U.S. OVERVIEW/UPDATE: EXASCALE PROJECT HAPPENINGS

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ECP WBS

1. Project Management
   1.1

2. Project Planning and Management
   1.1.1

3. Project Controls & Risk Management
   1.1.2

4. Business Management
   1.1.3

5. Procurement Management
   1.1.4

6. Information Technology and Quality Management
   1.1.5

7. Communications & Outreach
   1.1.6

8. Integration
   1.1.7

9. Application Development
   1.2

10. DOE Science and Energy Apps
    1.2.1

11. DOE NNSA Applications
    1.2.2

12. Other Agency Applications
    1.2.3

13. Developer Training and Productivity
    1.2.4

14. Co-Design and Integration
    1.2.5

15. Software Technology
    1.3

16. Programming Models and Runtimes
    1.3.1

17. Tools
    1.3.2

18. Mathematical and Scientific Libraries and Frameworks
    1.3.3

19. Data Management and Workflows
    1.3.4

20. Data Analytics and Visualization
    1.3.5

21. System Software
    1.3.6

22. Resilience and Integrity
    1.3.7

23. Co-Design and Integration
    1.3.8

24. Hardware Technology
    1.4

25. PathForward Vendor Node and System Design
    1.4.1

26. Design Space Evaluation
    1.4.2

27. Co-Design and Integration
    1.4.3

28. Co-design and Integration
    1.5.1

29. Testbeds
    1.5.2

30. NRE
    1.5.3

31. Exascale Systems
    1.5

Slide from R. Thakur (ANL)
ECP Software Technology Overview

• Build a comprehensive and coherent software stack that will enable application developers to productively write highly parallel applications that can portably target diverse exascale architectures

• Accomplished by extending current technologies to exascale where possible, performing R&D required to conceive of new approaches where necessary
  – Coordinate with vendor efforts; i.e., develop software other than what is typically done by vendors, develop common interfaces or services
  – Develop and deploy high-quality and robust software products
ST Projects (incl. ATDM) Mapped to Software Stack

- **Correctness**
  - Visualization: VTK-m, ALPINE, Cinema

- **Visualization**
  - Math Libraries/Frameworks:
    - ScaLAPACK, DPLASMA, MAGMA, PETSc/TAO, Trilinos, xSDK, PEEKS, SuperLU, STRUMPACK, SUNDIALS, DTK, TASMANIAN, AMP, FieCSI, KokkosKernels, Agile Comp., DataProp, MFEM

- **Data Analysis**
  - Tools:
    - PAPI, HPCToolkit, Darshan, Perf. portability (ROSE, Autotuning, PROTEAS), TAU, Compilers (LLVM, Flang), Mitos, MemAxes, Caliper, AID, Quo, Perf. Analysis

- **Applications**
  - Programming Models, Development Environment, and Runtimes:
    - MPI (MPICH, Open MPI), OpenMP, OpenACC, PGAS (UPC++, Global Arrays), Task-Based (PaRSEC, Legion, DARMA), RAJA, Kokkos, OMPTD, Power steering

- **Data Management, I/O and File System**
  - Node OS, low-level runtimes:
    - Argo Global OS enhancements, SNL OS project

- **System Software, Resource Management Threading, Scheduling, Monitoring, and Control**
  - System Software
    - Argo Global OS, Qthreads, Flux, Spindle, BEE, Spack, Sonar

- **Co-Design**
  - Memory and Burst buffer:
    - Chkpt/R estudio (VeloC, UNIFYCR), API and library for complex memory hierarchy (SICM)

- **Tools**
  - Hardware interface

Slide from R. Thakur (ANL)
The Kinds of Software Technologies ECP Apps Ask For…

**Tools** (debuggers, profilers, software development, compilers)

- LLVM/Clang, HPCToolkit, PAPI, ROSE, Oxbow, JIRA, Travis
- ASPEN (machine modeling), CMake, git, TAU, Caliper, GitLab, CDash, Flux, Spack, Docker, Shifter, ESGF, Gerrit
- GDB, Valgrind, GitHub, Jenkins (testing), DDT (debugger)

**Data Management and Workflows**

- Swift, MPI-IO, HDF, ADIOS, XTC (extended tag container), Decaf, PDACS, GridPro (meshing), Fireworks, NEDB, BlitzDB, CouchDB
- Bellerophon, Sidre, Silo, ZFP, ASCTK, SCR, Sierra, DHARMA, DTK, PIO, Akuna, GridOPTICS software system (GOSS), DisPy, Luigi
- CityGML, SIGMA (meshing), OpenStudio, Landscan USA
- IMG/KBase, SRA, Globus, Python-PANDAS

**Data Analytics and Visualization**

- VisIt, VTK, Paraview, netCDF, CESIUM, Pymatgen, MacMolPlt, Yt
- CombBLAS, Elviz, GAGE, MetaQuast
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Node OS, low-level runtimes
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Memory and Burst buffer
- Chkpt/Restart (VeloC, UNIFYCR), API and library for complex memory hierarchy (SICM)

Data Management, I/O and File System
- ExaHDF5, PnetCDF, ROMIO, ADIOS, Chkpt/Restart (VeloC, UNIFYCR), Compression (EZ, ZFP), I/O services, HXHIM, SIO Components, DataWarehouse

Resilience
- Checkpoint/Restart (VeloC, UNIFYCR), FSEFI, Fault Modeling

Tools
- Hardware interface
Data Management and Workflow Technology Areas (Dominant project themes)

• I/O Interfaces and Data Services
  – The ADIOS framework for Scientific Data on Exascale Systems, Klasky (ORNL)
  – Data Libraries and Services Enabling Exascale Science, Ross (ANL)
  – HXHIM Key-value Stores for Applications, Settlemyer (LANL)
  – Scalable I/O Components, Ulmer (SNL)

• Checkpoint/Restart
  – UnifyCR, Mohror (LLNL)
  – VeloC: Low Overhead transparent multilevel Checkpoint/restart, Cappello (ANL)

• Compression
  – ZFP: Compressed Floating-Point Arrays, Lindstrom (LLNL)
  – EZ: Exascale lossy compression for scientific data, Cappello (ANL)

• Workflow
  – Workflow Infrastructure for Increasing User Productivity, Laney (LLNL)
  – DataWarehouse: Asynchronous Data Management Layer, Ulmer (SNL)
Data Analysis and Visualization Technology Areas
(Dominant project themes)

• In Situ Data Reduction
  – ALPINE, Ahrens (LANL)
  – Cinema, Ahrens (LANL)

• Infrastructure Improvement
  – Scalable Visualization, Moreland (SNL)
  – VTK-m, Moreland (SNL)
Related Technologies in Other Software Areas (Dominant project themes)

• Virtualization and Scheduling
  – BEE: Virtual Environments for Applications, Sewell (LANL)
  – Operating System, Pedretti (SNL)
  – Argo: OS and Resource Management for Exascale, Beckman (ANL)
  – Flux Resource Manager, Ahn (LLNL)

• Programming and Runtime
  – Distributed Tasking for Exascale, Dongarra (UT Knoxville)
  – Enhancing and Hardening Legion for ECP, Shipman (LANL)
  – DARMA: Asynchronous Many-Task (AMT) Abstraction Layer, Bennett (SNL)

• Software Package Management
  – Spack Package Manager, Gamblin (LLNL)
CODAR: A Co-Design Center for Online Data Analysis and Reduction at the Exascale
Ian Foster (ANL)

- Address growing disparity between computation and I/O rates
  - Deliver high-performance products for data analysis and reduction
  - Quantify performance tradeoffs for offline vs. online analyses
  - Orchestrate online data analysis and reduction

- Partnership among Argonne, Brookhaven, Oak Ridge, Rutgers, Stony Brook, and Brown University

[Diagram of CODAR runtime and I/O system]

Simulation knowledge: application, models, numerics, performance optimization, …

Figure from I. Foster (ANL)
ExaGraph: Combinatorial Methods for Enabling Exascale Applications Co-Design Center
Mahantesh Halappanavar (PNNL)

• Focus on graph analytics – combinatorial (graph) kernels that play a crucial enabling role in many data analytic computing (DAC) application areas as well as several ECP applications
  – Graph matching
  – Graph coloring
  – Graph clustering: including clique enumeration, parallel branch-and-bound, and graph partitioning

• Partnership among PNNL, Berkeley, Sandia, and Purdue University

• Announced March 2!
THANKS!