The Harness Workbench:
Unified and Adaptive Access to Diverse High-Performance Computing Platforms

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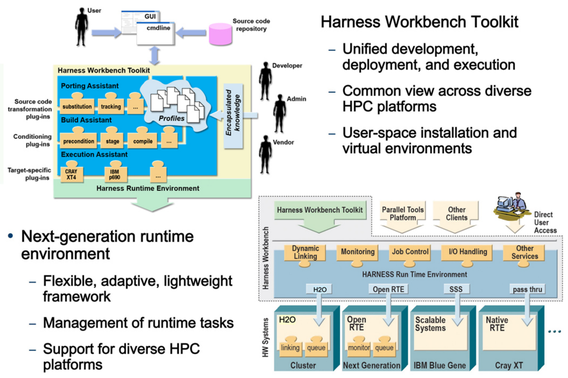
Harness workbench core components

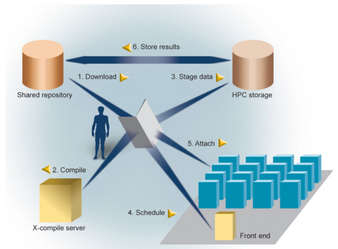


Harness Workbench Toolkit
- Unified development, deployment, and execution
- Common view across diverse HPC platforms
- User-space installation and virtual environments

- Next-generation runtime environment
  - Flexible, adaptive, lightweight framework
  - Management of runtime tasks
  - Support for diverse HPC platforms

Research and development goals

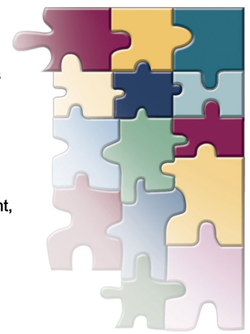
- Increasing the overall productivity of developing and executing computational codes
- Optimizing the development and deployment processes of scientific applications
- Simplifying the activities of application scientists, using uniform and adaptive solutions
- "Automagically" supporting the diversity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



Typical scientific application development, deployment, and execution activities

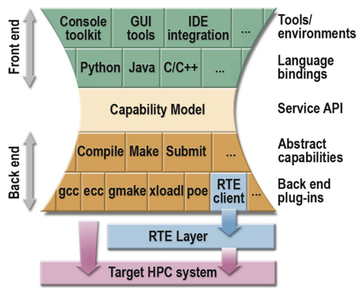
Harness workbench core technologies

- 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



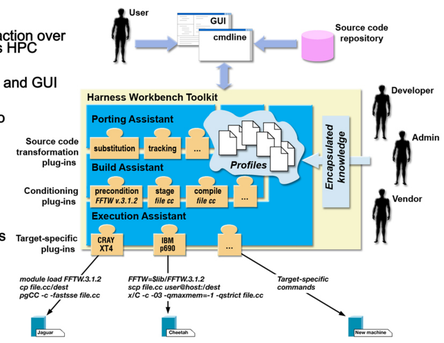
Common view across diverse platforms

- 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



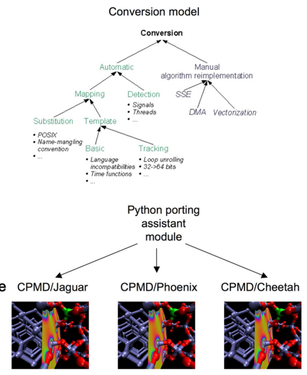
Harness workbench toolkit (HWT)

- 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



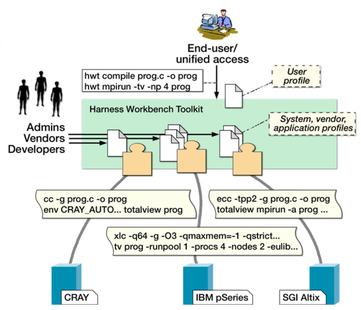
HWT porting assistant

- Facilitates source code adaptation through specialized plug-ins
  - Suggests safe conversions
  - Highlights manual code replacement areas
  - Guided by situation-specific profiles
- Prototype
  - Plug-ins as Python scripts
  - Ported CPMD across Jaguar (Cray XT3), Phoenix (Cray X1), Cheetah (IBM p690)
  - Example conversions: detection, function mappings, data type size changes



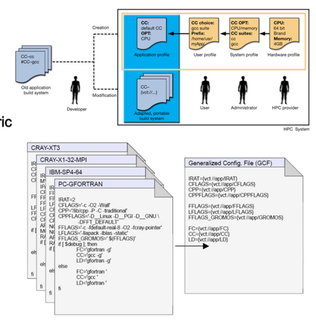
HWT virtualized command toolkit (VCT)
HWT build and execution layer

- Abstraction layer between users and platform-specific compilers, linkers, libraries, testing and debugging software, launching systems, etc
- End-users issue generic build commands that are processed to produce a target-specific set of commands
- Pluggable modules to deliver back-end functionality

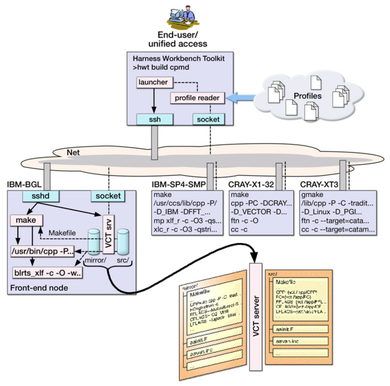


VCT prototype approach

- Target-specific knowledge encapsulated in profiles
- Generic build-related files
- *Late binding* – concretizing generic build files at runtime



VCT prototype architecture



VCT prototype use-case

Scenario

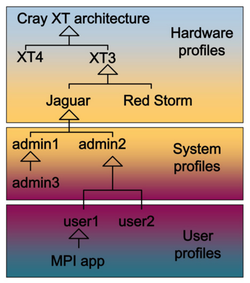
1. End-users stage-in application source codes with application's generic build system on the front-end node to 'src/'
2. HWT starts VCT server that mirrors 'src/'
3. The build system is launched on the front-end node in 'mirror/'
4. OS redirects filesystem operations to VCT server (e.g. reading Makefile)
5. To concretize generic files VCT server interacts with HWT and, based on profiles, resolves *vct references* at runtime through *late binding*

Implementation details

- VCT server exploits FUSE (Filesystem in USErspace)
- Python scripts
- Tested on CPMD

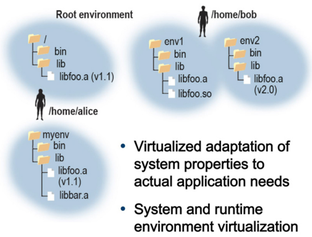
HWT profiles

- Declarative descriptions created by vendors, administrators, developers and adjusted by users
- Encapsulate target-specific knowledge at the system and application levels
- Support mechanisms
  - *Inheritance*
  - *Dynamic recursive resolution* to allow switching among predefined settings



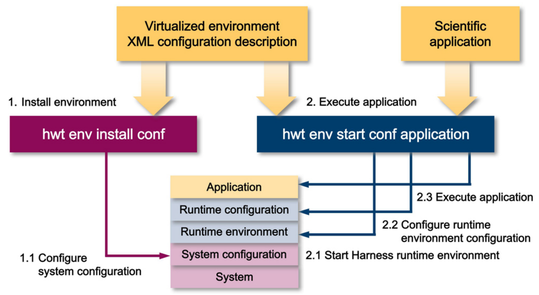
HWT virtualized environments

- 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.

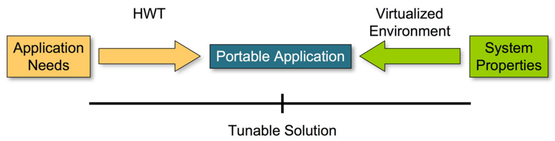


- Virtualized adaptation of system properties to actual application needs
- System and runtime environment virtualization

Configurable "sandboxes" for scientific applications



Tunable scientific application portability for day-one operation



- HWT for adaptation of application to HPC system properties
- Virtualized environment for adaptation of HPC system to application needs
- Tunable solution, where applications can move from one HPC system to another with initial minimal changes enabling day-one operation
- Continued adaptation to actual target platform properties assures eventual performance gains by gradually taking advantage of new system features

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