



Multitier Portal Architecture for Thin- and Thick-client Neutron Scattering Experiment Support

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OAK RIDGE NATIONAL LABORATORY
U. S. DEPARTMENT OF ENERGY



Funded by Spallation Neutron Source, Oak Ridge National Laboratory

- **Motivation**
- **Spallation Neutron Source Background**
- **Multitier Portal Architecture (MPA) Introduction**
- **Thin-client Tiers**
 - Tier I: Spallation Neutron Source Portal
 - Tier II: Spallation Neutron Source OGCE Portal
- **Thick-client Tiers**
 - Tier III: Eclipse RCP GumTree+ Application
 - Tier IV: Eclipse IDE
- **Conclusion**
- **Future Work**

- **Problem Identification**

- Providing robust authentication, authorization, and user group management.
- Providing the ability for user customizable portal interfaces that meet the expectations of researchers and scientists.
- Providing a scalable and flexible architecture for novice to sophisticated portal user groups.
- Providing an integrated application development, debugging, and execution environment.
- Integration of emerging technologies and design patterns into a portal architecture.

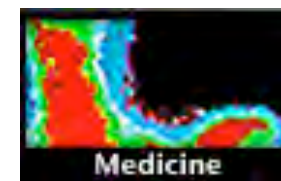
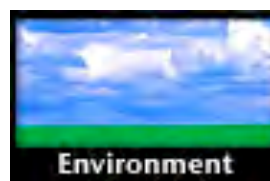
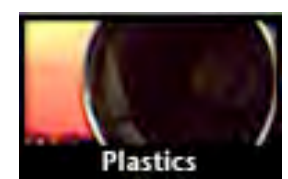
- **Solution Methodology**

- Utilize existing technologies wherever possible.
- Provide an architectural design that maximizes information technology service reuse while providing a customizable user interface that scales with user sophistication and requirements.
- Do not re-invent the wheel!

Spallation Neutron Source (SNS)



- **Facility Specifications and Construction**
 - \$1.5 Billion Dollars
 - 5 Years of Construction Project by Thousands of People...
 - World's Largest, Most Powerful Neutron Accelerator
 - Order of Magnitude Larger Than Any Existing Facility! (1.4 MW)
- **Use Neutrons to Determine Atomic or Molecular Structure**
 - Materials, Chemistry, Engineering, Polymers, Structural Biology, Superconductivity...



Spallation Neutron Source (SNS)



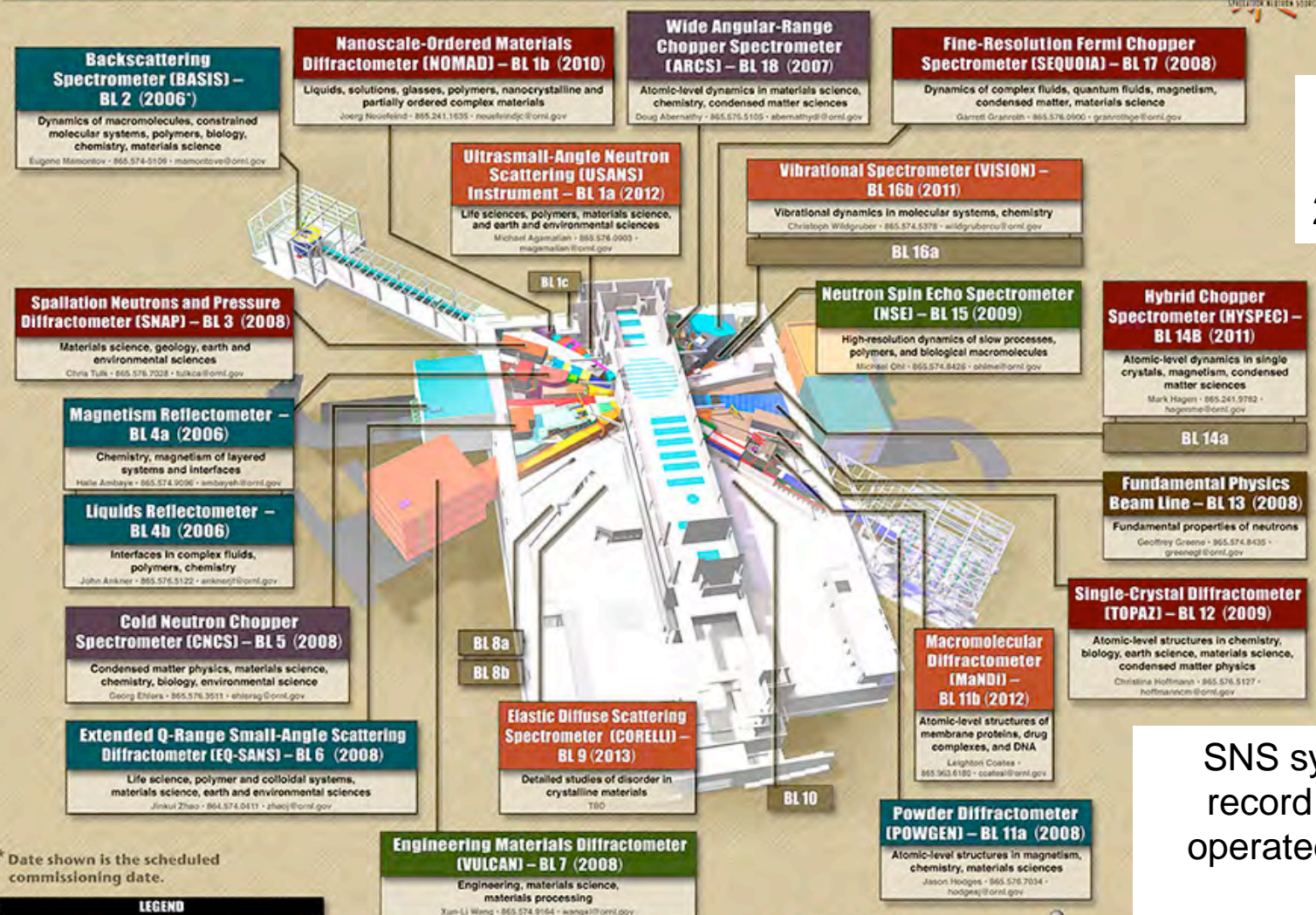
SNS Neutron Scattering Facility



Spallation Neutron Source (SNS)



Spallation Neutron Source

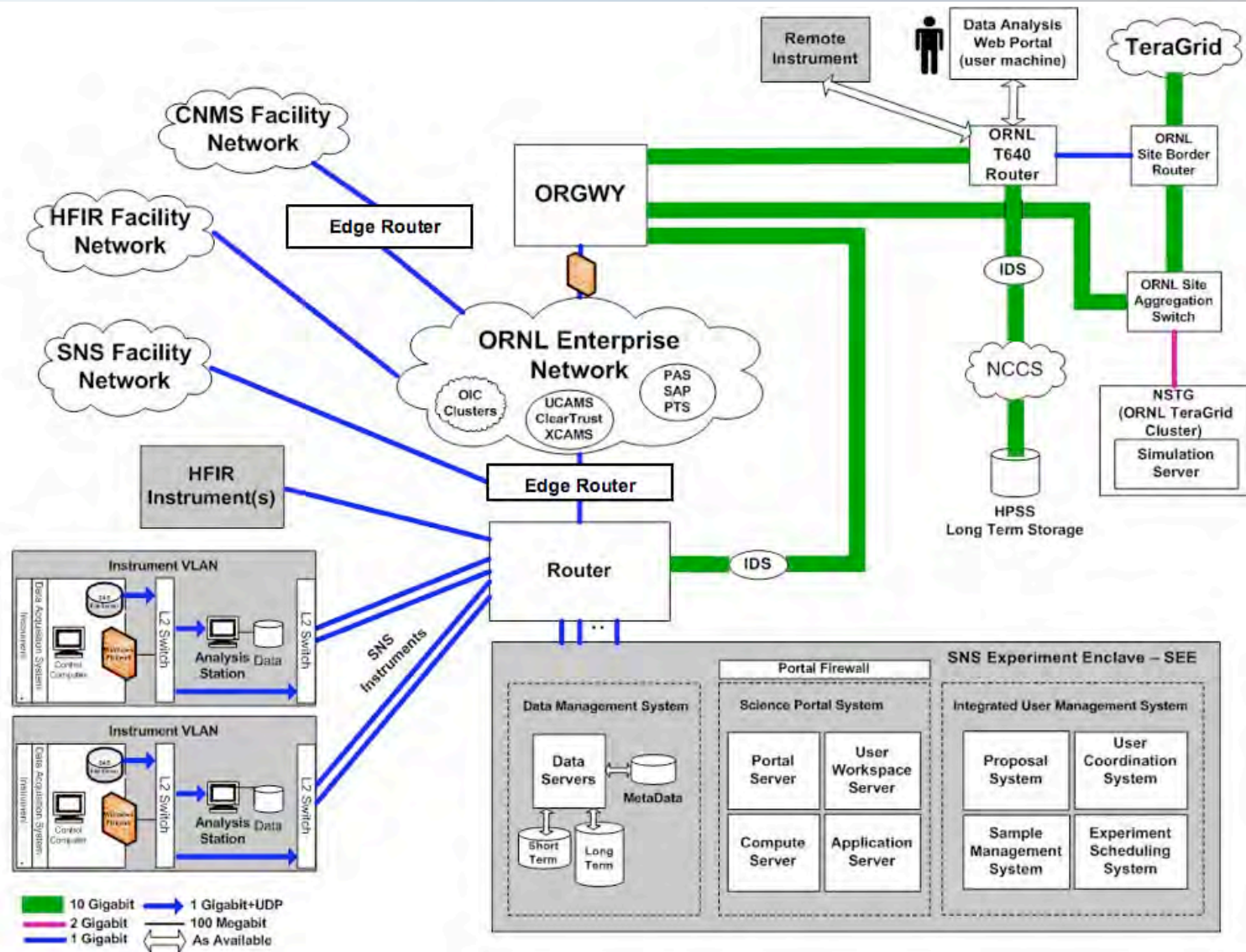


18 beam lines
with
24 instruments

SNS systems set world
record in August 2007
operated at 183 kilowatts

—
surpassing the previous
record established at the ISIS
research facility in the UK

Spallation Neutron Source (SNS)



Multitier Portal Architecture (MPA)



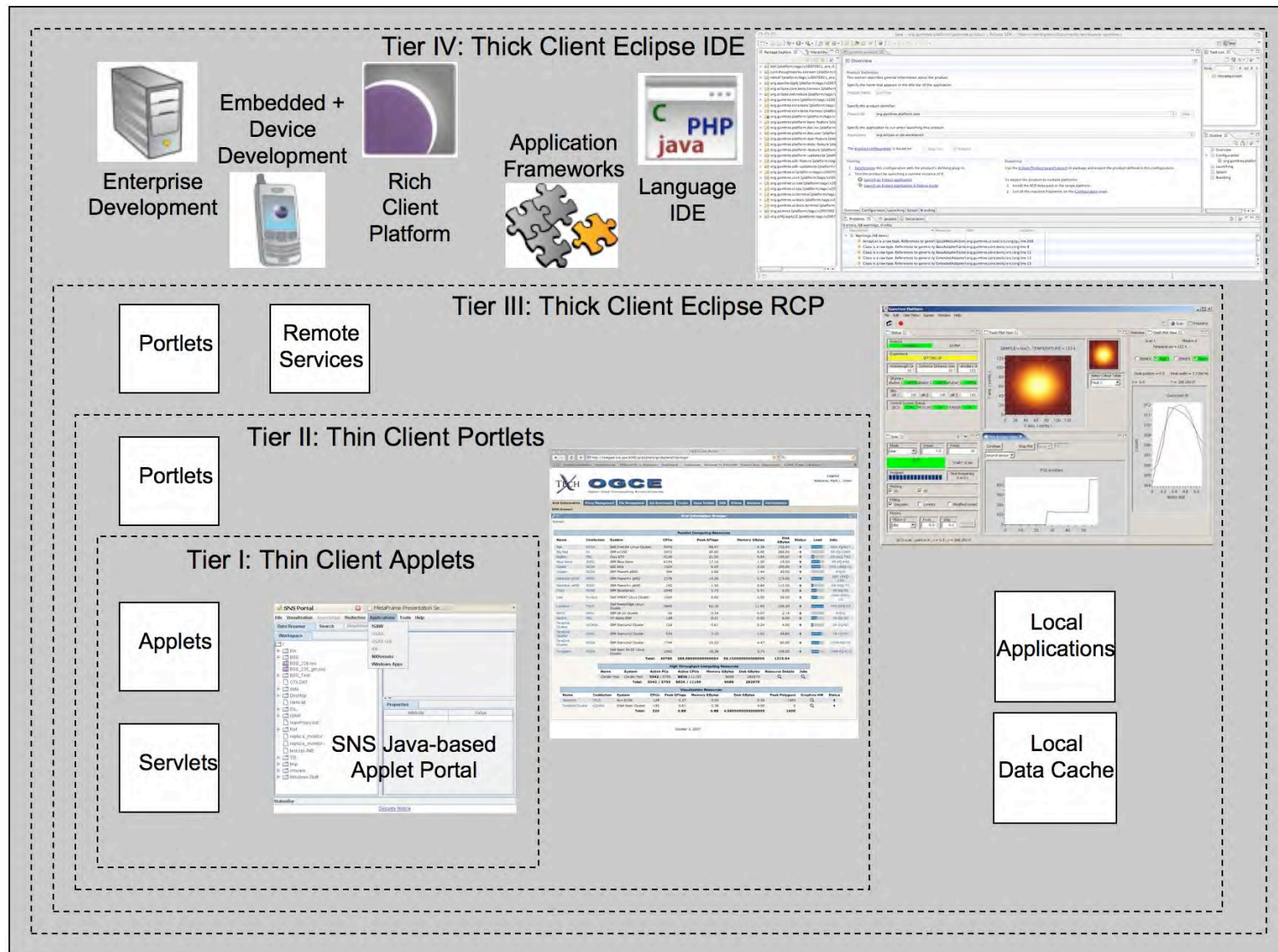
- **Thin-client Support**

- Tier I: SNS Java-based Science Portal
 - Java Web Start Applet Application
- Tier II: Open Grid Computing Environment
 - Gridsphere Portlet Based Environment

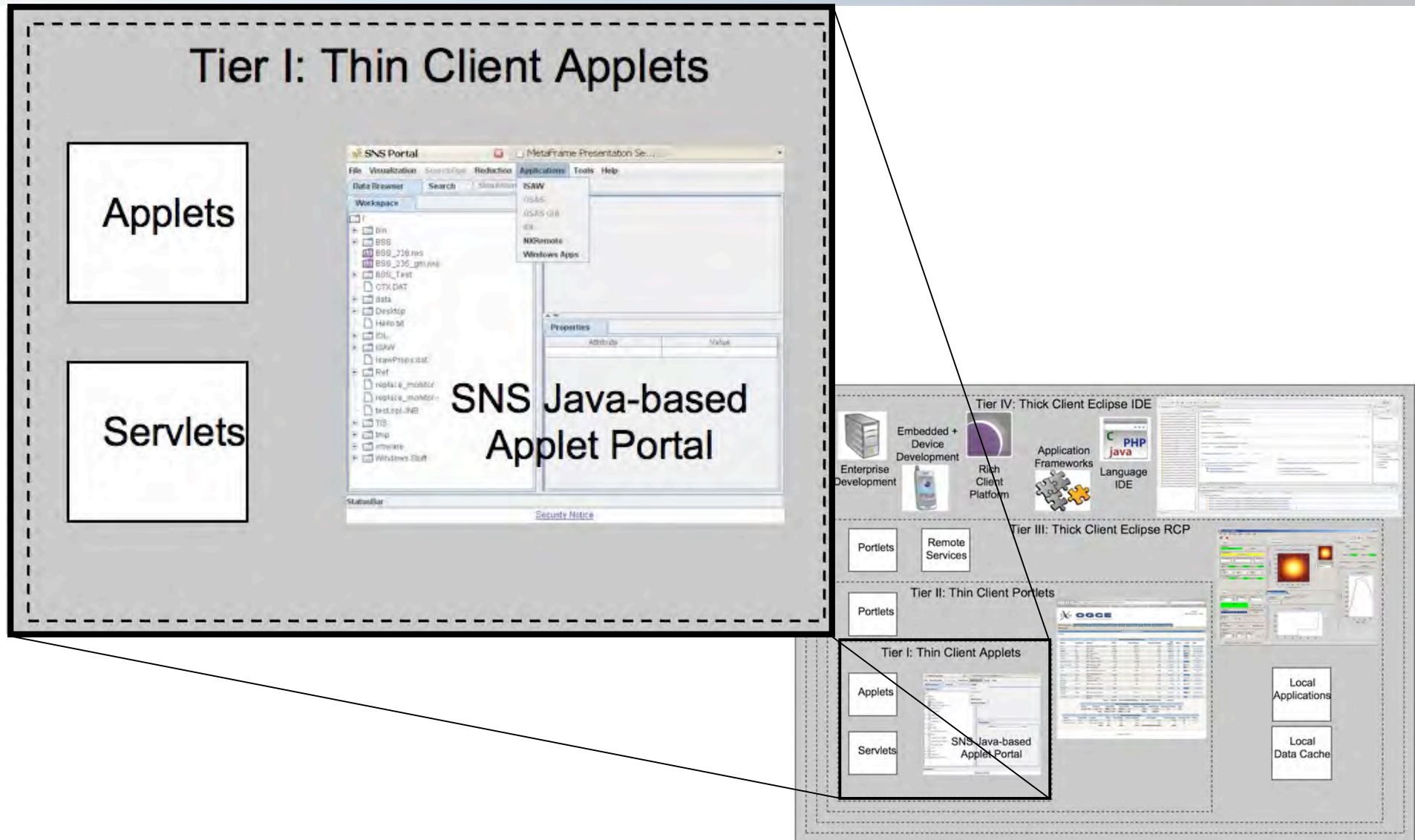
- **Thick-client Support**

- Tier III: GumTree Application
 - Eclipse Rich Client Platform Application
- Tier IV: Eclipse
 - Java, C/C++, Fortran, PHP, Python, etc. Integrated Development Environment

Multitier Portal Architecture (MPA)



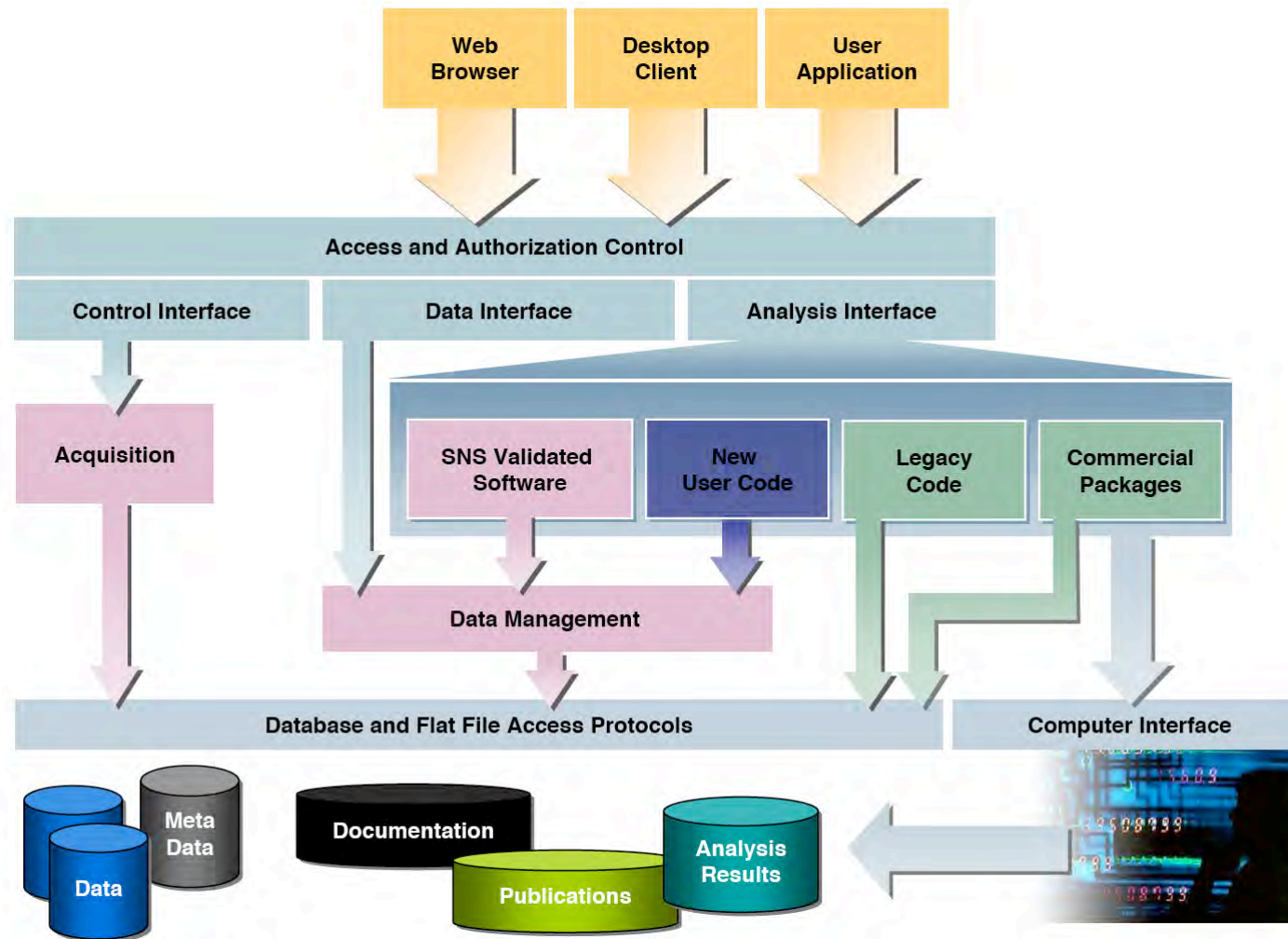
Thin-client MPA Tier I



Thin-client MPA Tier I: SNS Applet Portal



SNS Software Architecture



Thin-client MPA Tier I: SNS Applet Portal



- Spallation Neutron Source Applet Portal
 - <https://portal.sns.gov/snsportal/>

The screenshot displays the SNS Portal web application. The top navigation bar includes links for Getting Started, Latest Headlines, Apple, Amazon, eBay, Yahoo!, and News. The main menu contains File, Visualization, SearchOps, Reduction, Applications, Tools, and Help. The left sidebar features a Search Criteria section with dropdown menus for Facility List, Instrument List, and Search Criteria, along with a Search button. Below this is a Search Results table with columns for URI, TITLE, SAMPLE_NAME, and CREATE_TIME. The table lists various data entries, including Lysozyme D20 on c... Hydrated Proteins, with URIs starting with /SNS/BSS/IPTS-132... and creation dates ranging from 2007-09-01 to 2007-09-11. The right pane shows a file browser view of the workspace, displaying a tree structure with folders like data, public, SNS, ARCS, BSS, BSS_test, Ex07BSS, 5, 264, NeXus, BSS_264_example.nxs, 265, 288, 289, 290, 291, shared, IPTS-132, IPTS-234, IPTS-236, IPTS-241, IPTS-273, testing12345, DEMO, REF_L, REF_M, software, TESTING, Desktop, ISAW, IsawProps.dat, mysql-5.0.45.tar, and phpinfo.php. The Properties panel on the right shows details for the selected file, including signal (1), type (NX_UINT32[64,64,20001]), and target (/entry/instrument/bank1/data).

URI	TITLE	SAMPLE_NAME	CREATE_TIME
/SNS/BSS/IPTS-132...	Lysozyme D20 on c...	Hydrated Proteins	2007-09-01 16
/SNS/BSS/IPTS-132...	Lysozyme D20 on c...	Hydrated Proteins	2007-09-01 17
/SNS/BSS/IPTS-132...	Lysozyme D20 on c...	Hydrated Proteins	2007-09-01 18
/SNS/BSS/IPTS-132...	Lysozyme D20 on c...	Hydrated Proteins	2007-09-02 02
/SNS/BSS/IPTS-132...	Lysozyme D20 on c...	Hydrated Proteins	2007-09-02 05
/SNS/BSS/IPTS-132...	Lysozyme D20 on c...	Hydrated Proteins	2007-09-02 13
/SNS/BSS/IPTS-132...	Lysozyme D20 on c...	Hydrated Proteins	2007-09-02 20
/SNS/BSS/IPTS-132...	Lysozyme D20 on c...	Hydrated Proteins	2007-09-03 02
/SNS/BSS/IPTS-132...	Lysozyme D20 on c...	Hydrated Proteins	2007-09-03 08
/SNS/BSS/IPTS-132...	Lysozyme D20 on c...	Hydrated Proteins	2007-09-03 13
/SNS/BSS/IPTS-132...	Lysozyme D20 on c...	Hydrated Proteins	2007-09-03 18
/SNS/BSS/IPTS-132...	Lysozyme D20 on c...	Hydrated Proteins	2007-09-04 03
/SNS/BSS/IPTS-132...	Lysozyme D20 on c...	Hydrated Proteins	2007-09-04 08
/SNS/BSS/IPTS-132...	Lysozyme D20 on c...	Hydrated Proteins	2007-09-04 18
/SNS/BSS/IPTS-132...	Lysozyme D20 on c...	Hydrated Proteins	2007-09-05 03
/SNS/BSS/IPTS-132...	Lysozyme D20 on c...	Hydrated Proteins	2007-09-05 12
/SNS/BSS/IPTS-132...	Lysozyme D20 on c...	Hydrated Proteins	2007-09-05 20
/SNS/BSS/IPTS-132...	Lysozyme D20 on c...	Hydrated Proteins	2007-09-06 04
/SNS/BSS/IPTS-132...	Lysozyme D20 on c...	Hydrated Proteins	2007-09-07 12
/SNS/BSS/IPTS-132...	Lysozyme D20 on c...	Hydrated Proteins	2007-09-07 18
/SNS/BSS/IPTS-132...	Lysozyme D20 on c...	Hydrated Proteins	2007-09-08 06
/SNS/BSS/IPTS-132...	Lysozyme D20 on c...	Hydrated Proteins	2007-09-08 15
/SNS/BSS/IPTS-132...	Lysozyme D20 on c...	Hydrated Proteins	2007-09-08 21
/SNS/BSS/IPTS-132...	Lysozyme D20 on c...	Hydrated Proteins	2007-09-09 00
/SNS/BSS/IPTS-132...	Lysozyme D20 on c...	Hydrated Proteins	2007-09-09 04
/SNS/BSS/IPTS-132...	Lysozyme D20 on c...	Hydrated Proteins	2007-09-01 16

Thin-client MPA Tier I: SNS Applet Portal



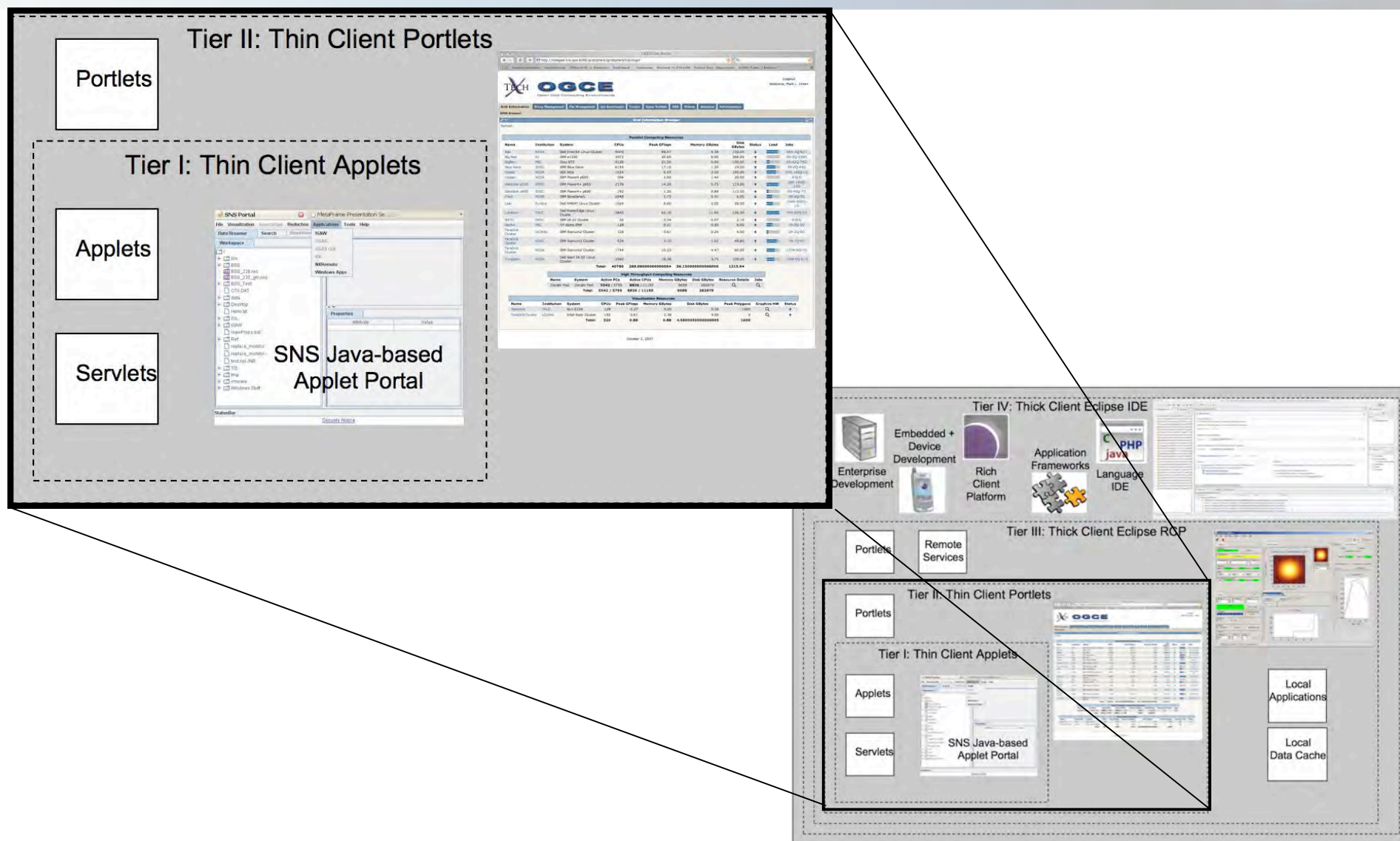
- **SNS manages**
 - Multiple instruments, multiple users (2000/year)
 - Multiple services:
 - Data, acquisition, analysis, simulation, and visualization
- **Portal is a common “gateway” to a complex set of services:**
 - Software analysis tools and applications for neutron science data
 - Instruments and data acquisition
 - Data repositories, file systems, and archives
 - Databases with metadata and provenance
 - High-performance computing resources — analysis and simulation
 - Collaborative services — interactive visualization, information sharing
- **Several access modes: web-based, desktop-applications...**

Thin-client MPA Tier I: SNS Applet Portal



- **Secure access to key services:**
 - Acquisition, analysis, visualization, simulation...
 - Data repositories, file systems and archives
 - Meta-data and provenance databases
 - High-performance computing resources
- **Software analysis tools for neutron science**
 - Web-based and programmatic desktop access
 - Integration of facility and community tools
- **Extensible software architecture**
 - Powerful data and application management

Thin-client MPA Tier II



Thin-client MPA Tier II: SNS OGCE Portal



- **The OGCE framework provides several features that are currently not available through the SNS Java-based Applet Portal including:**
 - Grid credential proxy management portlets;
 - Portlets for managing remote files through GridFTP and other file management systems;
 - Portlets for running jobs through Globus Toolkit versions 2.4 and 4.0 (both Web Service and pre-Web Service versions);
 - Storage Resource Broker (SRB) portlets;
 - Grid Portals Information Repository (GPIR) portlets and services; and
 - Condor job submission portlets.

Thin-client MPA Tier II: SNS OGCE Portal



OGCE Grid Portal

https://faregate.ornl.gov/gridsphere/gridsphere?cid=iframe-portlet

Getting Started Latest Headlines Apple Amazon eBay Yahoo! News

OGCE Open Grid Computing Environments

SNS SPALLATION NEUTRON SOURCE

TECH

Welcome Administration gpip-browser-2 sns-portlet srb-portlet proxymanager-portlet

OGCE SNS Portlet

Data Browser Search Simulation

Workspace

/

- data
 - public
 - SNS
 - ARCS
 - BSS
 - DEMO
 - REF_L
 - REF_M
 - EX07REF_M
 - 2
 - 1886
 - Analysis
 - NeXus
 - REF_M_1886_example.nxs
 - REF_M_8_boxes.nxs
 - REF_M_8a_boxes.nxs
 - REF_M_8sm_boxes.nxs
 - 1898
 - 1899
 - 1900
 - shared
 - REF_M_test
 - software
 - TESTING
 - Desktop
 - ISAW
 - IsawProps.dat
 - mysql-5.0.45.tar

entry

- bank1
- BSlit1
- BSlit2
- BSlit3
- collection_identifier
- collection_title
- definition
- duration
- end_time
- experiment_identifier
- instrument
- LSlit1
- LSlit2
- LSlit3
- monitor
- notes
- proton_charge

2-D View: /data/SNS/BSS/EX07BSS/5/264/NeXus/BSS_264_example.nxs

/entry/bank1/data [-, -]{0-20000}

data Default Unit

Intensity Slider

Pointed At

X [] Y []

Marker Overlay

Axis Overlay

Selection Overlay

Annotation Overlay

Selectors

Default

Add Selector

Panning Tool

X-Axis: x_pixel_offset

Y-Axis: y_pixel_offset

time_of_flight

0.0 66660.0 133320.0 199980.0

Integrated

Properties

Attribute	Value
name	REF_M_1886_example.nxs
location	/data/SNS/REF_M/EX07REF_M/2/1886/NeXus/REF_M...
type	application/x-NeXus
lastModified	Sun Nov 11 06:16:33 EST 2007
length	10086776 bytes
TITLE	Slit1 scan with L position=2.998400 and R position=3...
NOTES	18 of 80 scans
START TIME	2007-07-05T23:42:54-04:00
END TIME	2007-07-05T23:58:30-04:00
DURATION	936.328 second

Applet gov.ornl.sns.portal.PortalApplet started

faregate.ornl.gov

Thin-client MPA Tier II: SNS OGCE Portal



- The development of component based neutron science pre-experiment specific portlets is ongoing in collaboration with Tech-X, OGCE, and SNS for:
 - integration of an experiment protocol planner,
 - experiment sample scheduler,
 - Monte Carlo simulations,
 - sample activation calculator, and
 - group collaborative calendars for on-site trip planning.



Thick-client MPA Tier III: GumTree



- Australian Nuclear Science and Technology Organisation (ANSTO)**

Australian Government

Bragg Institute Development



- GumTree is:**

a multiple-platform rich client scientific workbench and an open source project and platform for software collaboration.

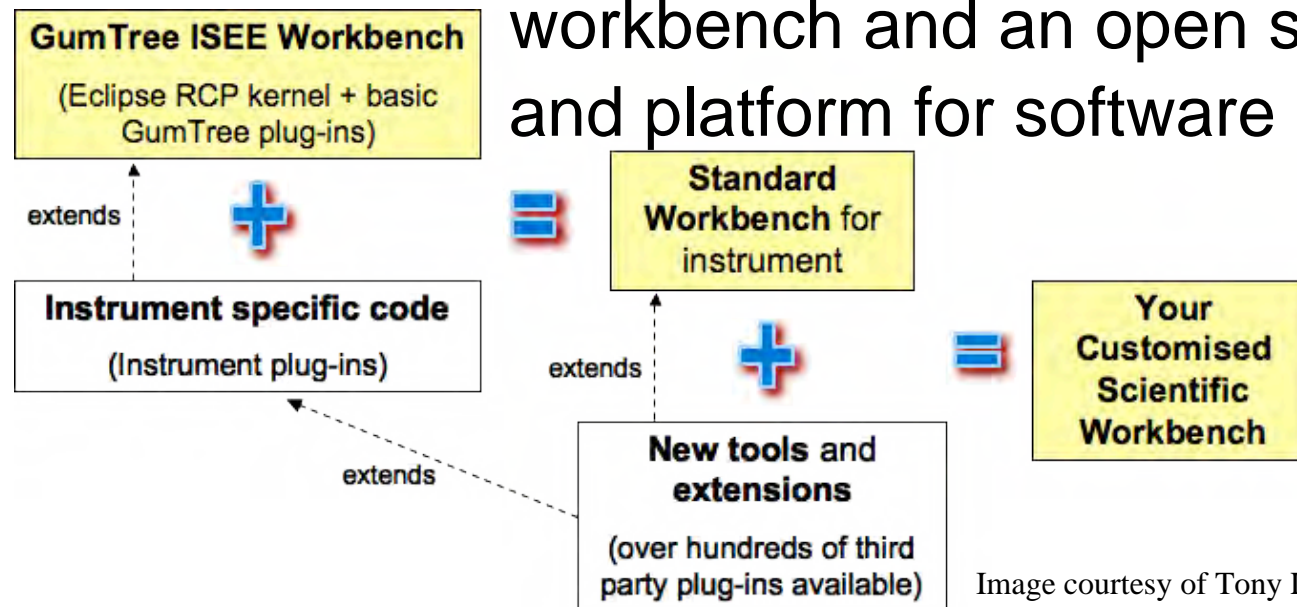
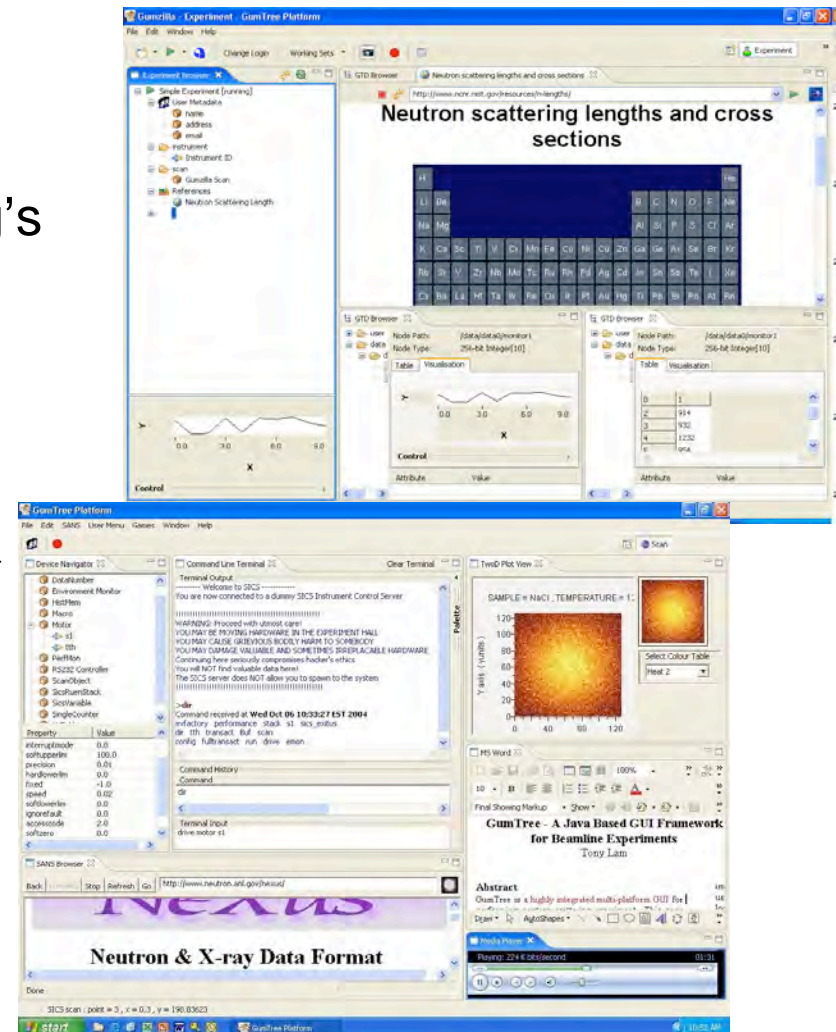


Image courtesy of Tony Lam eScience Workshop 2006 Presentation

Thick-client MPA Tier III: GumTree



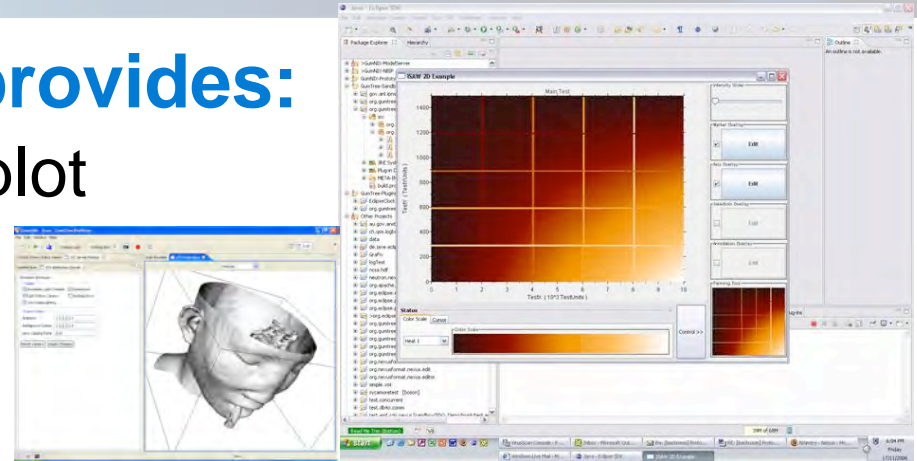
- **GumTree ISEE plans to offer:**
 - Instrument Control & Data Acquisition
 - SICS, EPICS, TANGO and Bragg's model server
 - Online and Offline Data Analysis
 - Centralized control of a complex data acquisition system
 - Electronic Laboratory Notebook & Report
 - Interacts with the word processor and graphical report tools
 - Collaborative environment for remote experiment
 - File sharing, chatting, shared whiteboard, remote workbench control



Thick-client MPA Tier III: GumTree



- **GumTree Visualization provides:**
 - OpenGL, VTK, ISAW, Ptpot capabilities for 1, 2, 3-D plotting and visualization.
- **GumTree Neutron / NeXus Instrument eXtension (GumNIX) provides:**
 - a generic library to support user requirements,
 - graphical interface for batched instrument control and data acquisition,
 - data access to NeXus data across network,
 - online data reduction (during data acquisition), and
 - is extensible and customizable.



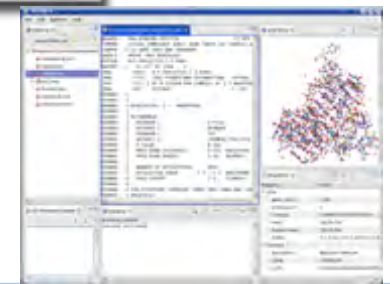
Thick-client MPA Tier III: GumTree



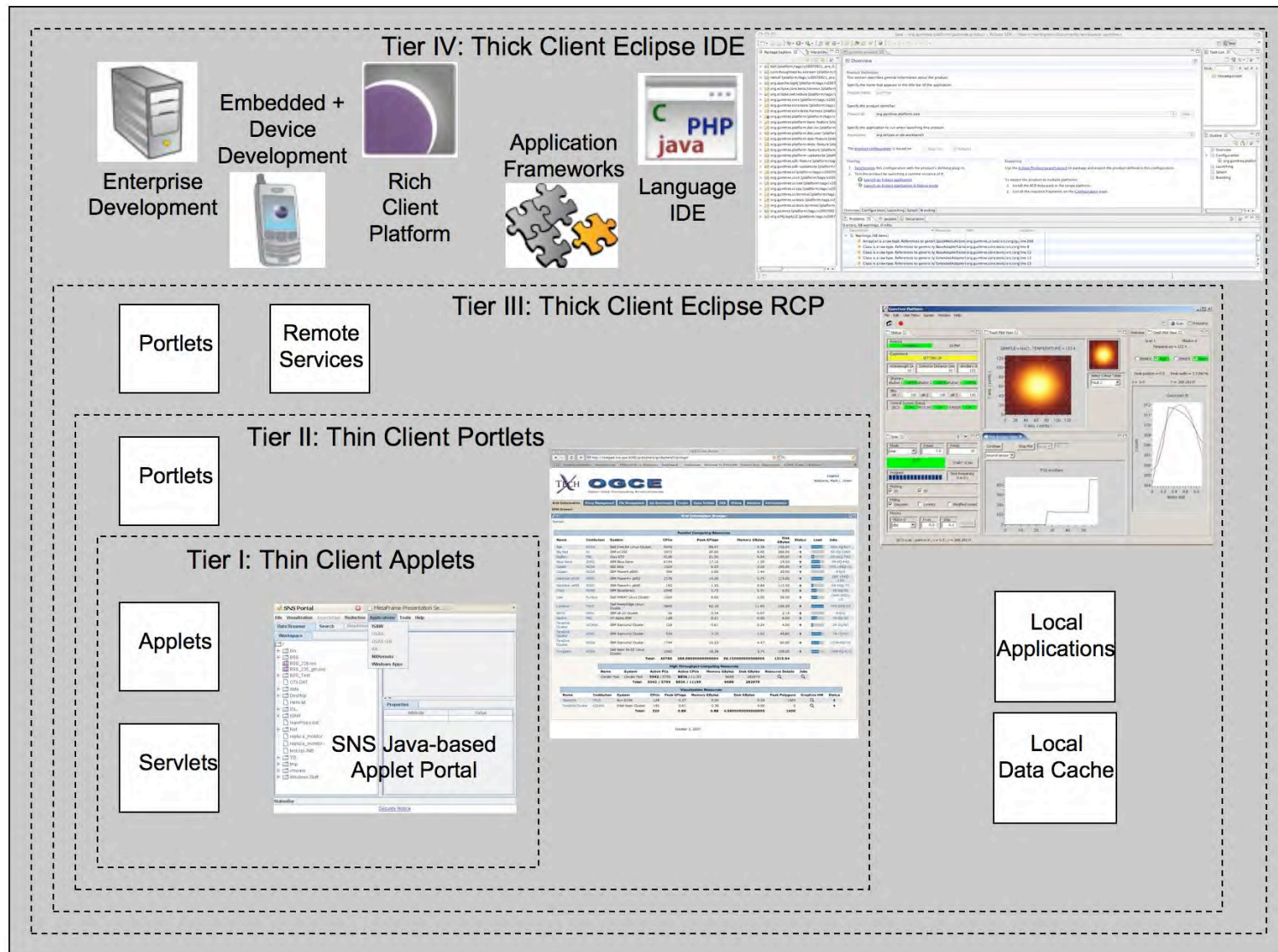
- **Many other projects leveraging Eclipse**
 - Providing a repository for plug-in exchange
- **g-Eclipse**
 - Users: desktop-like access to Grid resources
 - Providers: reduced the time-to-service
 - Developers: reduce the time-to-market for applications
- **Control System Studio**
 - The proposed next generation standard control system software EPICS GUI.
- **NASA Maestro**
 - Eclipse RCP used for mission planning, control, and image analysis.
- **Bioclipse**
 - 3D-visualization of molecules and proteins for chemo- and bioinformatics.



CSS
control system studio



Thick-client MPA Tier IV



Thick-client MPA Tier IV: Eclipse IDE



- **Eclipse Integrated Development Environment (IDE) incorporates**

features provided by the previous tiers in Eclipse based projects stored in a central Subversion code repository.

This tier is meant to provide access for very sophisticated users that have the desire to develop infrastructure and capabilities specific to their SNS instrument using the available plugins, servlets, portlets, and applications.

Currently integrating the Eclipse Parallel Tools Platform (PTP) project.

Thick-client MPA Tier IV: Eclipse IDE



- **The aim of the Parallel Tools Platform project is**
to produce an open-source industry-strength platform that provides a highly integrated environment specifically designed for parallel application development.
- **The project provides:**
 - a standard, portable parallel IDE that supports a wide range of parallel architectures and runtime systems
 - a scalable parallel debugger
 - support for the integration of a wide range of parallel tools
 - an environment that simplifies the end-user interaction with parallel systems

Thick-client MPA Tier IV: Eclipse IDE

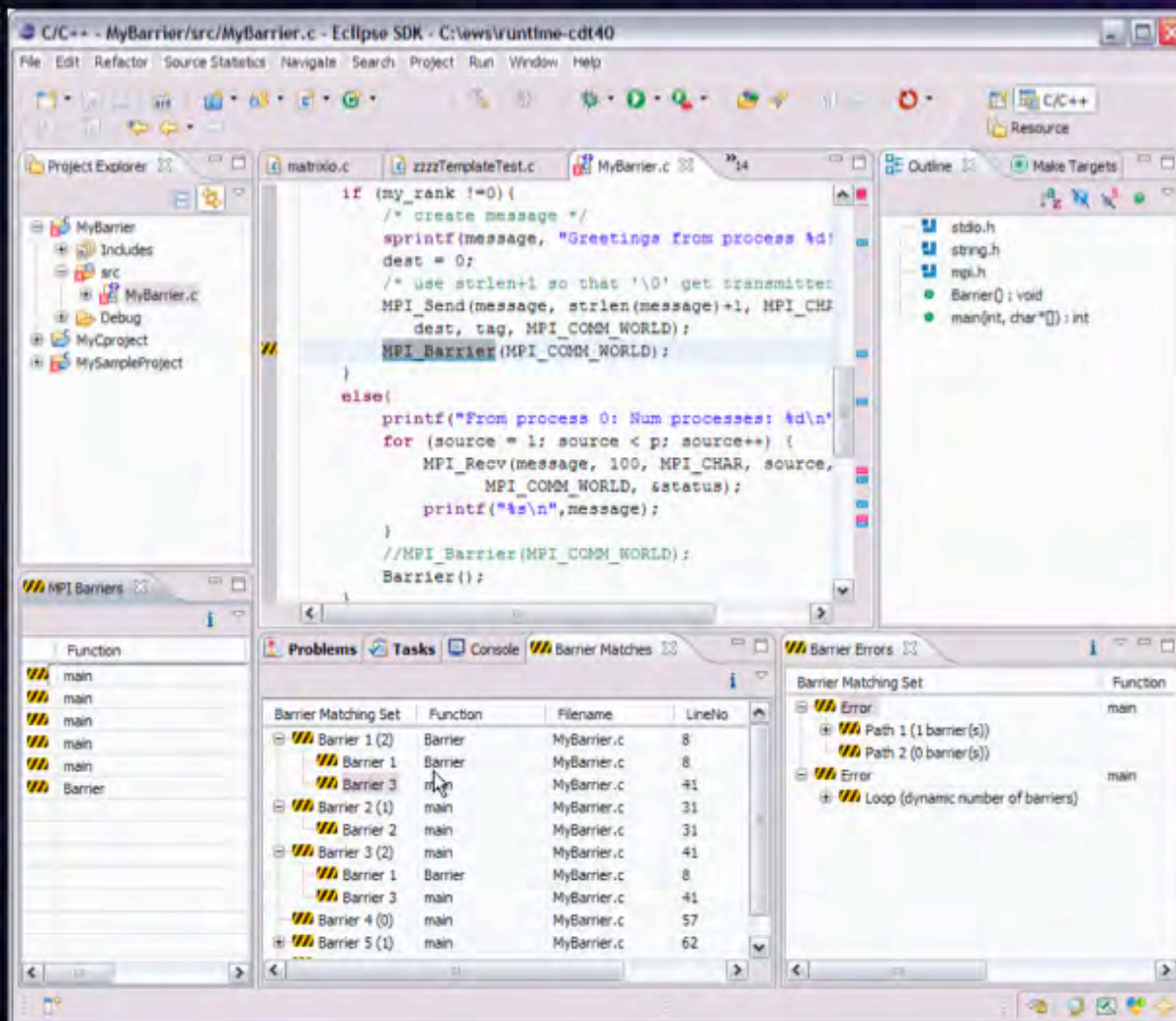


- **Eclipse**
 - Java Development Tools
 - Plug-in and Project Repository
- **Parallel Tools Platform (PTP)**
 - C/C++ Development Tools (CDT)
 - Fortran Development Tools (Photran)
 - OpenMPI or MPICH2
 - PTP Proxy
- **SNS FAREGATE.ORNL.GOV Integration**
 - Planning PTP Proxy Deployment for SLURM Managed Resources
 - Provided Authentication Resource Access and Debugging Capabilities for Instrument Scientist Parallel Application Development

Thick-client MPA Tier IV: Eclipse IDE



MPI Barrier Analysis



Verify barrier synchronization in C/MPI programs
Interprocedural static analysis outputs:

- ✦ For verified programs, lists barrier statements that synchronize together (match)
- ✦ For synchronization errors, reports counter example that illustrates and explains the error.

Thick-client MPA Tier IV: Eclipse IDE



System Monitoring

- ★ Machine status shown in **Machines** view
- ★ Node status also shown in **Machines** view
- ★ Hover over node to see node name
- ★ Double-click on node to show attributes

Resource Managers

ORTE@N.N.N.N (ORTE)

Machines

ORTE@N.N.N.N: localhost.localdomain - Root [64]

localhost.localdomain

0 10 20 30 40 50 60

Node Attributes

Attribute	Value
Name	node0
Node Number	0
Node State	UP

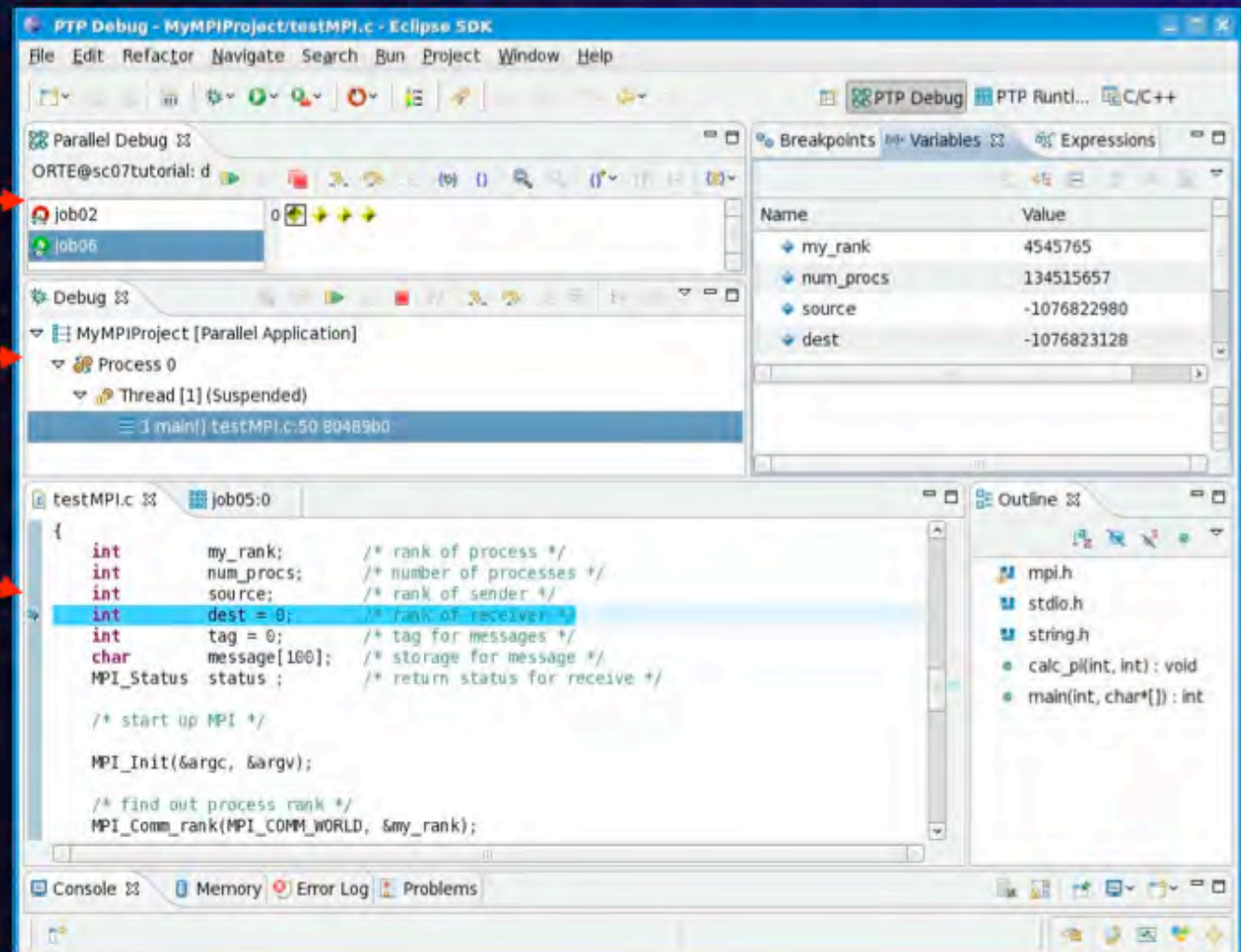
Process Info

Thick-client MPA Tier IV: Eclipse IDE



The PTP Debug Perspective (1)

- ★ **Parallel Debug view** shows job and processes being debugged
- ★ **Debug view** shows threads and call stack for individual processes
- ★ **Source view** shows a **current line marker** for all processes

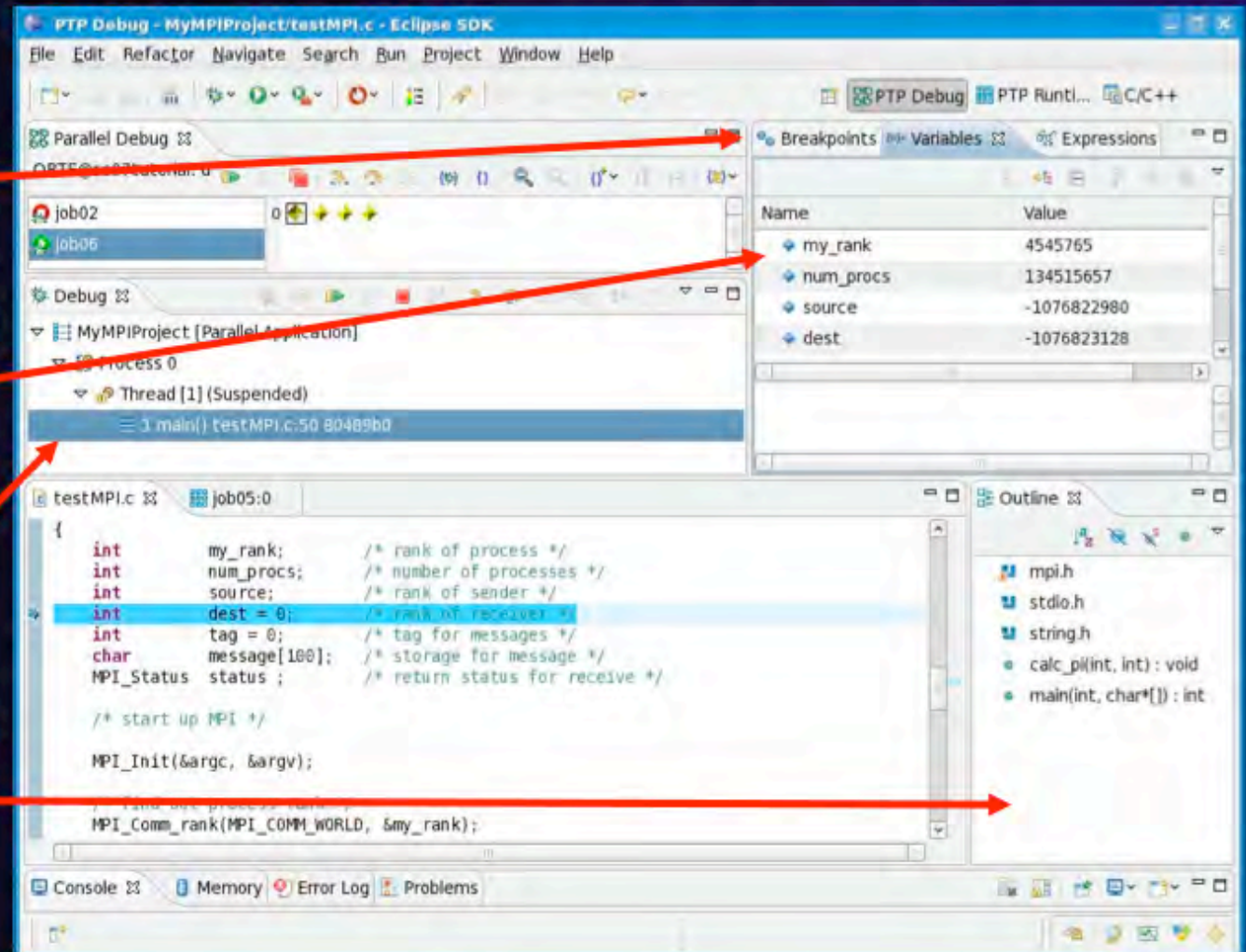


Thick-client MPA Tier IV: Eclipse IDE



The PTP Debug Perspective (2)

- ★ **Breakpoints view** shows breakpoints that have been set (more on this later)
- ★ **Variables view** shows the current values of variables for the currently selected process in the **Debug view**
- ★ **Outline view** (from CDT) of source code



Conclusion



- **The Multitier Portal Architecture (MPA):**
 - Has the potential to scale to the expertise and requirements level of the user.
 - Maximizes the reuse of the developed infrastructure and services in successive tiers.
 - Can incorporate open source portlets available from repositories and projects.
 - GumTree+ Project will provide significantly more thick-client capabilities (refer to paper for specific tasks).