Portal Development for High Performance Computing (HPC) at Maui High Performance Computing Center (MHPCC)

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Overview

- **Goals**

- **Long-term vision**

- **Application delivery**

- **Open frameworks**

- **Single sign-on**

- **User Interface Toolkit (UIT)**

- **CREATE-Kestrel Integration**

- **Matlab**

Goals

- **Attract new users by Providing High Performance Computing (HPC) software applications through a "portal environment"**
  - **HPC knowledge not required**
  - **MHPCC new mission focus, key alliances with ARL, ERDC, and CREATE**
  - **CREATE and Matlab apps are initial standup**
- **Provide secure unified access with single sign on**
- **Providing a centralized web-based interface for customers that requires no software installation on user workstations**
- **Work across multiple security enclaves, providing seamless navigation among components and across HPC resources**
- **Secure suite of access controls that secures each users' data**
- **Search capabilities across the domain**
- **Ability to scale and grow to accommodate new HPC software applications**
- **Ability to customize to address unique user requirements**

Long-Term Vision

- Long term vision guides near-term development to ensure the portal design is applicable and scalable to other domains in the future

- As networks and browsers continue to improve cloud-based application delivery appears well suited to the DoD
  - may be de facto delivery mechanism in the future

- Benefits of portal application delivery
  - No client software required on users machine
  - Eliminates all user configuration and maintenance
  - Seamless collaboration within groups
  - Extreme HPC scalability
  - Delivery is OS and device independent
  - Simplified security model

Application Delivery (Level 0)
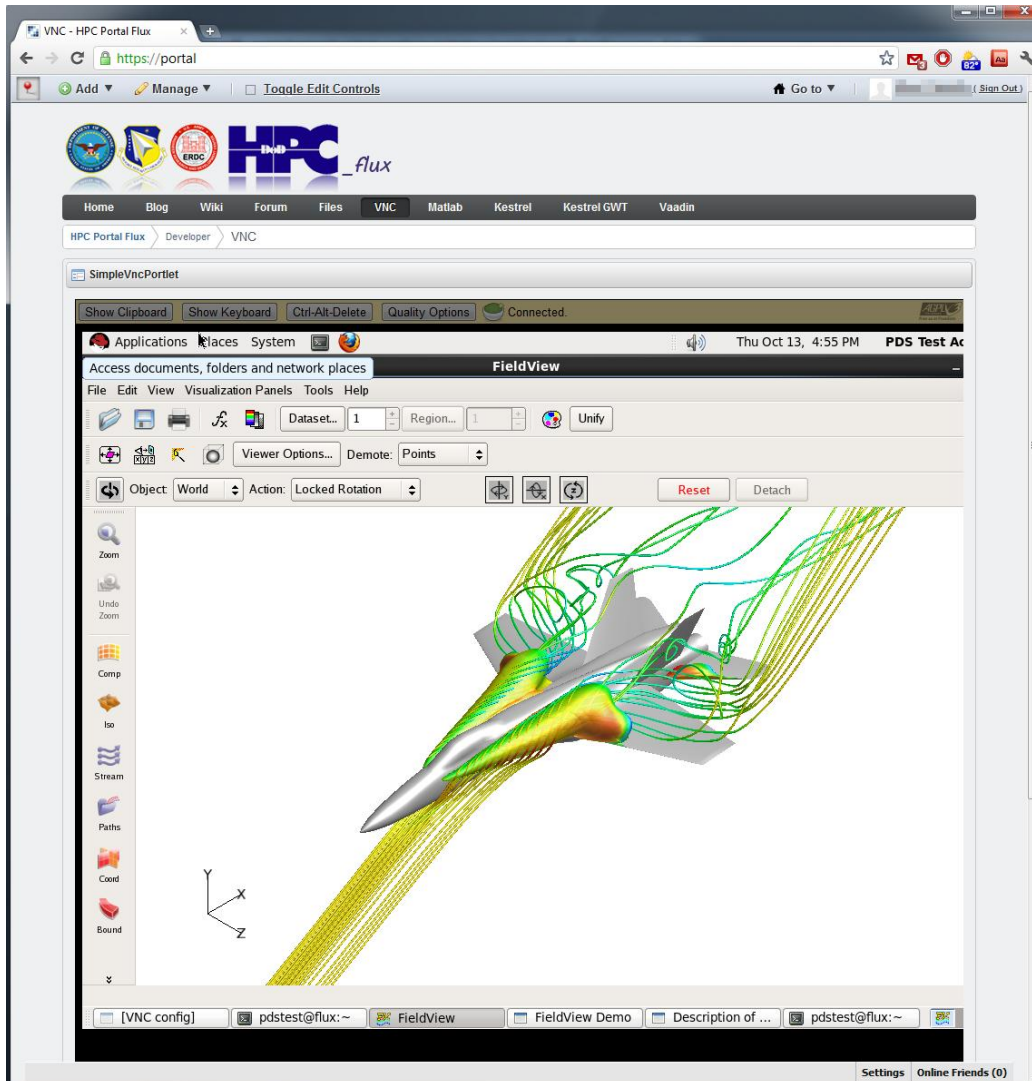
- **Quickest standup for legacy apps or COTS**

- **No SW changes**

- **All SW installed at DSRC**

- **Virtualized machine (Windows or Linux) running on a Linux server**

- **App delivered via "zero footprint" browser**

  - **HTML5 + JavaScript (AJAX) only**

  - **No plug-ins or client-side SW required**

  - **Eliminates user config and maintenance**

Application Delivery (Cont.)

- **Level 1**

  - **Hybrid between a clean slate web-based application design and Level 0**

  - **Used for CREATE Kestrel**
    - **Clean MVC architecture made for easy separation**
    - **Control logic remains on server**
    - **Server-side workflow integrated with portal framework**

- **Level 2**

  - **Native HTML5/JavaScript web-based application**

  - **Goal is to provide a bandwidth-aware software development kit (SDK)**
    - **Capability to view large datasets using level of detail technology**
    - **e.g. Google Maps supports efficient HTML5 / JavaScript implementations**

Portal SDK

- **Portal SDK itself is being developed for the DoD**

- **Developers share a common repository**

  - **MHPCC moderators**

- **SDK-framework (backend) for HPC resource access**

  - **files, job setup/status**

- **SDK-appUI (frontend) provides common look and feel interface components**
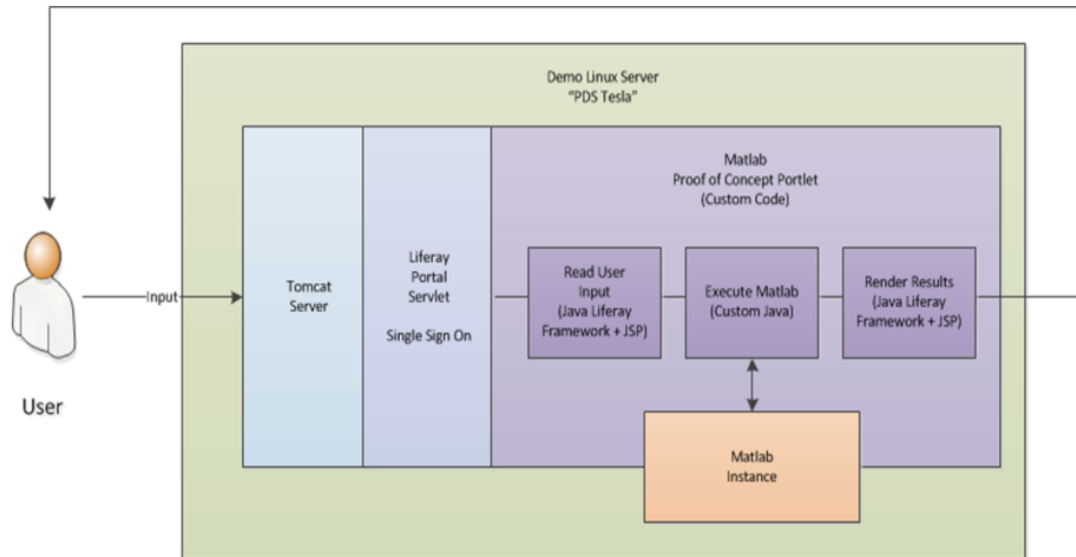
  - **Includes data quicklook capabilities**

Proof-of-concept background

- Drag and drop matlab script into portal window
- Server executes script and returns results including figures and plots to user
- Upload multi-file matlab package for execution
- .mat file download for 3d viewing

- **Matlab Proof-of-concept implemented in frameworks including Liferay, WSO2, Drupal, and Joomla**

- **Liferay selected for superior collaboration & content/identity management**
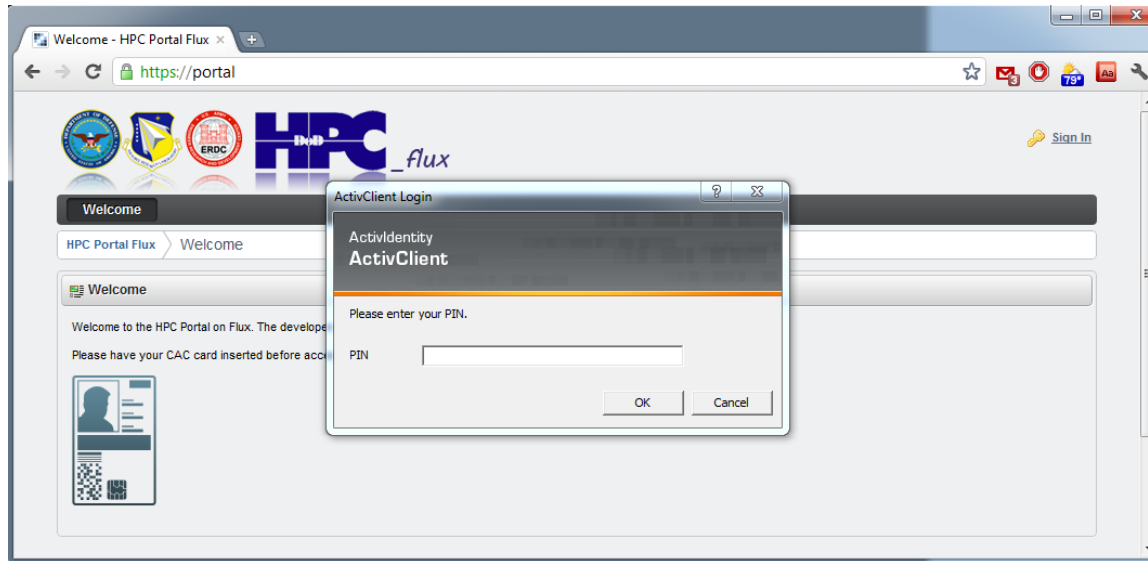
Matlab Proof-of-Concept Using Liferay Delivered to Non-Traditional Devices
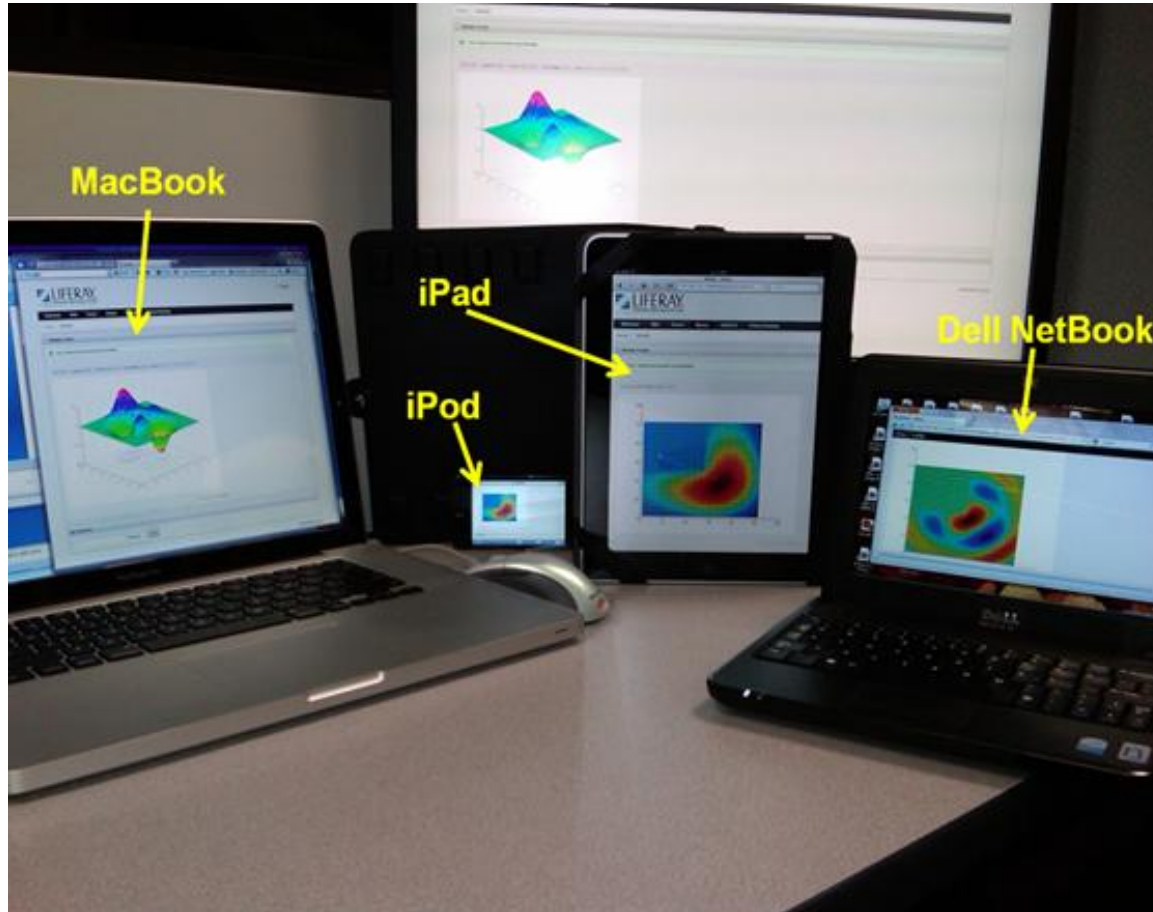
- Drag-and-drop matlab code

- Browser displays HTML results

Single-Sign-On (SSO)

YubiKey

- **In support of "*Enhancements to HPCMP Authentication and Authorization Services*" memo (5 April 2011) OpenID is used for SSO**

- **DoD high security standards require HW token (CAC or Yubikey) for SSO**
  - **CAC SSO today, Yubikey SSO soon**

- **YubiKey selected as a lower cost, higher reliability alternative hToken and secureID**

Portal able to access HPC systems on a user's behalf
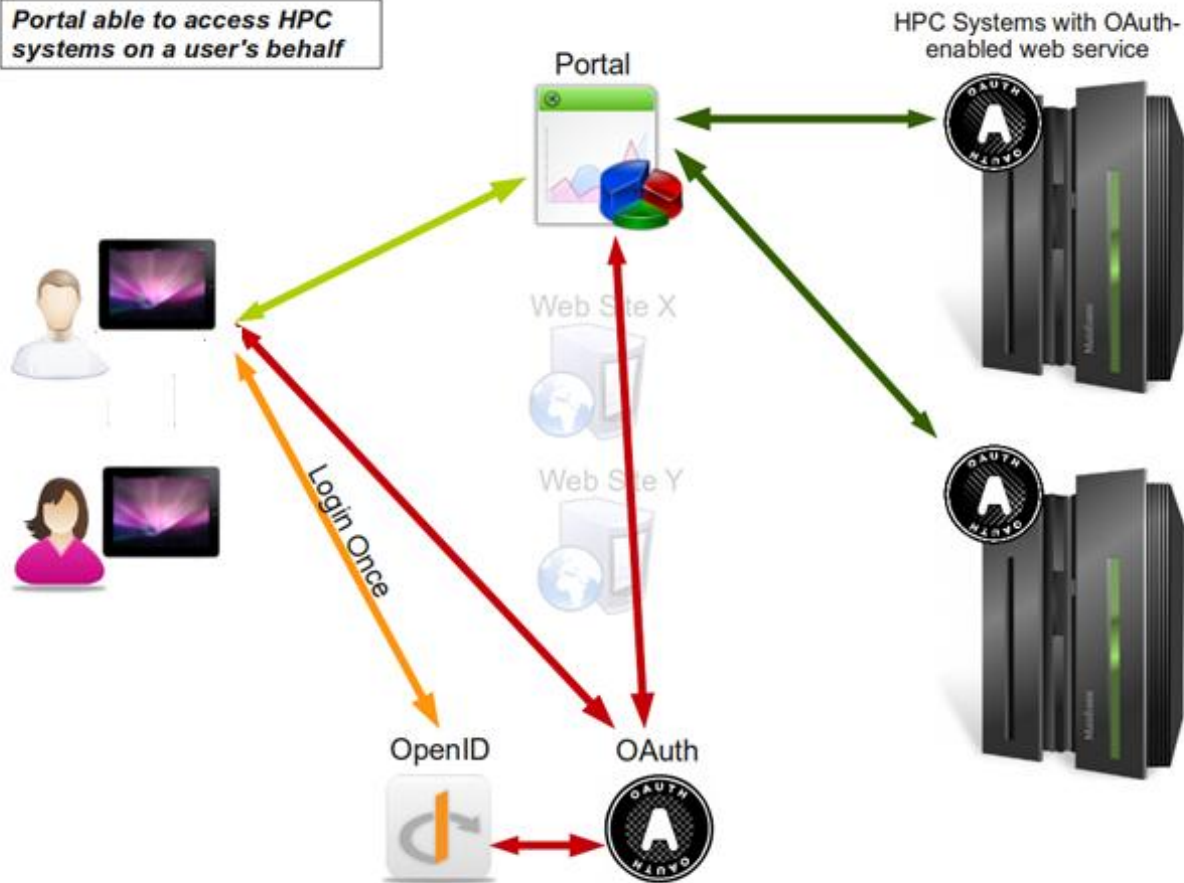
- **Portal leverages updated UIT for remote resource access and authentication**

- **Updated UIT supports OpenID and Oauth in place of Kerberos**

- **Allows access to remote resources across DSRCs**

- **FY12 Concept demonstration of seamless resource management between MHPCC and ERDC**

CREATE-Kestrel Integration
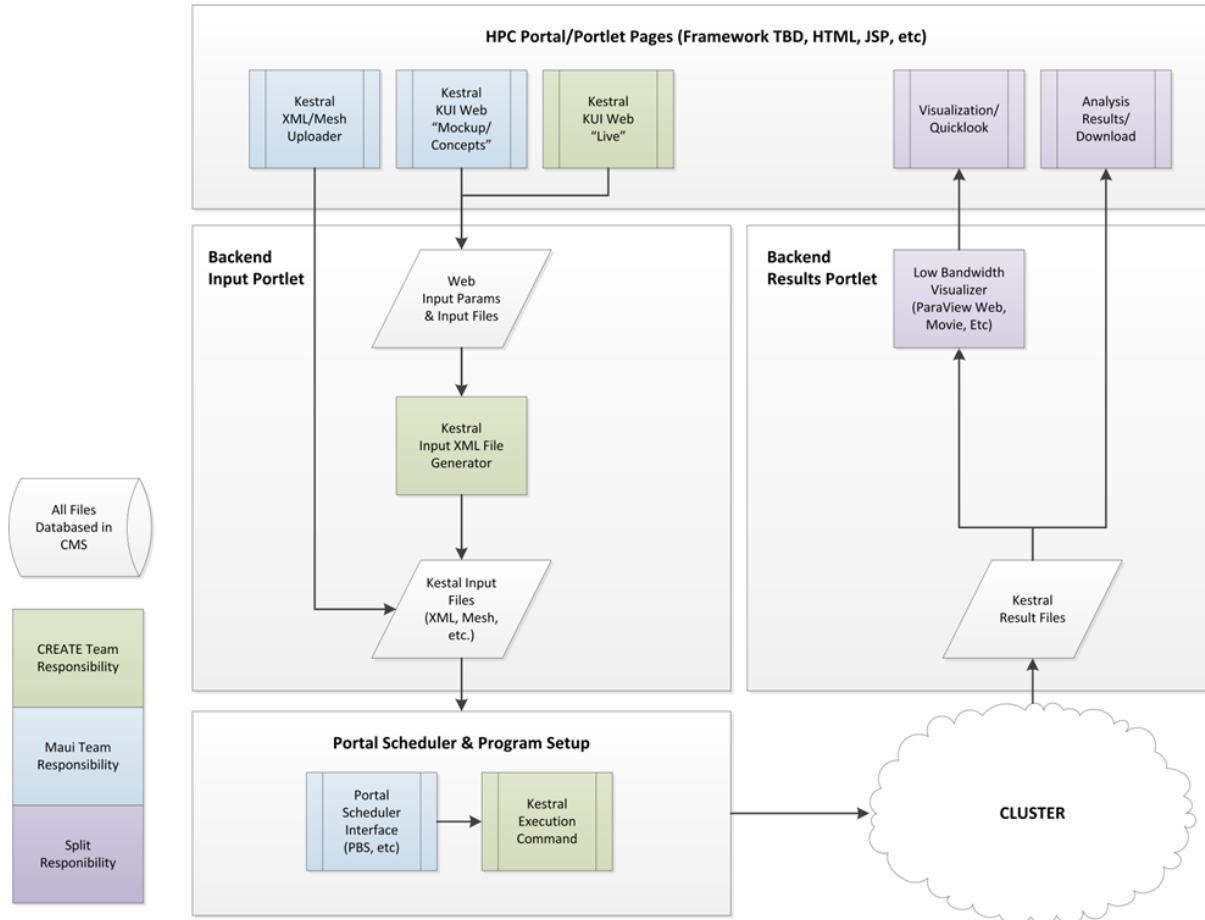
- **Kestrel is first CREATE app to be integrated with the portal**

- **Existing MVC architecture provided clean separation**

- **Stand-alone UI is available for product team development**

- **File management, job workflow, and quicklook handled by SDK**
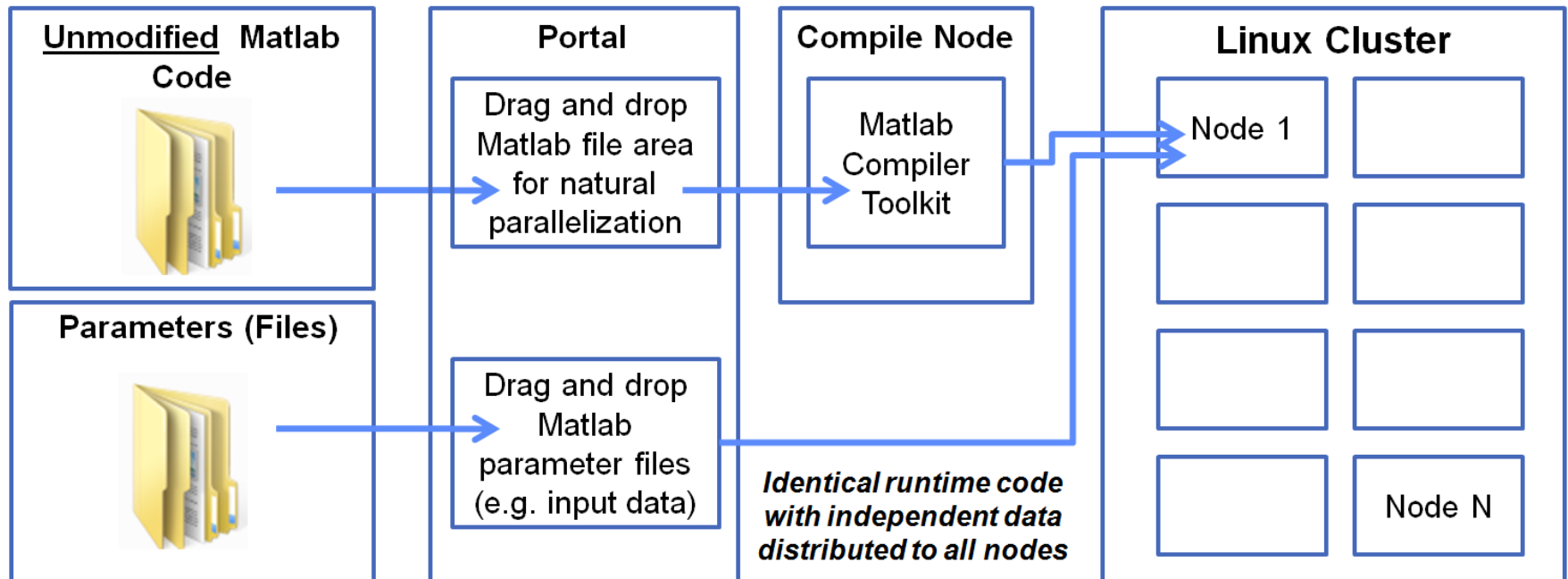
CREATE-Kestrel Integration
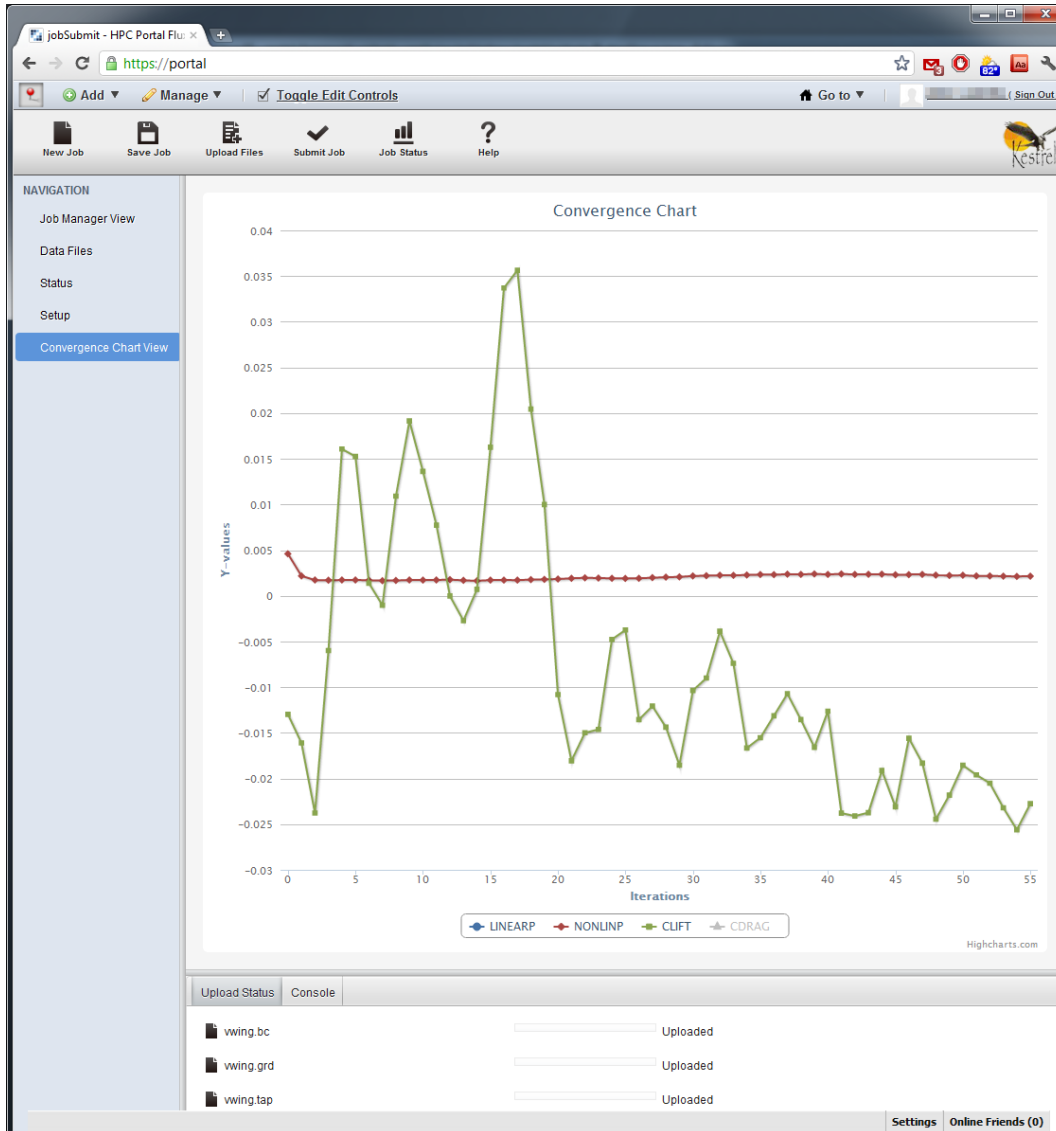
- **Dynamic status display shows convergence in real time**

- **Cursor driven data display provided with mouse over**

- **Legend is also active to provide rescaled plots**

Matlab for Naturally Parallel Jobs

- **High-speed short integration frames are collected for multiple satellite / missile pass to freeze atmospheric effects**

- **Research algorithm to remove atmospheric effects written in Matlab requires processing multiple passes for comparison to other techniques (10 to 100 frames are used for each final image in box car fashion)**

- **Portal will provide researcher capability to immediately use HPC for this naturally parallel problem without knowledge parallel programming**

Unmodified Matlab Code	Portal	Compile Node	Linux Cluster
	Drag and drop Matlab file area for natural parallelization	Matlab Compiler Toolkit	Node 1
Parameters (Files)	Drag and drop Matlab parameter files (e.g. input data)		Node N

Identical runtime code with independent data distributed to all nodes

Matlab Example 1 (Naturally Parallel)

- **Example parametric study of sensitivity of deconvolution to blur rate and angle**

- **User code runs unmodified across all cores available after "drag-and-drop"**

- **User supplies runFunc(iter) which maps integer (iter) to blur angle and rate**

- **Run functions are typically < 10 lines of Matlab**

- **Portal framework handles job, job status**

- **Optionally captures all output (text and graphics) to an html file as each run completes**

- **Automatic quick look provides displays of graphical output**

Matlab Example 2 (Naturally Parallel)

- **DoD Time-domain Analysis Simulation for Advanced used to determine accurately simulate reflectance and scattering of satellite materials Tracking (TASAT)**

- **Each iteration generates new light curve with different geometry**

- **>500 Matlab source files**

- **Also Includes compiled Fortran modules**

Matlab Example For Deep Parallel Processing

- **Matlab on current gen i7 processor**
  - **>> tic; fft2(rand(10000)); toc;**
    Elapsed time is 7.320237 seconds.
- **Typical MFBD image processing will require hundreds of forward and inverse 2-D fft's to estimate a single Object and PSF**
- **2D fft (one of many examples) is a naturally parallel**
- **Useful, for example, for near real-time image processing**

Matlab Node

```
image = zeros( 10000, 10000)
while ~converge

    limage = fft2( image);
    estimage = limage * Ppsf;
    .
    .
    errEst =
end
```

<u>Unmodified</u> User Script

Mex interface overloads default fft2

If data size sufficiently large invokes HPC Cluster fft else default Matlab fft2

Linux Cluster

Node 1	
	Node N

- **Example Multi-Frame Blind Deconvolution (MFBD)**

- **fft2 Matlab function is overridden to use compute cluster when warranted by data size and cluster loading**

- **Concept demonstration will be extended to other functions**
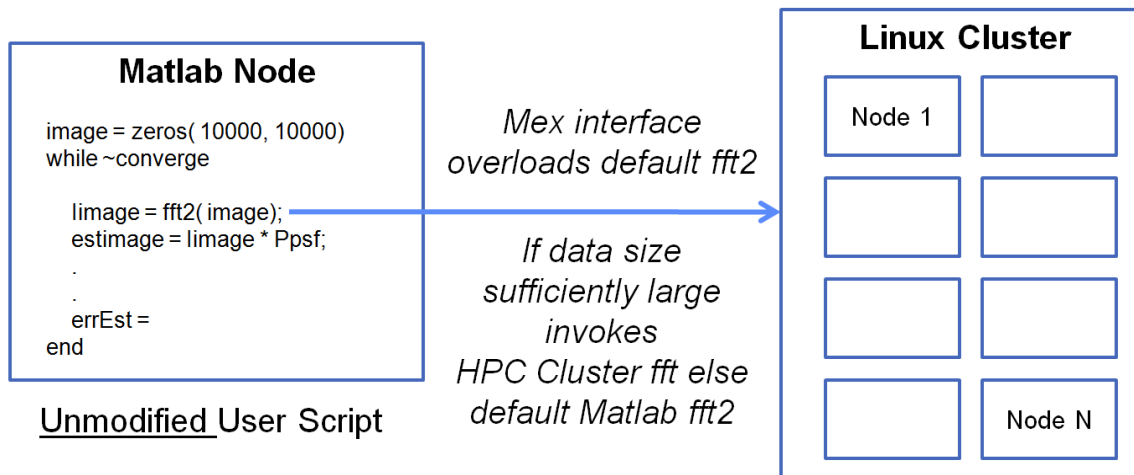
Future Capabilities

- **Concept demonstration portal live at MHPCC for a limited number of Kestrel and Matlab users (1K to 5K cores TBD) Q1 of 2012.**

- **Additional CREATE applications**

- **Incorporation of Utility Server functionality for web server scalability including HW/SW switching for redirection. VTK and ParaView technologies will be explored using the specialized Utility Server nodes that provide large memory and graphical processing capabilities while retaining the zero footprint requirement.**

- **Concept demonstration of how portal could automatically scale using resources across DSRCs (ERDC and MHPCC initially) without requiring user interaction.**

- **Enhanced Data Management will investigate more sophisticated data sharing with the storage initiatives such as the HEUE Center Wide File System (CWFS) and SRB implementations within the HPCMP.**

- **Graphical parallel programming for Matlab. Drag and drop capabilities are extended to include synchronization and shared memory concepts that once components are interconnected graphically automatically interface to HPC resources.**

- **Naturally parallel programming infrastructure for other languages**

Summary

- **Concept demonstration Portal is on track to demonstrate the high utility in providing HPC services for CREATE and Matlab applications**

- **Three prototype projects using Kestrel at MHPCC have been identified within the AF Aeronautical Systems Center (ASC)**

- **HPC Matlab that does not require HPC knowledge should attract a new user base**

- **AF Space Vehicles Directorate plans to explore the potential of permanently providing TASAT/PowerTASAT capabilities within the portal environment**

- **Our longer term effort is to work closely with other Government sponsors and targeted HPC user communities to identify additional applications that should be migrated to the portal environment**

Thank You

AFRL/RDSM

Questions?
www.maui.afmc.af.mil