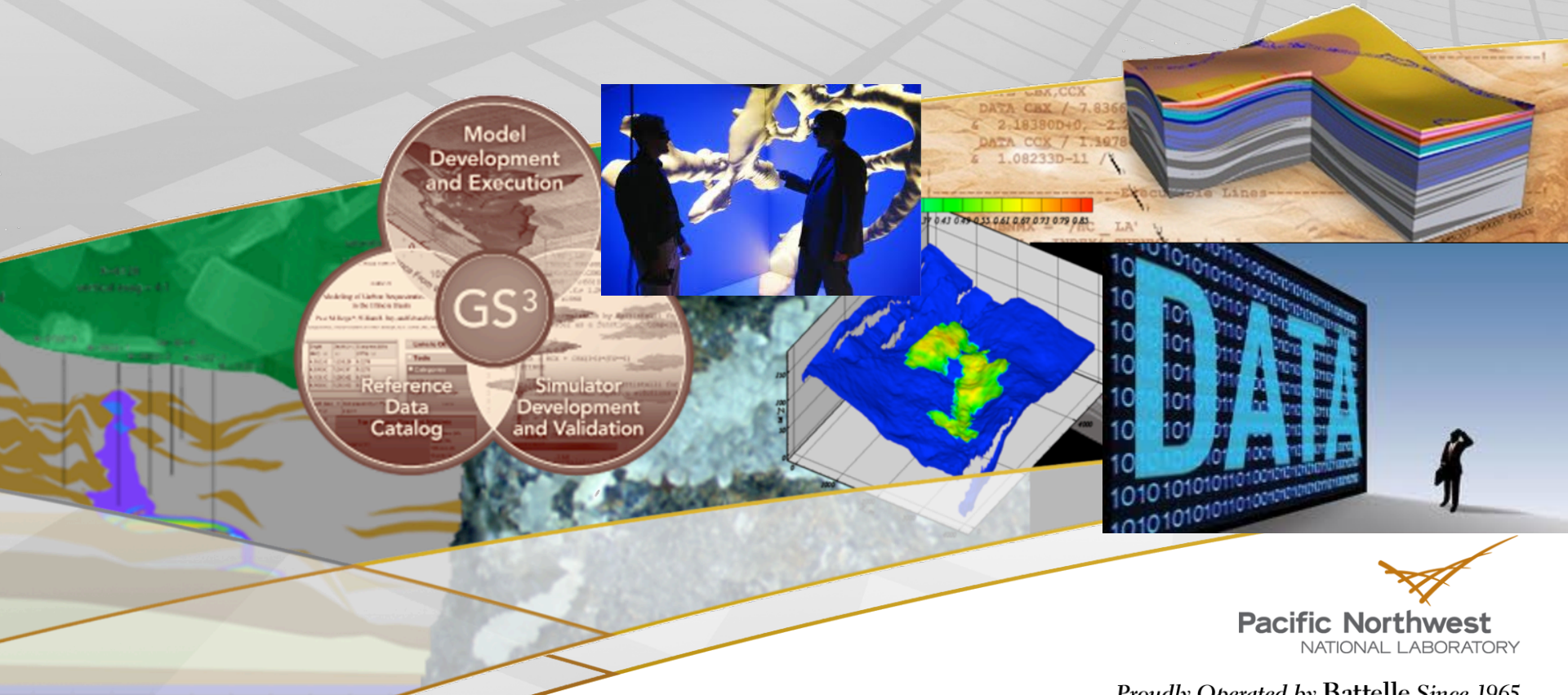


Velo: Knowledge and Tool Integration for Collaborative Scientific Projects

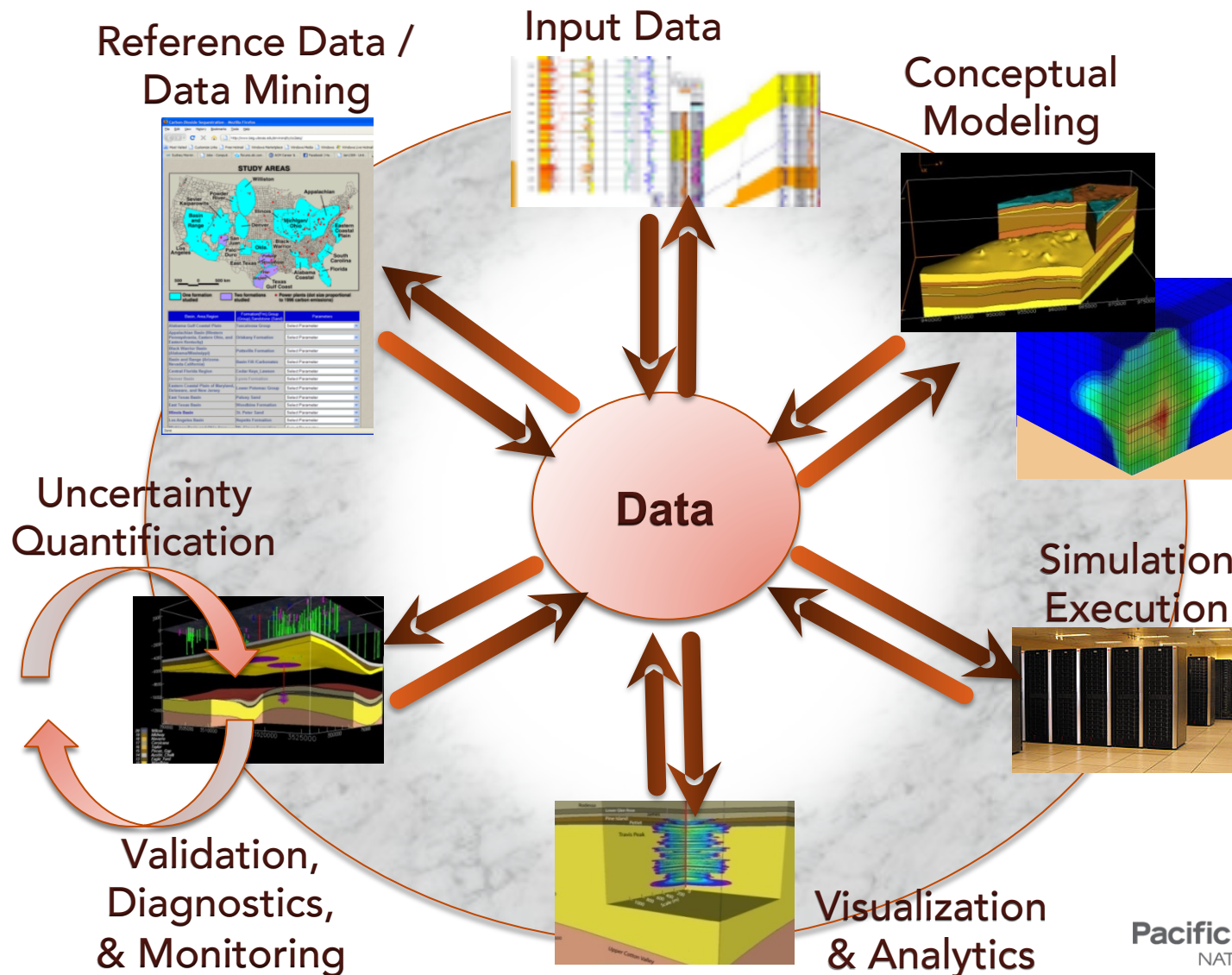
Carina Lansing, Kerstin Kleese van Dam



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Scientific Project Life Cycle

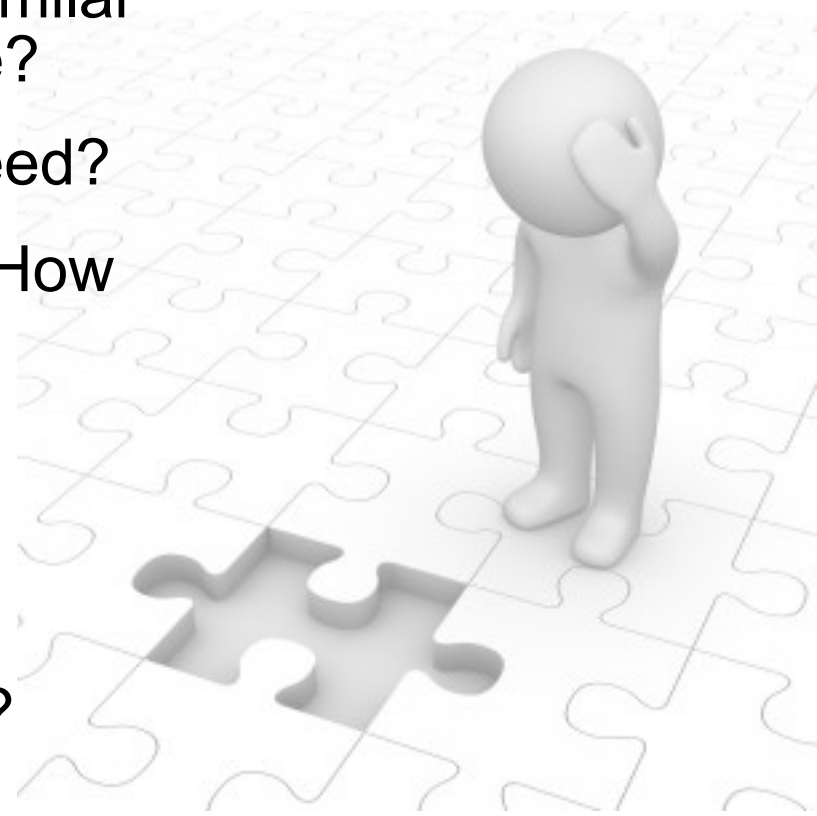


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Challenges to Scientists

- ▶ Has someone done something similar before? Is there a good example?
- ▶ How do I find the information I need?
- ▶ What are the best tools to use? How do I use them?
- ▶ I have to write another data converter<sigh>
- ▶ Can I reproduce my results?
- ▶ What did I do and how did I do it?
- ▶ How can I share my project “process” and data with others?
- ▶ Where is my data?

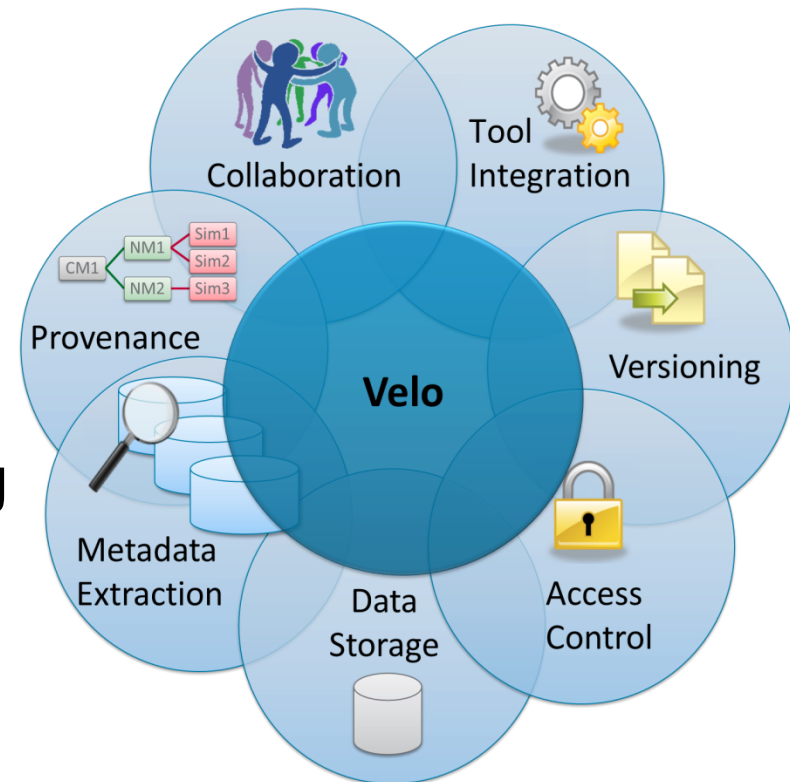


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Velo's Solution

- ▶ Full life cycle, integrated support for modeling, simulation, analysis, and visualization at any scale
- ▶ Data/metadata/relationship management
- ▶ Tool Integration
 - Connect tools to data
 - Chain tools together
- ▶ Simulation management, including UQ ensembles
- ▶ Collaboration across multi-disciplinary teams
- ▶ Provenance – who did what, when
- ▶ Open, Extensible, & Customizable

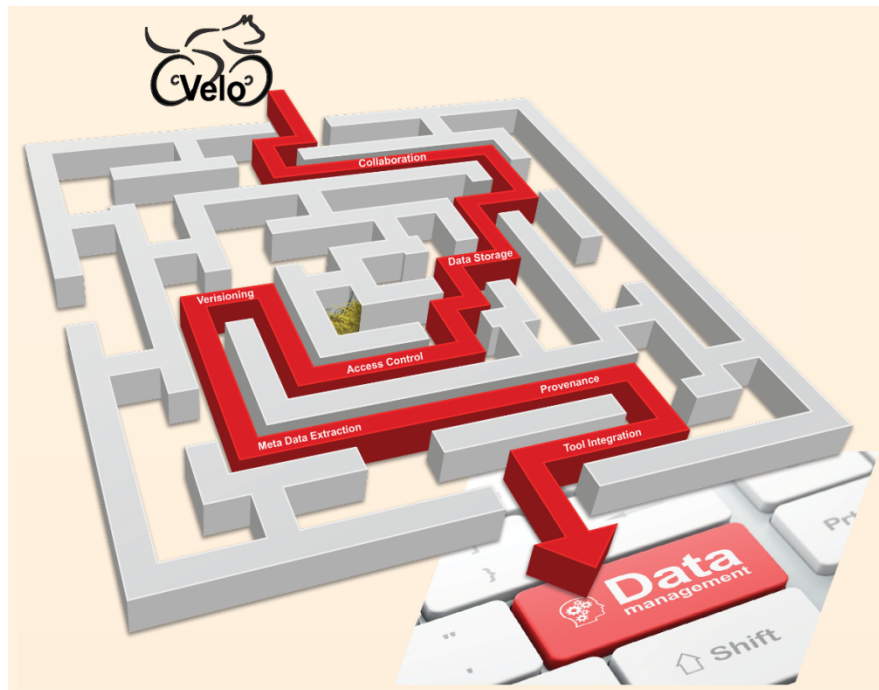


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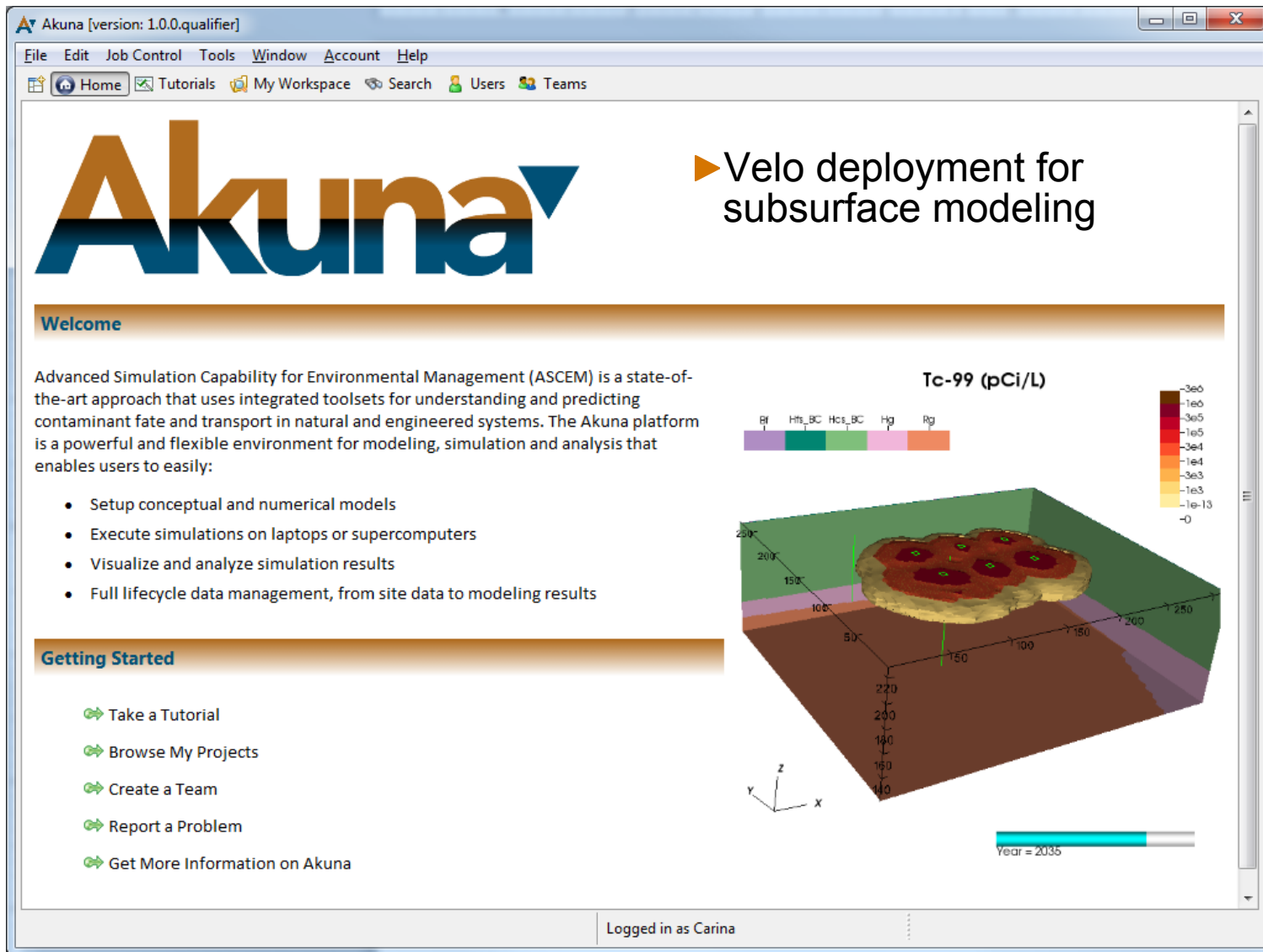
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Benefits

- ▶ Users can easily keep track of their scientific projects, even if data, tools, and collaborators are geographically distributed
- ▶ Low barrier of entry for HPC systems
- ▶ Easy to share data and tools (AppStore for science)
- ▶ Reproducible results
- ▶ Less time spent in data orchestration tasks = more time for science
- ▶ Reduce project costs, deploy new sites in weeks



Velo Use Case: Akuna



The screenshot displays the Akuna software interface. The title bar reads "Akuna [version: 1.0.0.qualifier]". The menu bar includes "File", "Edit", "Job Control", "Tools", "Window", "Account", and "Help". Below the menu bar are navigation buttons for "Home", "Tutorials", "My Workspace", "Search", "Users", and "Teams".

Akuna

Welcome

Advanced Simulation Capability for Environmental Management (ASCEM) is a state-of-the-art approach that uses integrated toolsets for understanding and predicting contaminant fate and transport in natural and engineered systems. The Akuna platform is a powerful and flexible environment for modeling, simulation and analysis that enables users to easily:

- Setup conceptual and numerical models
- Execute simulations on laptops or supercomputers
- Visualize and analyze simulation results
- Full lifecycle data management, from site data to modeling results

Getting Started

- Take a Tutorial
- Browse My Projects
- Create a Team
- Report a Problem
- Get More Information on Akuna

Logged in as Carina

Tc-99 (pCi/L)

Legend: Bf, Hts_BC, Hcs_BC, Hg, Pg

Color scale: -3e6, -1e6, -3e5, -1e5, -3e4, -1e4, -3e3, -1e3, -1e-13, 0

Year = 2035

The 3D model shows a subsurface cross-section with a central plume of Tc-99. The vertical axis (z) ranges from 140 to 220. The horizontal axes (x and y) range from 50 to 250. A color scale on the right indicates concentration levels from 0 to -3e6 pCi/L. A legend above the model identifies different material types: Bf (blue), Hts_BC (green), Hcs_BC (yellow), Hg (orange), and Pg (red). A "Year = 2035" indicator is shown at the bottom right of the model.

Velo Use Case: Akuna

The screenshot displays the Akuna software interface (version 1.0.0.qualifier) with a menu bar (File, Edit, Job Control, Tools, Window, Account, Help) and a toolbar. The main workspace shows a file explorer view of the path `/User Documents/D3k870/Richard-1D-transport_exa/monte-carlo`. The left sidebar shows a tree view of the workspace structure, including folders like `3D.PE`, `BC_Cribs`, `lightning`, `Richard-1D-transport_exa`, `monte-carlo [Success]`, `morris-one-at-a-time [Success]`, `single-run [Success]`, `Richard-1D-transport_exa-old`, `tutorial`, `Developers`, `Dtixier`, and `projects`. The main pane shows a table of files:

Name	Size	Type	Creator	Creat
Analysis		cmsfile/collec...	D3k870	05/21
Inputs			D3k870	05/21
Outputs		cmsfile/collec...	D3k870	05/21

Below the file explorer, there are two tabs: `Summary: monte-carlo` and `Preview: monte-carlo`. The `Summary: monte-carlo` tab is active, showing the following job state information:

Job State:

- Job ID: 6873204.hopque01
- Code ID: UQ
- Status: Success [Plot](#)
- Job User: vfreedma
- Job Machine: hopper.nersc.gov
- Queue: debug
- Processors: 2400
- Time Limit: 0:30:0
- Run Dir: /global/homes/v/vfreedma/scratch/amanzi/Richards-1d/UQ_monte-carlo_121313_201340
- Start Time: Fri Dec 13 20:17:25 PST 2013
- Stop Time: Fri Dec 13 21:00:02 PST 2013

At the bottom of the window, it says "Logged in as Carina".

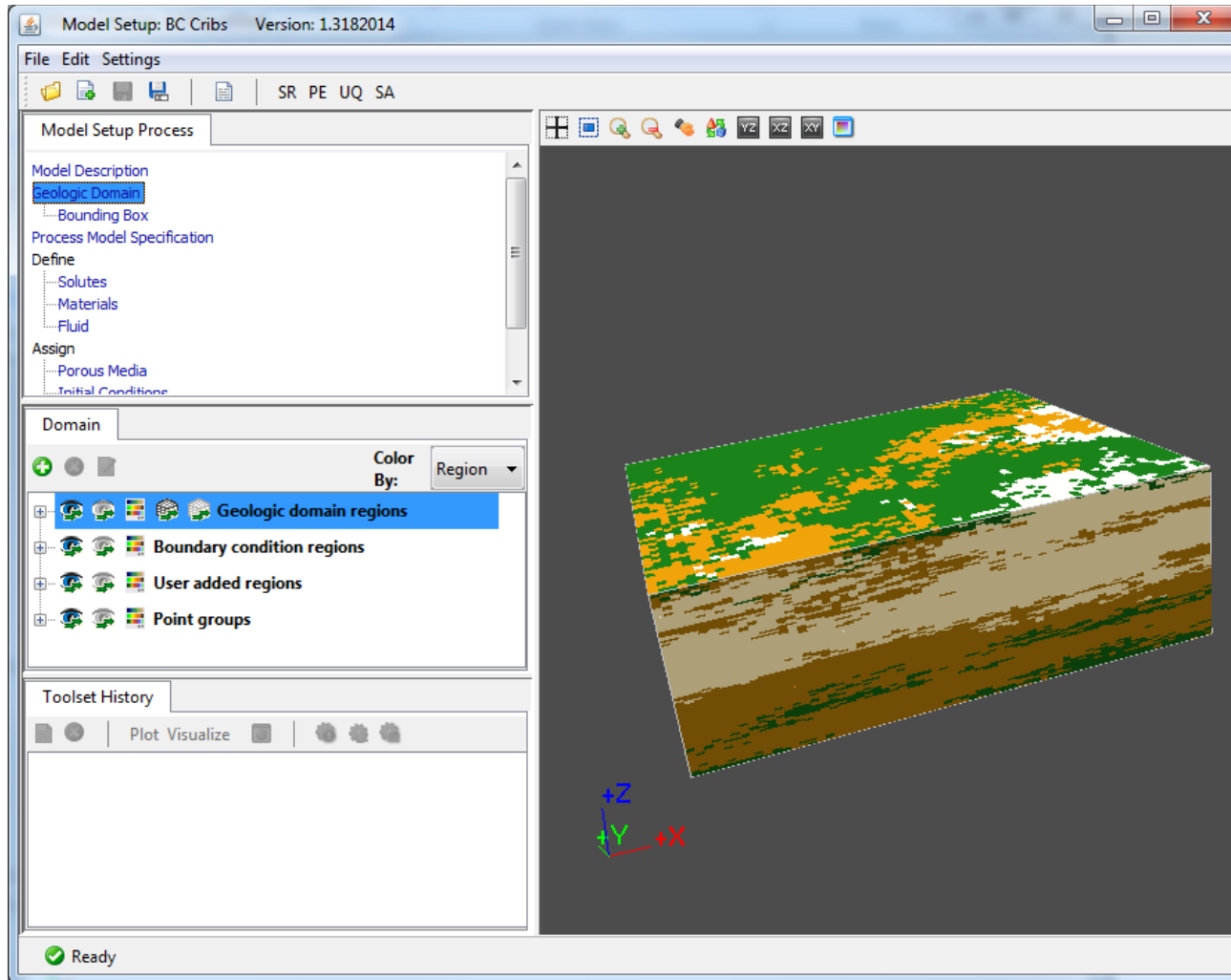
- ▶ Manage modeling projects, individual or collaborative
- ▶ View provenance information for each simulation run
- ▶ Simple explorer-like look and feel



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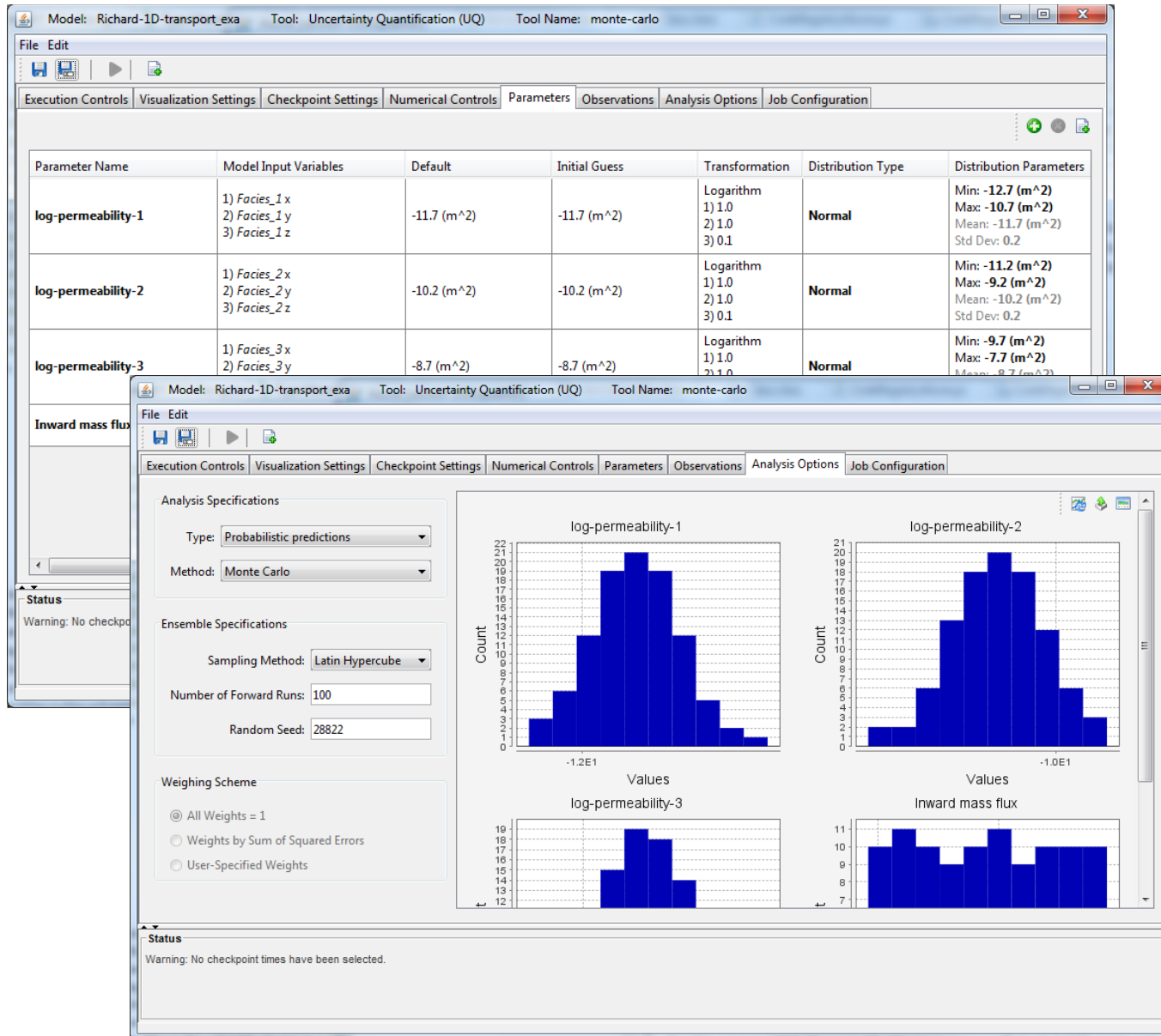
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Velo Use Case: Akuna



- ▶ Integrate 3D setup tools for defining conceptual model and input parameters
- ▶ Includes mesh generation
- ▶ Alternatively can define setup via input files for advanced users

Velo Use Case: Akuna



- Integrated ensemble configuration tools for controlling statistical ensembles such as uncertainty quantification and sensitivity analysis



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Velo Use Case: Akuna

The screenshot shows a software window titled "Model: Richard-1D-transport_exa Tool: Single Run (SR) Tool Name: single-run-newAmanzi". The window has a menu bar with "File" and "Edit", and a toolbar with icons for file operations and execution. Below the toolbar is a tabbed interface with tabs for "Execution Controls", "Visualization Settings", "Checkpoint Settings", "Numerical Controls", "Parameters", "Observations", and "Job Configuration". The "Job Configuration" tab is active, showing the following settings:

Machine: hopper.nersc.gov

Machine Settings:

Run Directory:

Username: Allocation Account: Job Queue:

Wall Time: hours minutes seconds

Processors: [1..]

Processors per Task: [1..]

Agni Parameters:

Agni Command:

Amanzi Command:

Max Simultaneous Simulations:

Agni verbosity level:

Status

Warning: No checkpoint times have been selected.

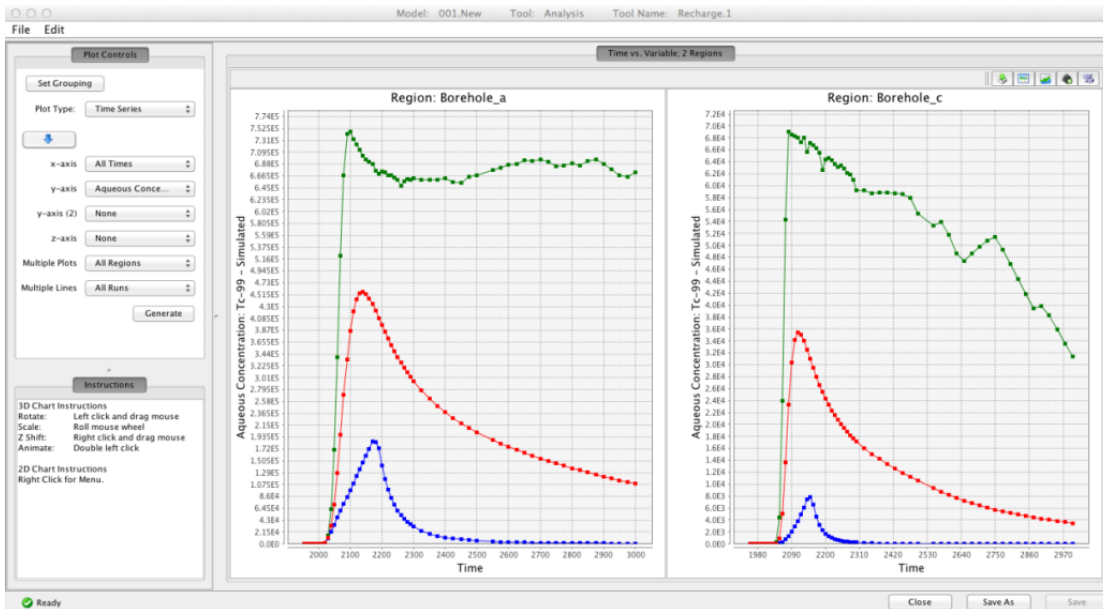
- ▶ Integrated HCP job configuration
- ▶ Simple user interface – “one click” launch
- ▶ Real-time run monitoring
- ▶ Automated capture of provenance information and output data
- ▶ Integration of outputs into analytic tools



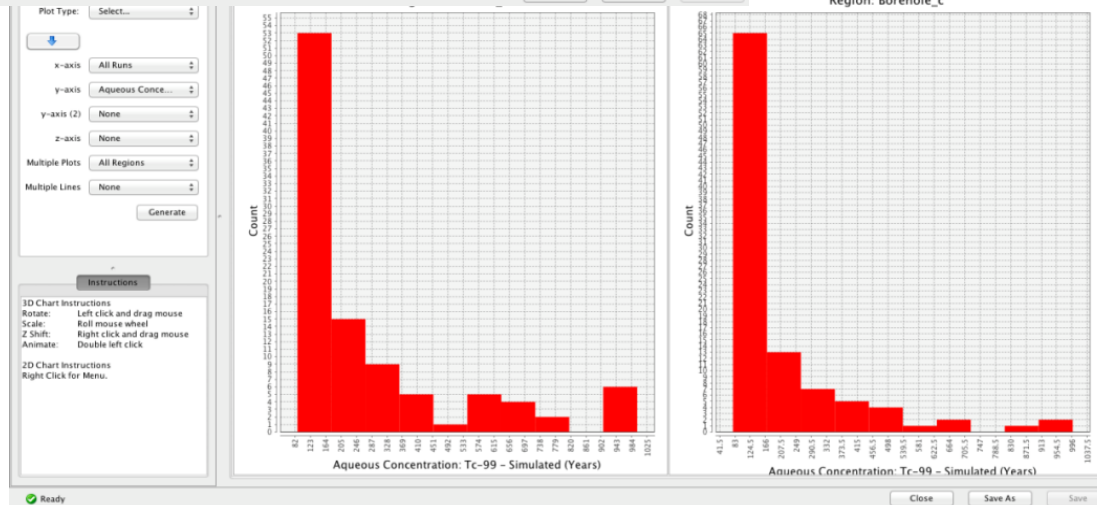
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Velo Use Case: Akuna



► Analyze/compare statistical ensemble runs with integrated temporal analysis tools

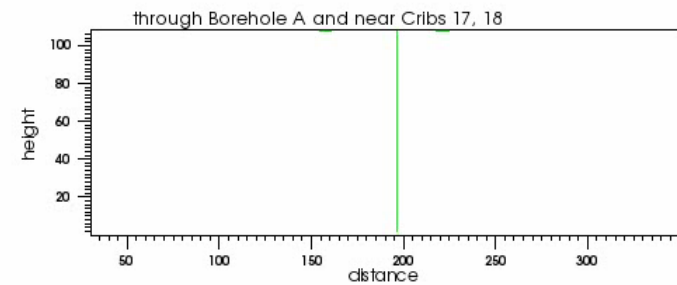
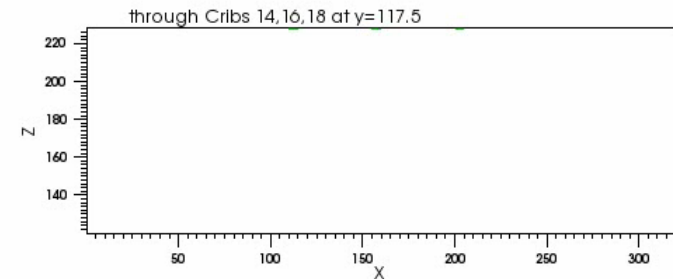
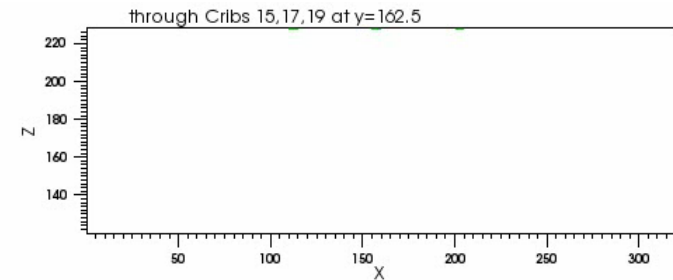
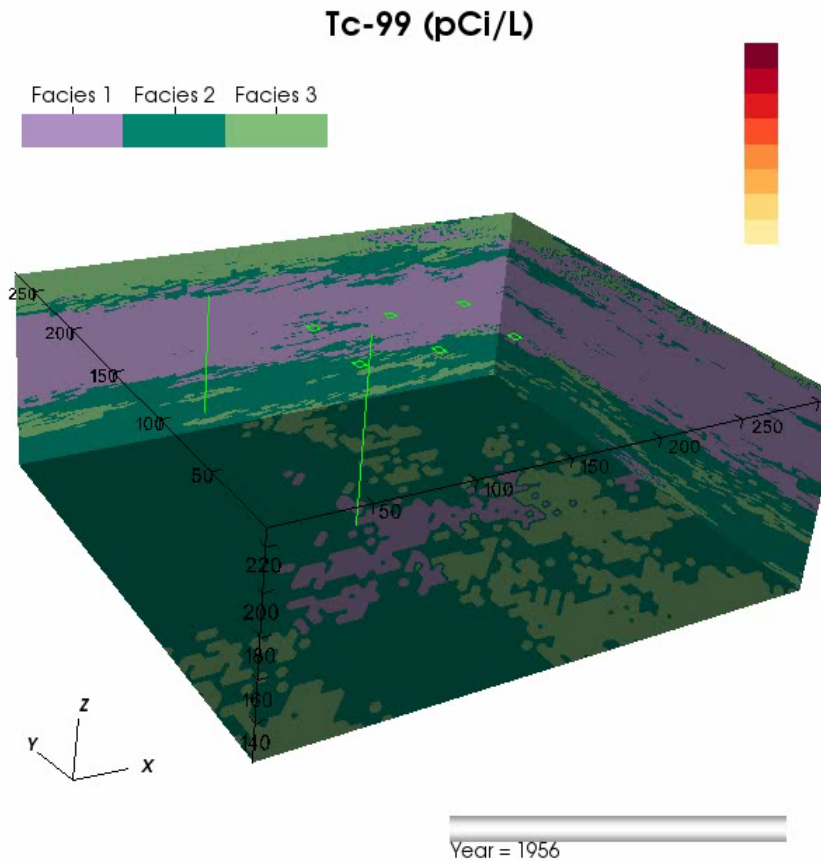


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Velo Use Case: Akuna

- ▶ Analyze simulation results with integrated spatial visualization via VisIt 3D cluster-based visualization

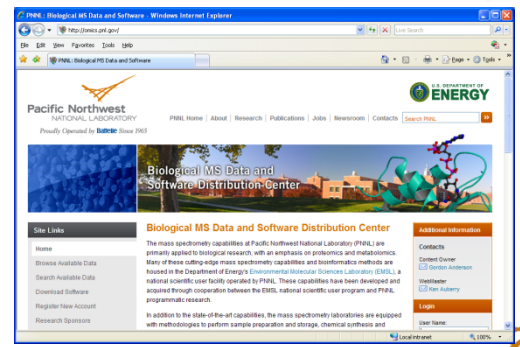
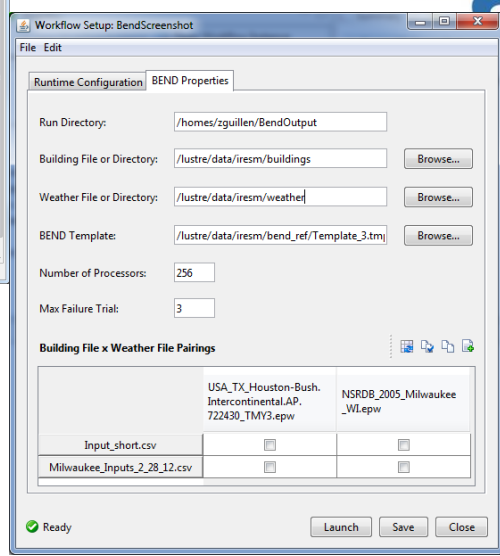
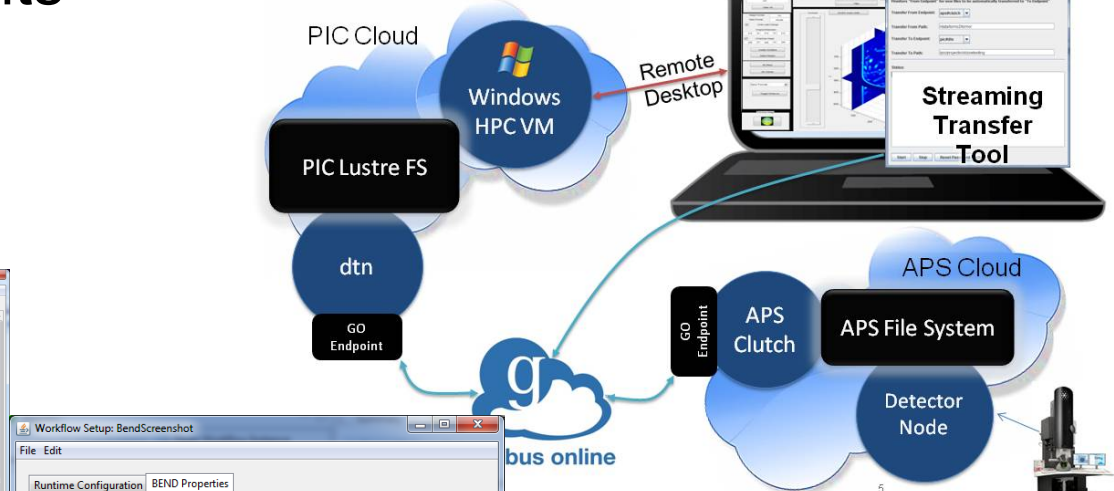
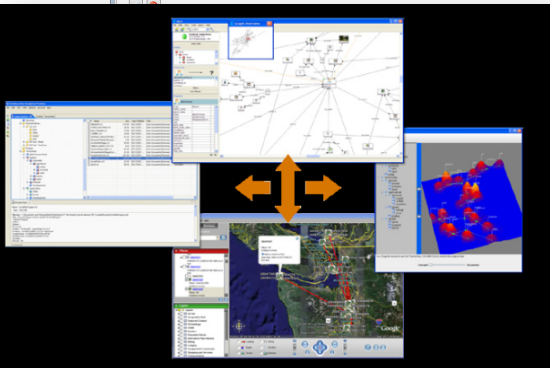
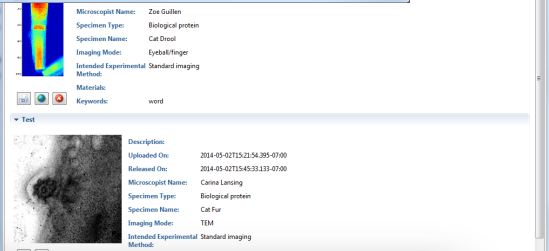
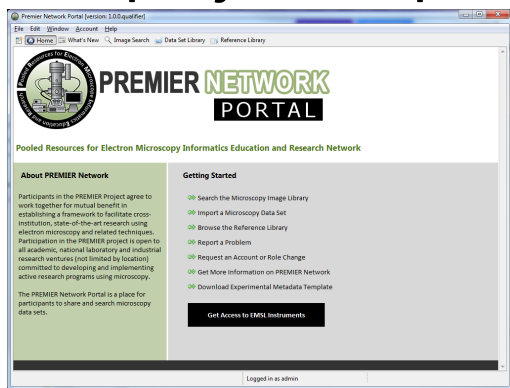


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Velo's Different Faces

- ▶ Velo is highly customizable and each deployment has its own set of capabilities and look and feel, dependent on project requirements



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