04.1
Cray Scientific and Math Libraries - FFTW	3.3.8.10	3.3.8.9
Perftools (CPMAT)	21.05.1	21.02.0
Performance API (PAPI)	6.0.0.7	6.0.0.6
Cray Debugging Support Tools – gdb4hpc	4.13.1	4.12.4
Cray Debugging Support Tools – STAT	4.11.1	4.10.1
Cray Debugging Support Tools – ATP	3.14.1	3.13.1

CPE 2021 ROADMAP FOR CRAY EX, APOLLO

Theme	CPE 21.02, 21.03 (January-March 2021)	CPE 21.04, 21.05, 21.06 (April-June 2021)	CPE 21.07, 21.08, 21.09 (July-September 2021)	CPE 21.10, 21.11, 21.12 (October-December 2021)
Hardware	• Grizzly Peak A100 • Apollo/DL with Slingshot-10 fabric* • Apollo/DL MI-100*	• Apollo/DL Gen10+ Milan • Apollo/DL MI-100 (Tech Preview)	• Cray EX with Slingshot-11 fabric • Next Gen AMD • Apollo/DL Gen10+ Icelake	• Next Gen Intel • Next Gen AMD
CSM (OS support)	• SHASTA V1.3, V1.4	• COS 2.1 (SLES15 SP2)	• COS 2.2 (SLES15 SP3)	• COS 2.2 (SLES15 SP3)
HPCM (OS support)	• SLES15 SP2 (EX) • RHEL 8 (Apollo/DL)	• COS 2.1 (EX) • RHEL 8 (Apollo/DL)	• COS 2.2 (EX) • RHEL 8 (Apollo/DL)	• COS 2.2 (EX) • RHEL 8 (Apollo/DL)
CPE Features	• MPI GPU-to-GPU support for NVIDIA A100 and AMD MI-100 • gdb for HPC support for PBSpro with HPCM • Support for 'cpe' module on EX • Support LMOD on Apollo	• CCE 12.0 with additional OpenMP 5.0 features • SPACK environment enablement • OpenSHMEMX 1.5 compliance • ROCm 4.1 support • Perftools support for OpenMP target offload for AMD MI-100 • LibSci OpenMP threaded kernel updates for AMD CPU targets on EX and Apollo • Transition from module collections to metamodules • Module support for 3 combinations of Intel OneAPI compilers	• MPI support for HPE NIC traffic classes, scalable startup, Rosetta hardware collectives • Perftools support for next Gen AMD • Code parallelization assistant tool scoping and OpenMP device directive generation	• CCE 13.0 with full OpenMP 5.0 support
3rd Party compilers	• NVIDIA HPC SDK (PrgEnv-nvidia)	• Intel OneAPI (PrgEnv-intel) • ROCm compilers (PrgEnv-amd)		

Limited availability

HPE CRAY PROGRAMMING ENVIRONMENT

- A cross-compiler environment
  - Compiler runs on a User Access Node (UAN)
  - Executable runs on the compute nodes

- Cray written compiler driver scripts
  - HPE Cray OS compiler options
  - HPE Cray OS system libraries and header files
  - Compiler specific programming environment libraries

- Modules utility
  - Consists of the `module` command and module files
  - Initializes the environment for a specific compiler
  - Allows easy swapping of compilers and compiler versions
  - Spock and Frontier will use Lmod modules based on Lua

PROCESSOR, ACCELERATOR, AND NETWORK MODULES

Module	Contents
`craype-x86-rome`	Specifies CPU Target of AMD EPYC 2nd Generation CPU - Rome
`craype-x86-milan`	Specifies CPU Target of AMD EPYC 3nd Generation CPU - Milan
`craype-accel-amd-gfx908`	Sets options and paths to build for the AMD MI100 GPU
`craype-network-ofi`	Sets options and paths for network to use libfabric from OpenFabrics Interfaces (OFI)
`craype-network-ucx`	Sets options and paths for network to use Nvidia (Mellanox) HPC-X toolkit using Unified Communication X (UCX)

COMPILER DRIVER SCRIPTS

- Do not call compilers directly; use Cray compile drivers
  - `ftn`
  - `cc`
  - `CC`

- Driver actions:
  - Select compiler version
  - Add system libraries and header files
  - Add compiler-specific programming environment libraries
  - Execute the actual compiler command with added options

- Use vendor man pages for details of compiler options
  - HPE Cray man pages: `crayftn`, `craycc`, `crayc++`
  - GCC man pages: `gfortran`, `gcc`, `g++`

Spack is a different story in development beyond the scope of today's training