Existing scientific application development and deployment issues

• The diversity of HPC platforms and associated software complexity often pose challenges that lead to slow or hampered scientific discovery.

• Application scientists expend considerable time and effort dealing with development, deployment, and runtime interfacing activities.

• Additionally, the short HPC system deployment and upgrade interval requires frequent redeployment of scientific application to different system software stacks.
Research and development goals

- Increasing the overall productivity of developing and executing computational codes
- Optimizing the development and deployment processes of scientific applications
- Simplifying the activities of application scientists, using uniform and adaptive solutions
- “Automagically” supporting the diversity of existing and emerging HPC architectures
Harness workbench core components

• Harness Workbench Toolkit
  – Unified development, deployment, and execution
  – Common view across diverse HPC platforms
  – User-space installation and virtual environments

• Next-generation runtime environment
  – Flexible, adaptive, lightweight framework
  – Management of runtime tasks
  – Support for diverse HPC platforms
Harness workbench core technologies

• Automatic adaptation using pluggable modules
  – Harness Workbench Toolkit plug-ins
  – Runtime environment plug-ins

• Development environment and toolkit interfaces
  – Easy-to-use interfaces for scientific application development, deployment, and execution
Common view across diverse platforms

- Various interfaces and bindings to external development and deployment tools and environments

- Generalized model for unified access to common development and deployment activities

- Mapping of generalized activities onto platform-specific toolkits and runtime environments (RTEs) via pluggable modules
Harness Workbench Toolkit

- Unifying abstraction over heterogeneous HPC resources
- Command line and GUI tools
- Translation into fine-tuned invocations of native toolkits
- Behavior encapsulated in plug-ins
- Configurable through profiles
- Tunable by end users
Next-generation runtime environment

- Uniform interface to various front-end systems
- Virtualized baseline platform runtime environment capabilities
- Advanced runtime environment capabilities via high-level plug-ins
Virtualized environments

• Problem:
  – Application dependencies may cause conflicts with system-wide installed libraries.

• Solution:
  – Use co-existing, alternative user-space installations.

• Approach:
  – Provide isolated installation environments ("sandboxes").
  – These can inherit from one another to build nested hierarchies.

• Virtualized adaptation of system properties to actual application needs
• System and runtime environment virtualization
Configurable “sandboxes” for scientific applications

Virtualized environment
XML configuration description

1. Install environment
hwb – env install conf

1.1 Configure system configuration

2. Execute application
hwb – env start conf application

2.1 Start Harness runtime environment
2.2 Configure runtime environment configuration
2.3 Execute application

Scientific application

Application
Runtime configuration
Runtime environment
System configuration
System
The Harness workbench: Unified and adaptive access to diverse HPC platforms

- Virtualized adaptation of system properties to actual application needs
- System and runtime environment virtualization
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