Bridging the Gap between Scientific Workflow Tool to High-End Computing Capability

Course: Architecture and Design, 96-705
Semester: Fall 2012
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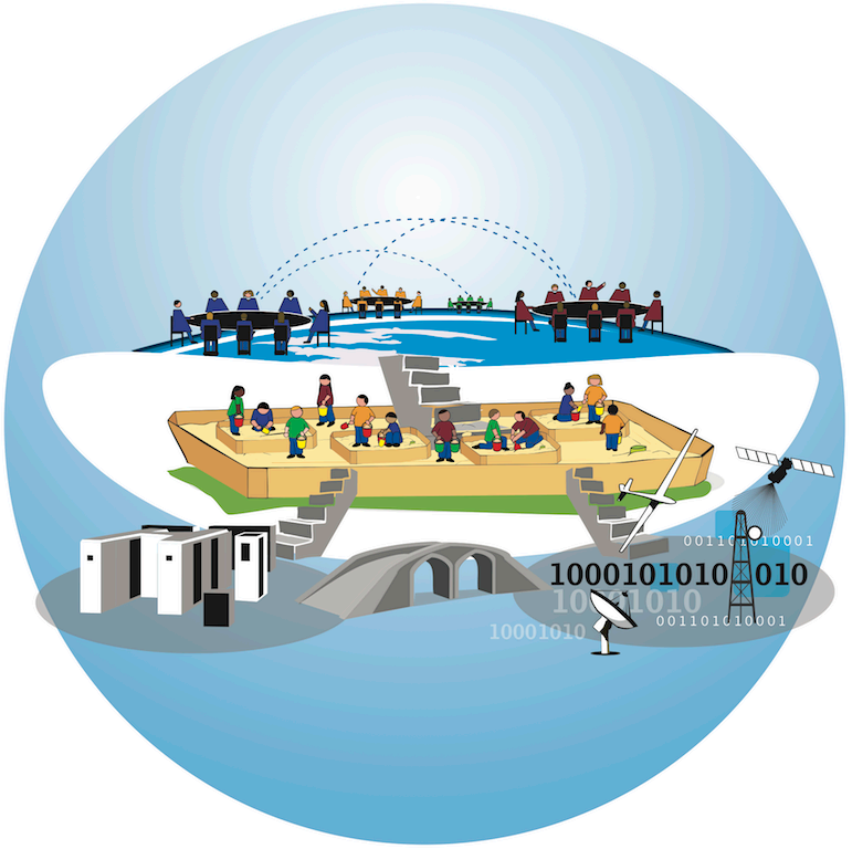
Roadmap

- Background
- Motivation & Goals
- Design
- Implementation
- Conclusions

NASA Earth Exchange Platform



A collaborative compute platform that improves the availability of Earth science data, models, analysis tools and scientific results through a centralized environment that fosters knowledge sharing, collaboration, innovation and direct access to compute resources.

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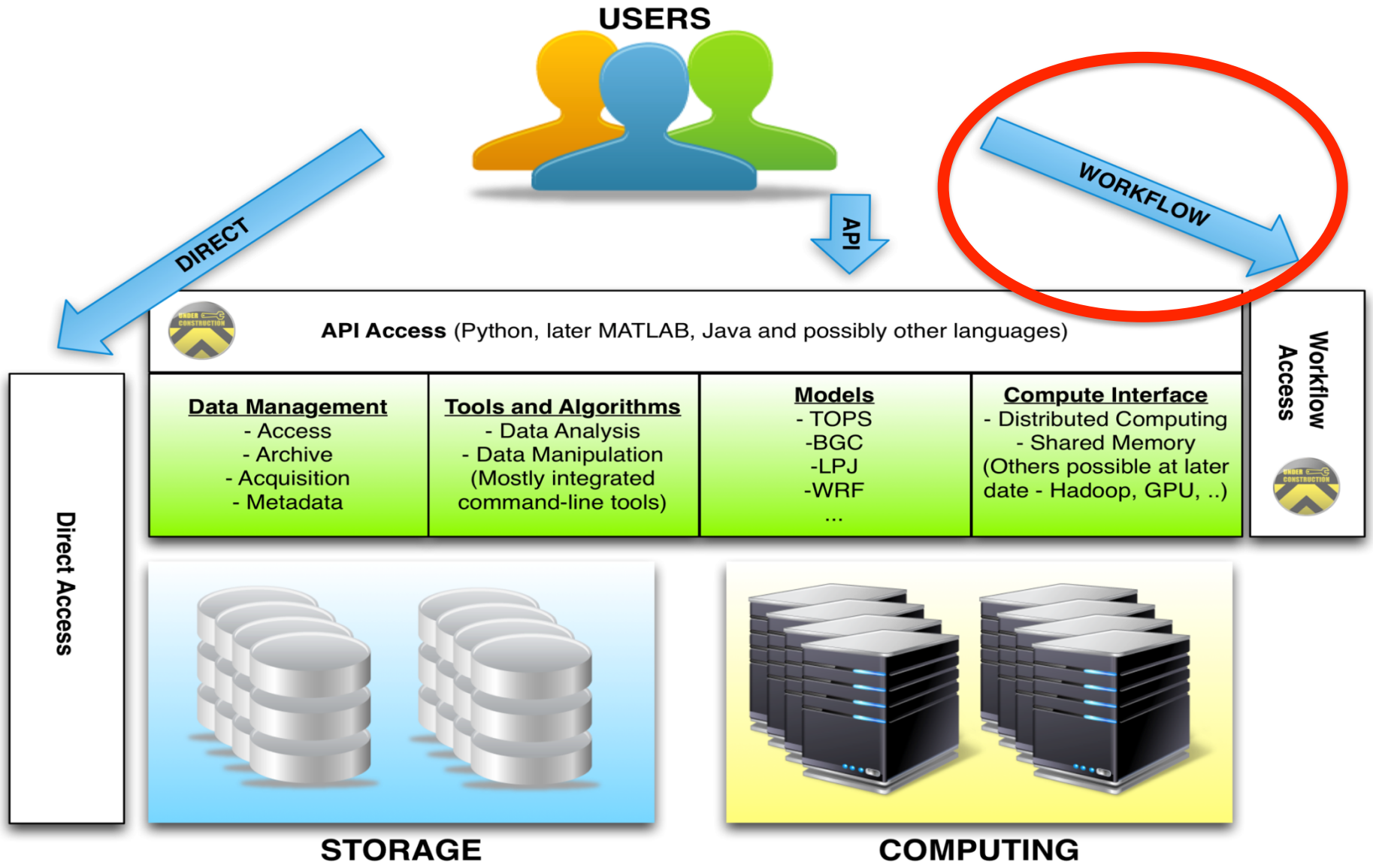
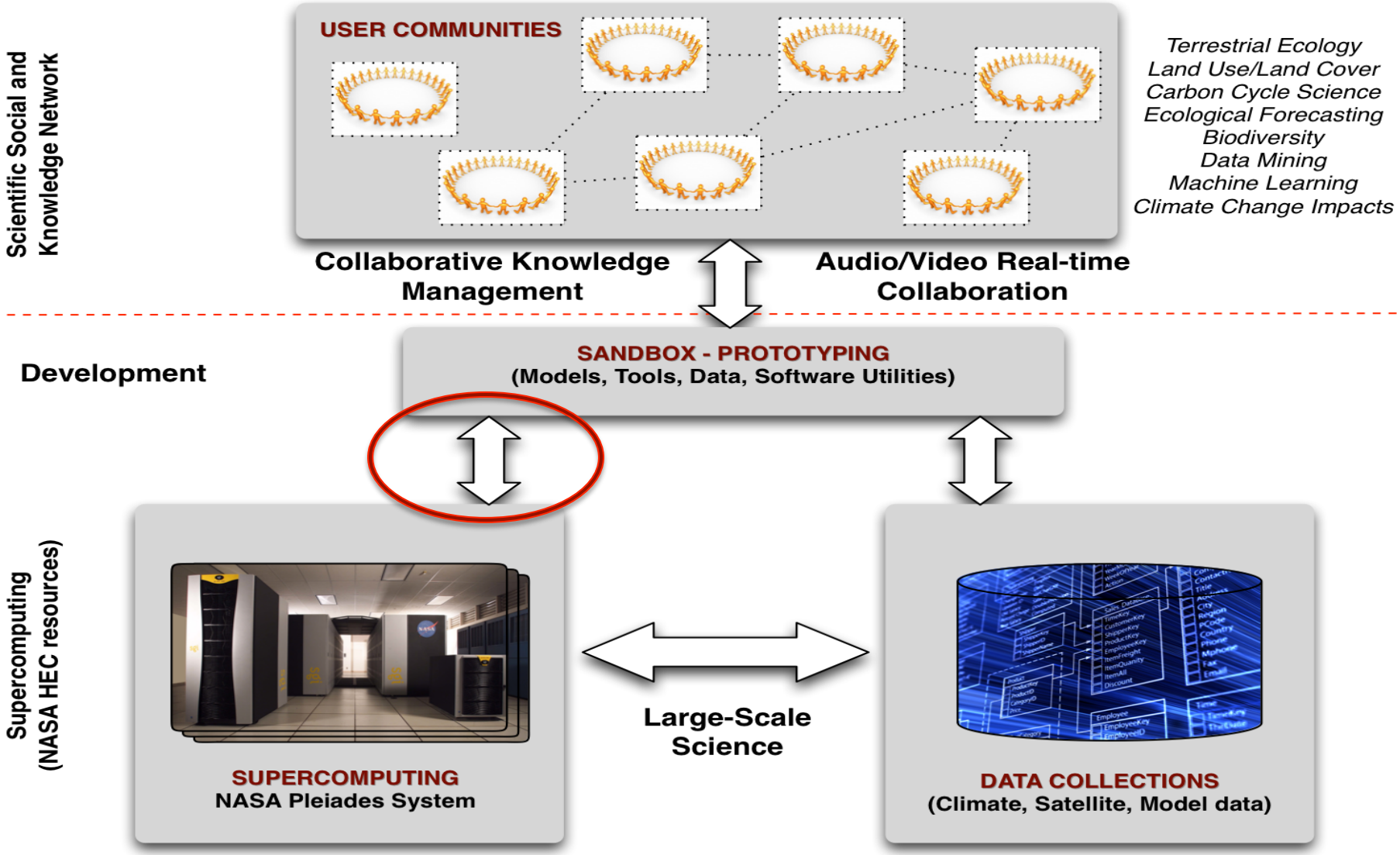
Single Access Point



Workflow Context



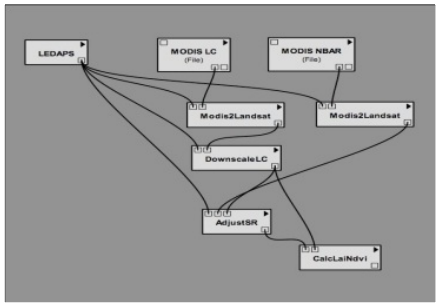
Project Motivation and Goal

- Motivation:
  - Vistrails is a scientific workflow management system
  - NEX scientists are currently using VisTrails workflow management system, but VisTrails does not link to HECC directly

- Goal: Bridge the gap between VisTrails and HECC
- Advantages
  - Leverage the supercomputing capabilities
  - Automate the process of moving code and computation from development environment to supercomputing environment
  - Scientists focus on science
  - NEX released from technical support

Bridge Between VisTrails & HECC

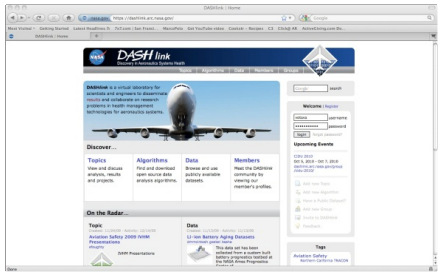
Workflow Design using VisTrails



Iterative Refinement/
Distributed Collaboration

Full-scale Execution

On-Line Result Sharing and
Process Re-use



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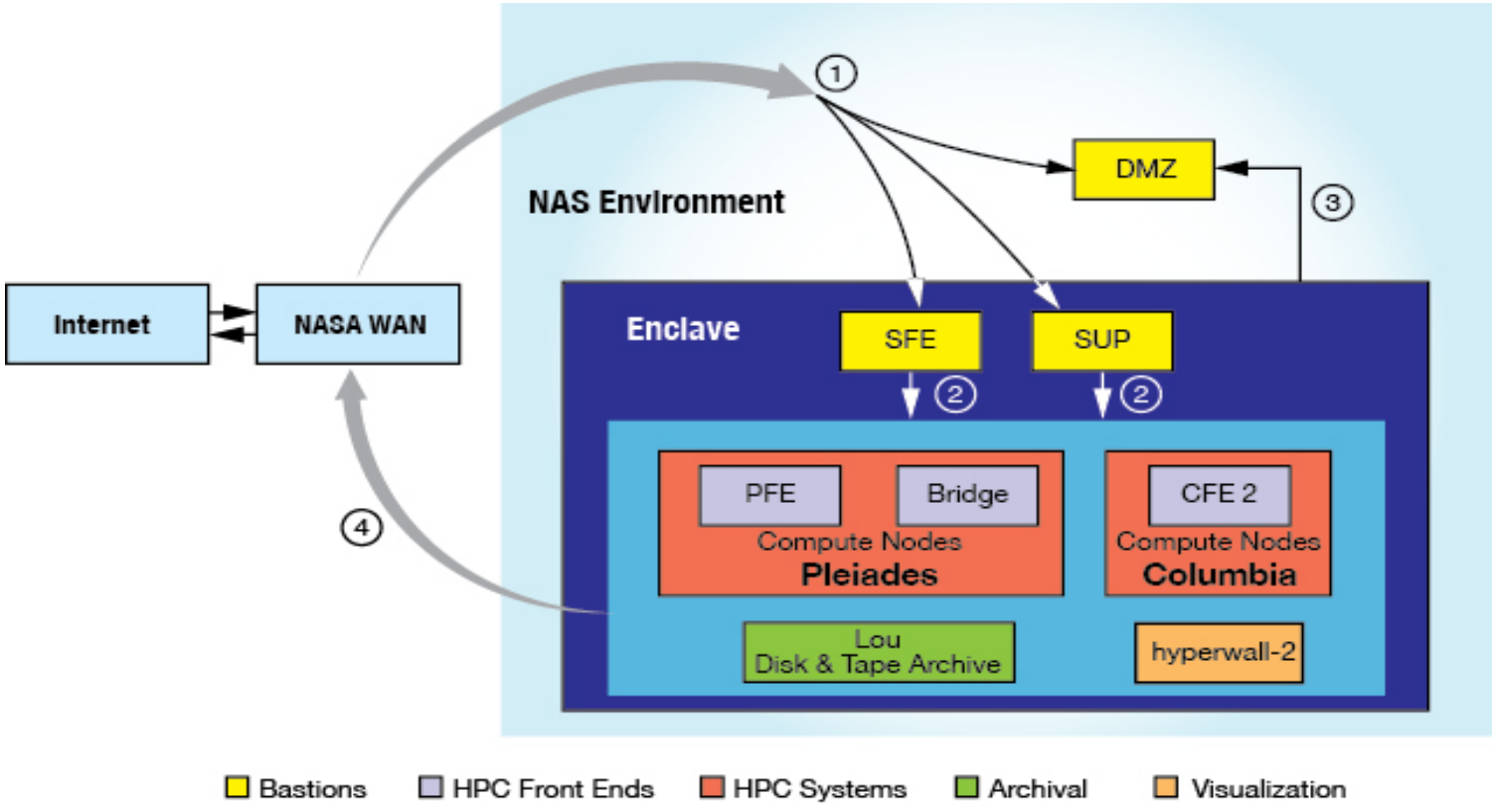
HECC Environment

- Types of Nodes
  - Secure Front-End (SFE) Nodes
  - Pleaides Front-End (PFE) and Bridge Nodes
  - Portable Batch System (PBS) Nodes
  - Four Types of Compute Nodes
- Access Limitation
  - Users can only access the computing platform through SFE
- PBS
  - Users can access PBS using qsub/qstat commands from PFE or bridge nodes

NAS Architecture



1. Inbound traffic going to the NAS bastions: SFEs, SUP, or DMZ;
2. Inbound traffic from an SFE or SUP to a Pleiades or Columbia front-end system (bridge, PFE or cfe2);
3. Outbound file transfers through the DMZ
4. Outbound traffic from Pleiades or Columbia directly to remote systems.

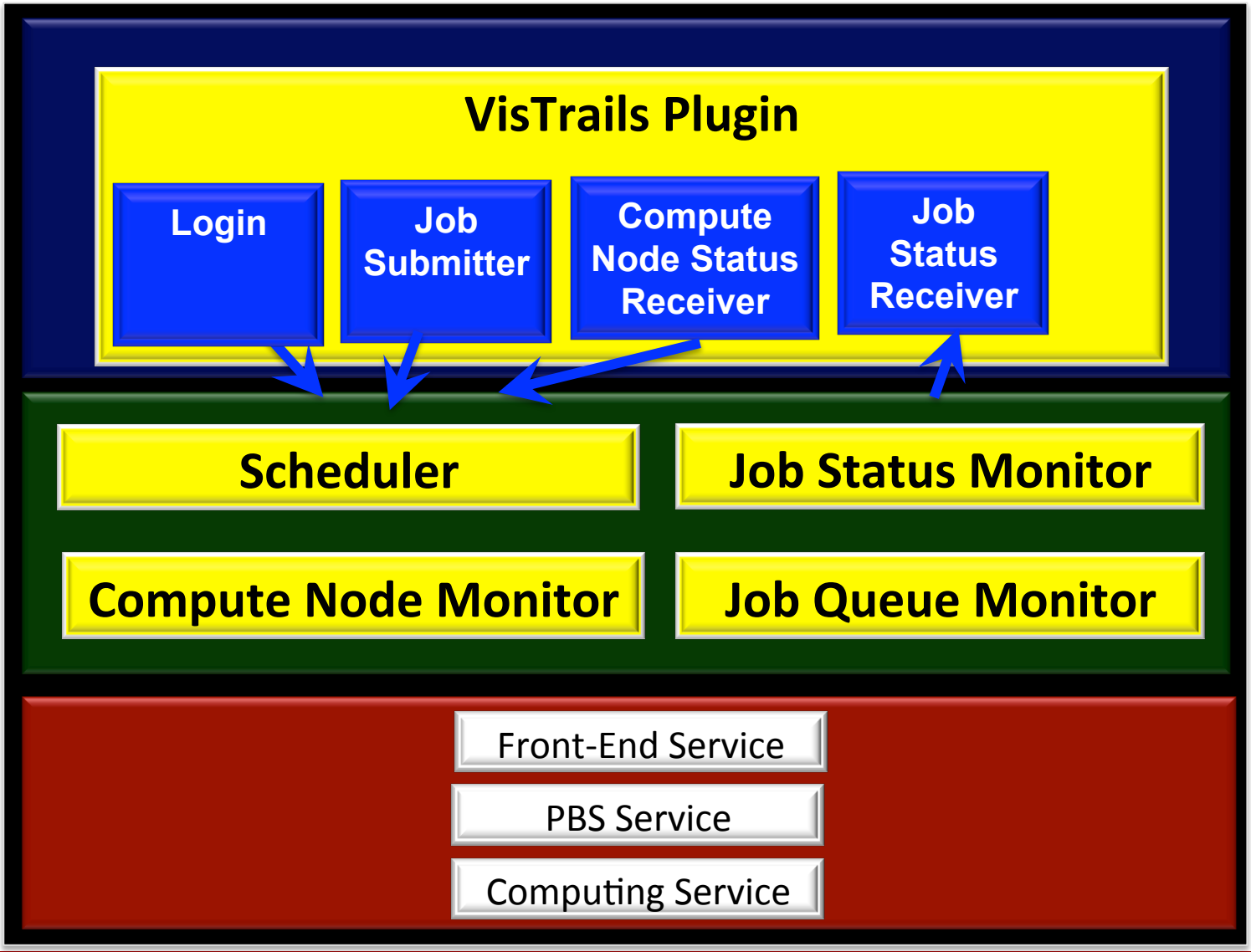
Issues, Constraints, and Strategies

- Issues & Constraints
  - Security (only SSH access from outside)
  - HECC access only through a PBS scheduler
  - Handle a large group of users and work items
  - 4 different types of nodes running on Pleiades
    - Differ in CPU types, number of nodes, memory size/node, speed
- Strategies
  - Identified relevant quality attributes
  - Design the system around the identified attributes
  - Validate our design with ATAM
  - Gather feedback from our client

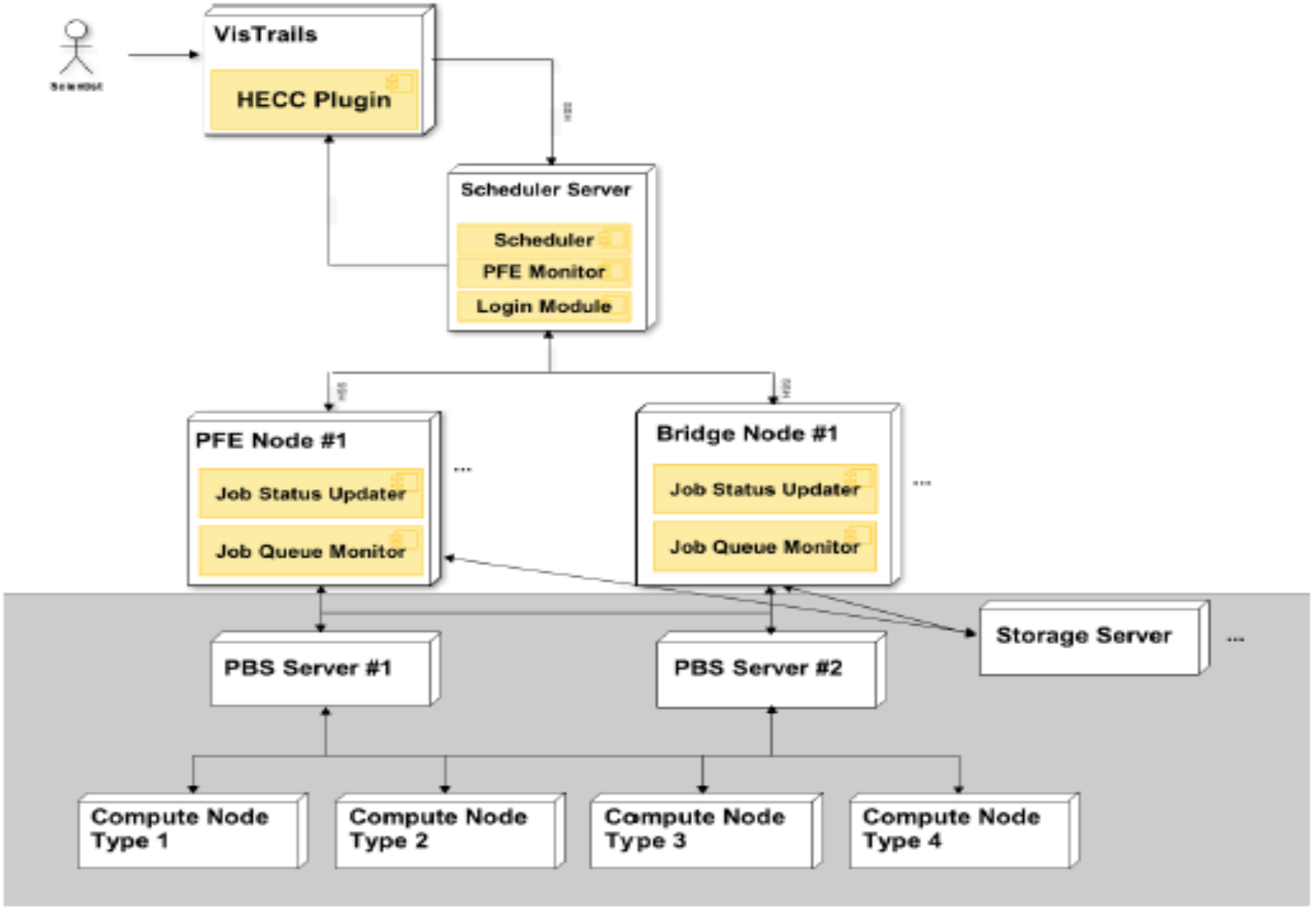
Strategy: ATAM Attributes

Quality Attribute	Description
Security	The system is protected from unauthorized access and data confidentiality is ensured.
Reliability	The system is stable and data integrity is guaranteed.
Availability	The system service is available on a 24/7 basis.
Usability	The system is easy to configure and use.
Performance	The system effectively utilizes computing resources.
Scalability	The system can accommodate a large number of users and data.
Extensibility	The system's functionalities are easy to extend and enhance.
Interoperability	The system can interface with different scientific workflow management software and commodity hardware.
Asynchronous Mode	The client can asynchronously retrieve job execution result from the system.

Architectural model



Deployment View



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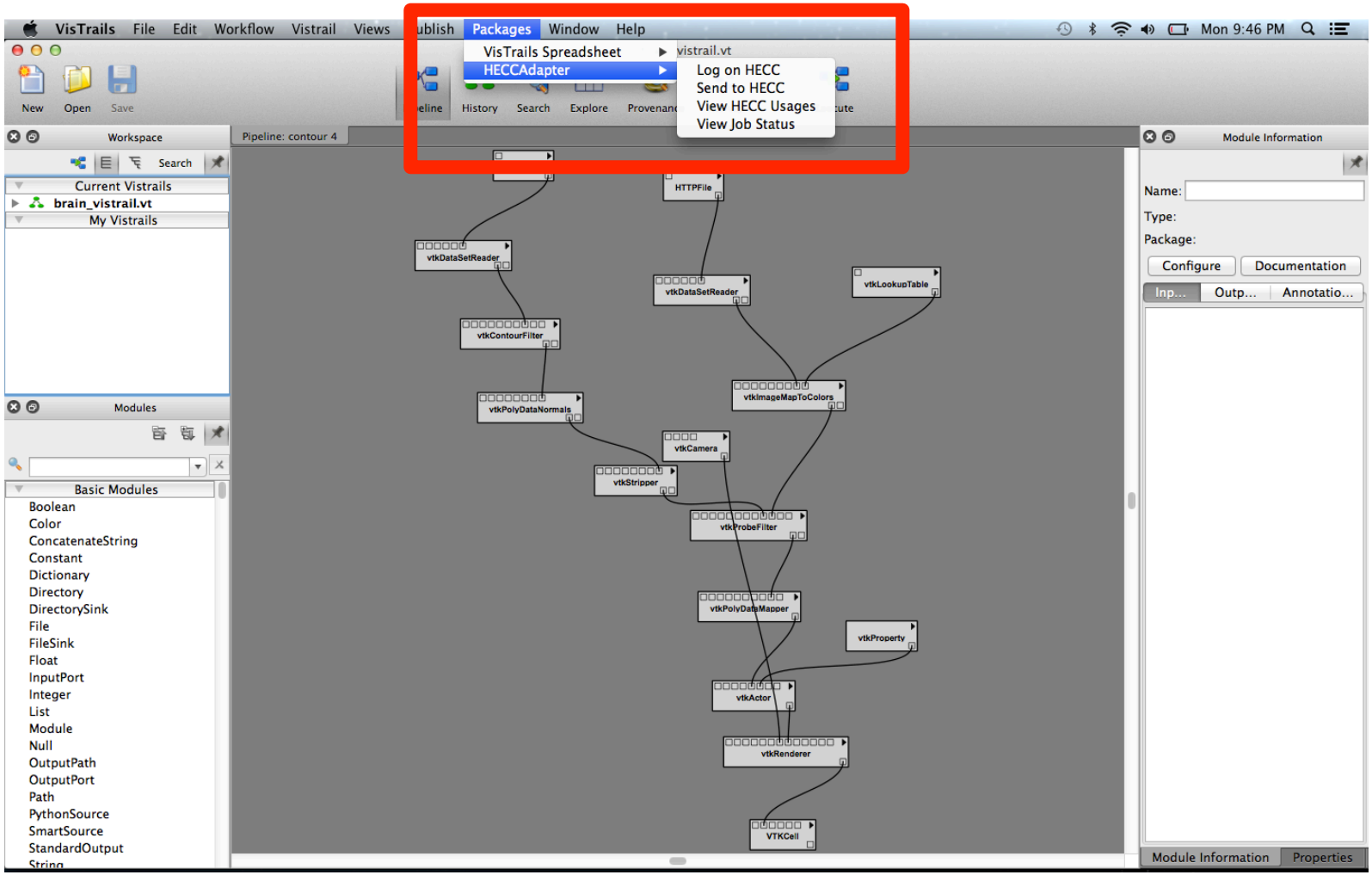
Prototype


VisTrails File Edit Workflow Vistrail Views
Packages Window Help
VisTrails Spreadsheet
HECCAdapter
vistrail.vt
Log on HECC
Send to HECC
View HECC Usages
View Job Status
Mon 9:46 PM
New Open Save
History Search Explore
Workspace
Search
Current Vistrails
brain_vistrail.vt
My Vistrails
Modules
Basic Modules
Boolean
Color
ConcatenateString
Constant
Dictionary
Directory
DirectorySink
File
FileSink
Float
InputPort
Integer
List
Module
Null
OutputPath
OutputPort
Path
PythonSource
SmartSource
StandardOutput
String
Pipeline: contour 4
HTTPFile
vtkDataSetReader
vtkDataSetReader
vtkLookupTable
vtkContourFilter
vtkImageMapToColors
vtkPolyDataNormals
vtkCamera
vtkStripper
vtkProbeFilter
vtkPolyDataMapper
vtkProperty
vtkActor
vtkRenderer
VTKCell
Module Information
Name:
Type:
Package:
Configure
Documentation
Inp...
Outp...
Annotatio...
Module Information
Properties

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Conclusions

- The project will help We provide a working base to future teams
  - Collect relevant information
  - Design and create prototype
  - Prototype 1: Run VisTrails in an external server, Monitor job statuses, Retrieve job results, UI Mockup
  - Prototype 2 (Current): Login module, Front-End node connection, Job completion notification, PBS conficuration
  - Release Candidate 1

- Long-term goals
  - Gain more accessibility to NASA's resources
  - Increase the number of scientists adopting NASA's computing ecosystem