Flexible HPC Environments

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Los Alamos NATIONAL LABORATORY EST.1943

Accelerating Scientific Discovery by Enabling Diverse Workloads on HPC Clusters

BACKGROUND & MOTIVATION

New computational paradigms require new tools and environments

- A new class of data-analysis tools are available for scientists
- These tools do not integrate well with traditional HPC resource management systems
- Differing and often conflicting requirements exist
- Some fields require validated environments
    - High energy physics
    - Cosmology

INNOVATION

Flexible supercomputing resources enable the next generation of scientific discovery

- Simulation and data analysis in one workflow
- Traditional simulation workloads will be supported alongside new data-intensive workloads and user-defined environments
- Users can request the software resources they require or provide their own

DESCRIPTION

By adopting cloud technologies in an HPC environment we are merging the compute-intensive and data-intensive worlds in one converged system

Early implementation of flexible environments

- Charliecloud
    - lightweight virtual machine-based environment
    - LANL-developed
    - integrated with existing slurm resource manager
    - http://charliecloud.lanl.gov

Current avenues of investigation

- OpenStack, Docker, Kubernetes, NERSC Shifter
    - open source projects developed to manage virtual machines, linux containers and chroot environments
    - provide operating system environment flexibility
- Apache Mesos
    - open source project developed to manage workload frameworks
    - provides workload execution flexibility

Challenges

- Integrating the environment and workload managers into a comprehensive system
- Performance and security of virtual machines and linux containers is improving
- Providing users with an easy-to-use interface to a complex system

Current Technology Readiness Level (TRL): 4

- All components of the system have been tested and a prototype preproduction system in being built

ANTICIPATED IMPACT

HPC Systems will support a Larger Set of Technologies

- Scientists will be able to leverage the latest tools on HPC resources at previously unavailable scales
- User-defined environments will enable rapid experimentation and adoption of emerging tools
- HPC systems will support a consolidated workflow from simulation to analysis and discovery
- HPC systems will have increased utility to a broader set of users

PATH FORWARD

- **Investigate** current state of the art technologies
- **Identify** candidate technologies and their shortcomings
- **Communicate and Collaborate** with public and industry partners in computing and resource management to mature existing technologies and develop new ones

Potential End Users:

- DOE data scientists
- Early adopters of new software
- LANL users pursuing work for others

Point of Contact: Tim Randles, HPC, 505-667-0680, trandles@lanl.gov

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