# Experiences with
# OGCE Workflow Suite Empowering
# LEAD, GridChem, BioVLAB, UltraScan Science Gateways

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Look to the future of high-performance computing.

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# Acknowledgements

- OGCE Workflow Suite is inherited from a decade of work by Extreme Computing Lab and many PhD's under the guidance of Dr. Dennis Gannon.

- Special Thanks to Dennis Gannon, Beth Plale , Kelvin Droegemeier and the LEAD TEAM.

- Includes contributions from: Alek Slominski, Satoshi Shirasuna, Gopi Kandaswamy, Yi Huang, Yogesh Simmhan, Wei Lu,  Srinath Perera, Chathura Herath, Lavanya Ramakrishnan, Eran Chinthaka, Thilina Gunarathne and the Lanka Software Foundation.

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# Nancy's Outline

- Choices made in evaluating and selecting a workflow tool

- Description of how these tools are implemented in a gateway

- Presentation of the user interface

- Description of tasks performed behind the scenes

- Discussion of experience with tools - pros and cons
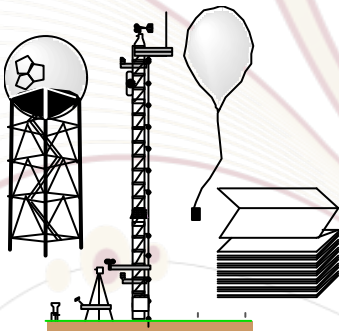
# High Level LEAD Architecture
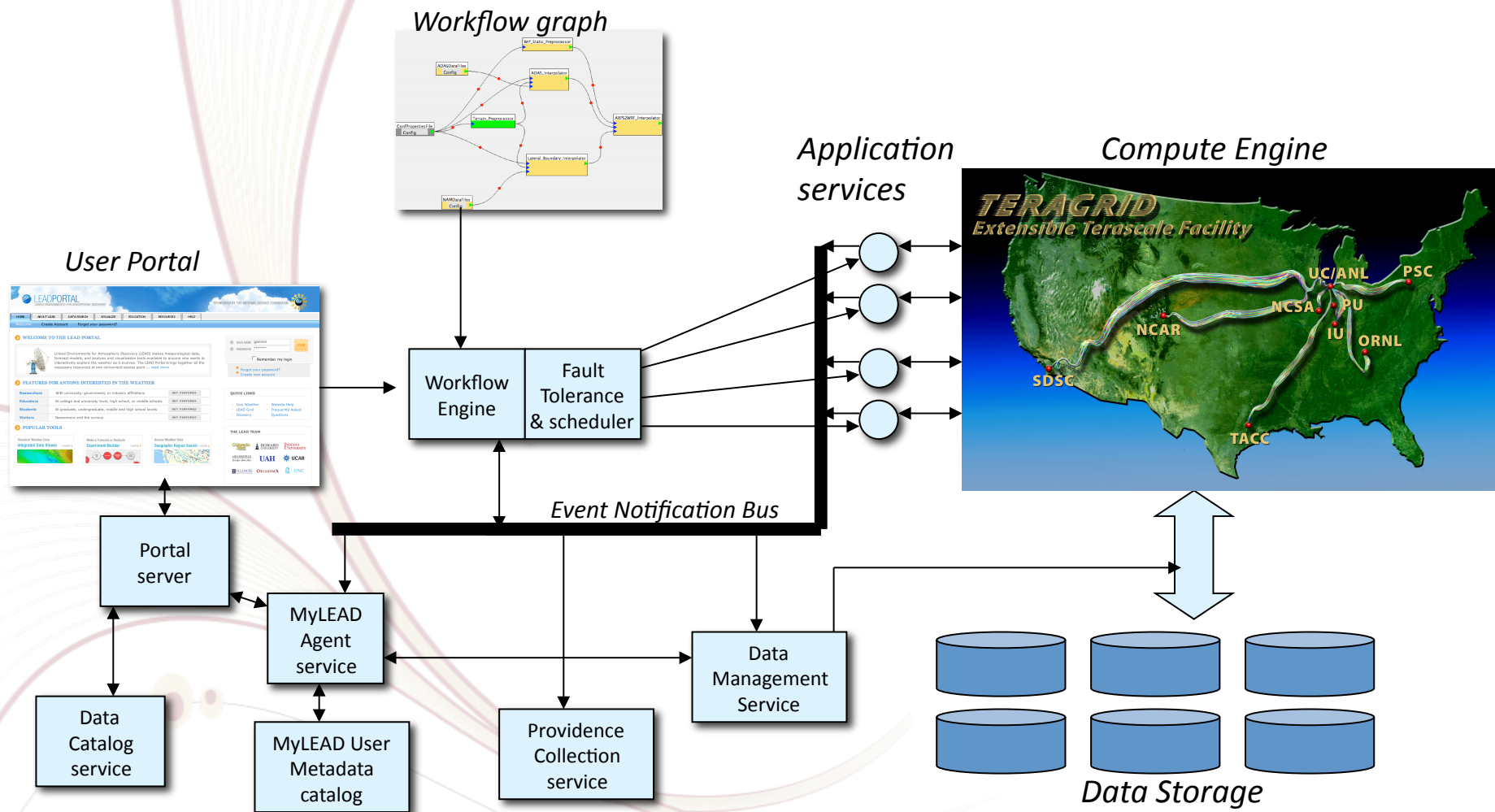
# Scientists and Educational Interactions

Application Developers (typically Scientists)

Researchers

Lowering the barrier for using complex end-to-end technologies

Democratize

Empower

Facilitate

End Users

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LEADPORTAL
LINKED ENVIRONMENTS FOR ATMOSPHERIC DISCOVERY

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HOME | MY WORKSPACE | ABOUT LEAD | DATA SEARCH | RESOURCES | HELP

Welcome

**Analyze & Predict**

**Discover &Visualize**

**Research & Reproducibility**

**Education & Outreach**

WELCOME TO THE LEAD PORTAL

Linked Environments for Atmospheric Discovery (LEAD) makes meteorological data, forecast models, and analysis and visualization tools available to anyone who wants to interactively explore the weather as it evolves. The LEAD Portal brings together all the necessary resources in a convenient access point ... read more

FEATURES FOR ANYONE INTERESTED IN THE WEATHER

| Research | affiliations | GET FEATURES |
| Education | or middle schools | GET FEATURES |
| Student | high school levels | GET FEATURES |
| Visitors | Newcomers the curious | GET FEATURES |

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MyLEAD

QUICK LINKS

Live Weather
LEAD Grid
LEAD Blog
Glossary

Website Help
Frequently Ask Questi
LEAD (pass prote

POPULAR TOOLS

Visualize Weather Data
**Integrated Data Viewer** | MORE >

a Forecast or Analysis
riment Builder | MORE >

Access Weather Data
**Geographic Region Search** | MORE >

THE LEAD TEAM

Colorado State | HOWARD UNIVERSITY | INDIANA UNIVERSITY
MILLERSVILLE | UAH | UCAR
ILLINOIS | OKLAHOMA

CT US | LOGOUT

# LEAD Workflow Requirements

- Run jobs on-demand on TeraGrid.

- Deadline driven workflows (severe weather tracking)

- Users ranging from 8th grade students to seasoned researchers.

- Run jobs on Multiple TeraGrid resources to increase turn-around time.

- Must be able to integrate to Portal with very user friendly web interface.

# Workflow Survey in 2003

(http://www.extreme.indiana.edu/swf-survey/)

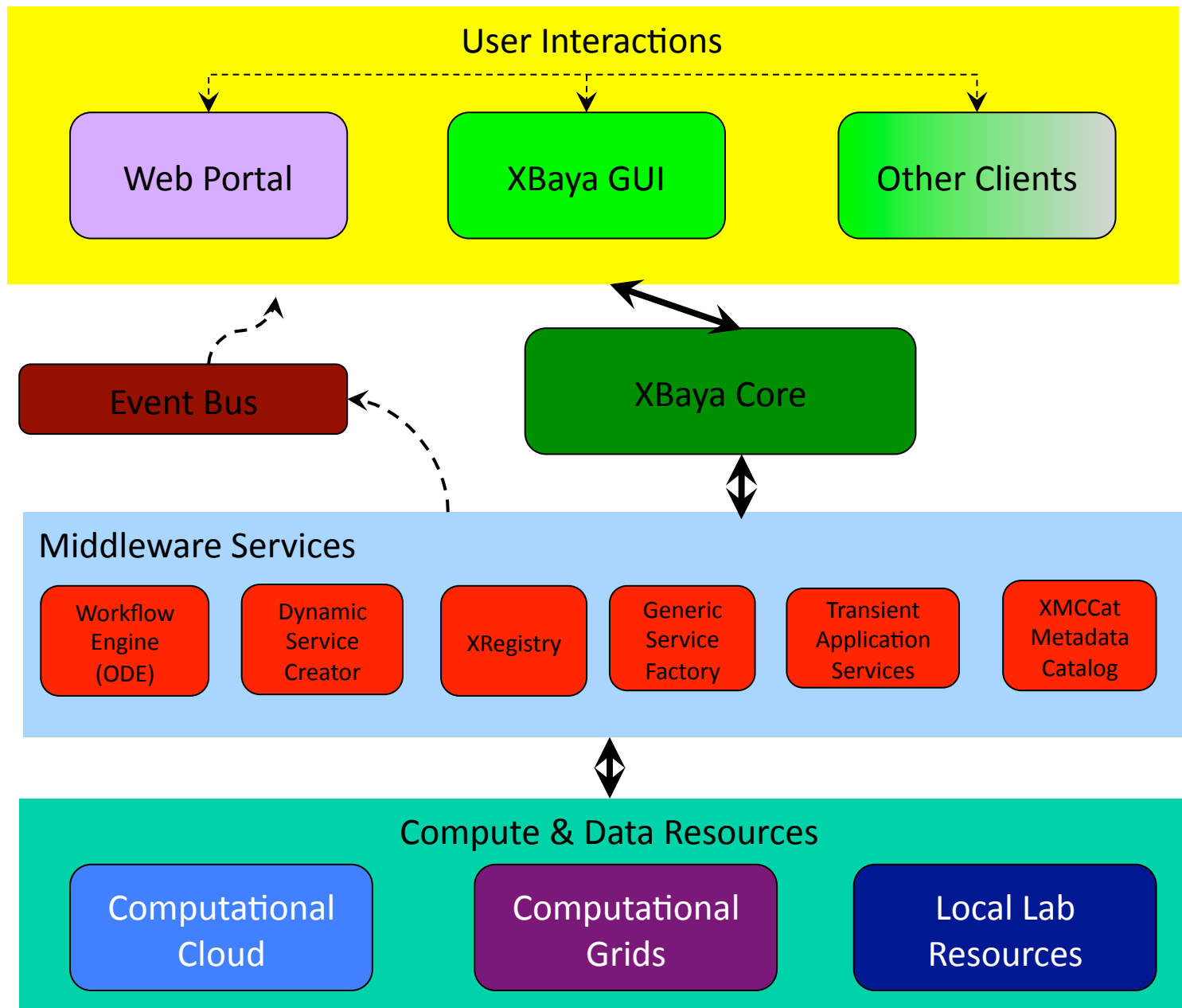## List of Scientific Workflows (Alphabetical)

| Name (link to background info) | Status, availability | Prerequisites | Tooling | Workflow Standards | Grid integration | Portal integration | Comments |
|---|---|---|---|---|---|---|---|
| Askalon | N/A | Java SDK 1.4, CoG | Java GUI | Custom XML language (AGWL) | GT3, CoG | NA | A Grid runtime for AGWL that has resource broker, resource monitoring, (meta)-scheduler etc. |
| AGWL | NA | NA | NA | NA | NA | NA | AGWL is an abstract Grid workflow language for describing workflows (graphs with loops) at a high level of abstraction used in Askalon |
| BioOpera | | | | | | | |
| Chimera | | Condor DAGMan | ? | NA | Condor | ? | Built on top of Condor, workflow as solution to provide on-demand data generation ("virtual data") |
| D2K | Multiple License | JDK 1.3.1 | Java GUI | NA | ? | ? | Modules composed into data flow optimized for data mining and KDD (Knowledge Discovery in Databases) |
| DAGMan | Part of Condor, source code under GPL | Condor | Integrated with Condor command line tools | NA | Condor, can run on top of GT2 (Condor-G) | Under work | Part of Condor, very well integrated |
| DDBJ | | | | | | | |
| DiscoveryNet | | | | | | | |
| EUROGRID | | | | | | | |
| Fiswidgets | GPL | Java (version?) | Java GUI | custom XML | not yet | no | domain independent, but designed for processing neuroimaging analyses |
| GRID superscalar | Binaries available upon request (license?) | | | | GT2 | | Simple makefile like data dependency to describe and execute grid tasks |
| GridAnt | Soon? | Java JDK 1.4, CoG | Graphical workflow visualizer (ANL) | Built on top of Apache ANT | via CoG | NA | Merged ANL GridAnt and NCSA OGRE |
| GridPort | 3.0 alpha | J2EE, CoG, JBoss | N/A | NA | via CoG | NMI OGCE, Jetspeed, Hotpage 3.0 | Non standard description of job sequences |
| GridNexus | 1.0.0 (to be released under open source license) | Java JDK 1.4 | Built on top of PtolemyII Java GUI | Internal DAG is transformed to new scripting language called JXPL (XML based) | GT3 | Under investigation | Main focus on making Drag-and-drop Grid GUI |
| Grid Service Broker | Part of the Gridbus Broker, code available under GPL | Java, CoG | Command line, Java based Grid API, | | GT2, Alchemi | Yes, with G-monitor that support multiple devices (?) | Supports parametric computing for compute and data grids applications. being extended to support advanced workflows. |
| GRMS | GPL | Java, CoG | command line and GridSphere Web portlet | DAG/PetriNet | Pre-WS GT | yes (GridSphere) | GRMS is a persistent GSI-enabled Web Service in GridLab project |
| GSFL | NA (only paper) | | | | | | Extended WSFL to add Grid support |
| JOpera for Eclipse | BSD | Java 1.4 (or above) | Eclipse 3.1 | Directed Cyclic Labeled Graphs, stored in custom XML format (Graph Flow Diagrams) - supports cycles | WSDL, WSRF, GT4, SSH, Condor | Built-in monitoring tools (Eclipse RCP and Web based) | Grid workflows fully integrated with the Eclipse user experience; Extensible with your own plugins to call any kind of service |
| ICENI | SISSL (open source license - certified?) | Java | Java GUI | | | | Component based dataflow |
| I-Lab | Soon? | Java? | Java GUI (Visual Grid Job Authoring) | GADL is based on Petri Nets | GT2 | Job Builder | Allows graph refinement during execution (such as add file transfer node) |
| INFORMNET | Summer'04? | Java? | Visualizer? | NA | GT3 | ? | uses XML based DAG |
| Karajan | CoG2 CVS (see CoG2 Manual for details) | Java 1.4, CoG2 | command line, API, GUI? | Ant like | GT2.4, GT3.02, SSH (future targets: Condor, GT4.0, Unicore) | NMI OGCE.org | Aims to be as easy to use as ANT but more workflow oriented |
| Pegasus | ? | Condor DAGMan | | | Condor | | Pegaus translates Abstract Workflow (AW) to produce a Concrete Workflow (CW) submitted to Condor's DAGMan |

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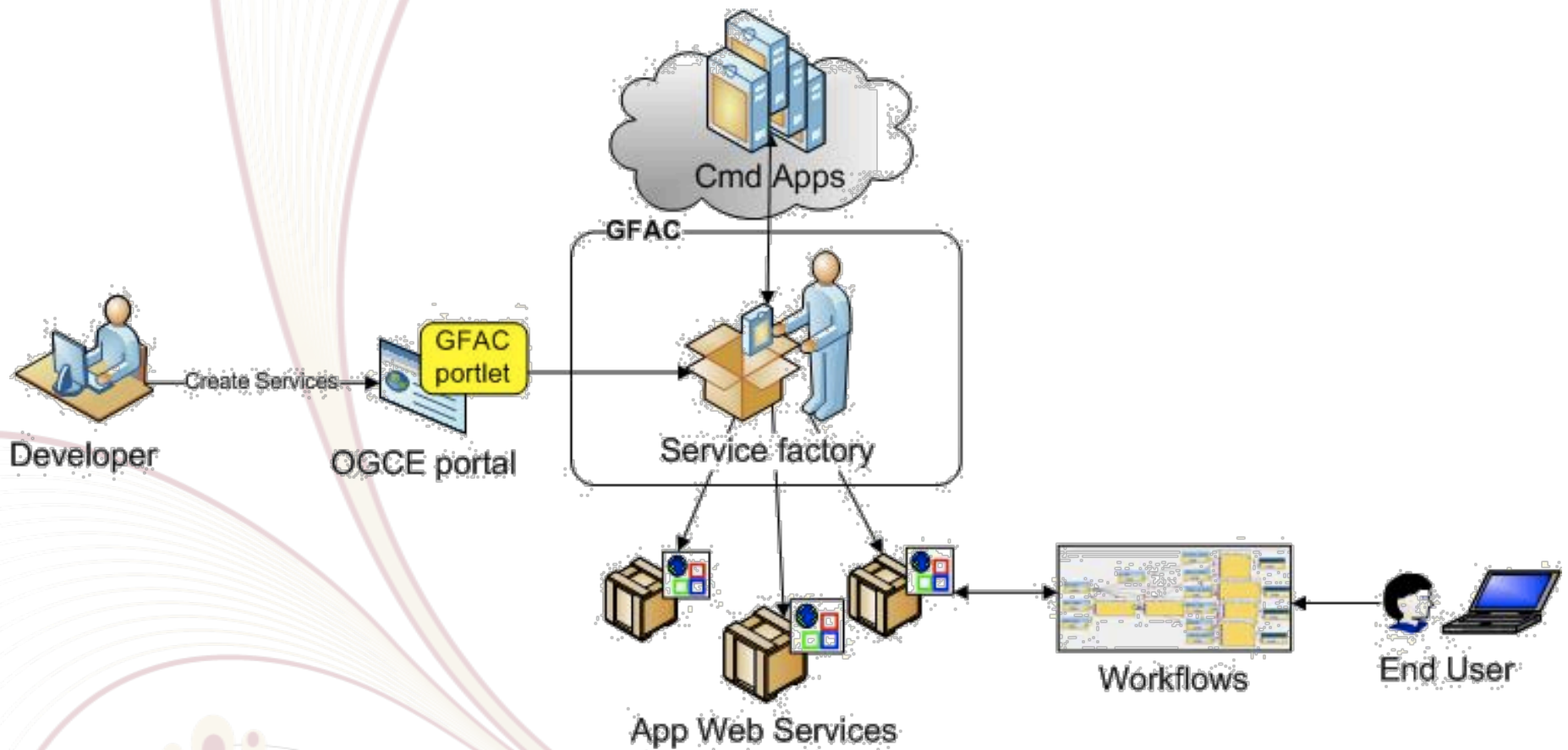Open Grid Computing Environments

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# OGCE Workflow Suite
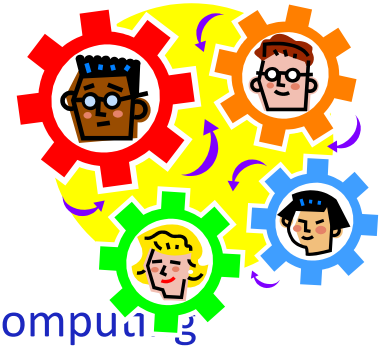
- Generic Service Toolkit
  - Tool to wrap command-line applications as web services
  - Handles file staging & job submission and monitoring
  - Extensible runtime for security, resource brokering & urgent computing
  - Generic Factory service for on-demand creation of application services
- XRegistry
  - Information repository for the OGCE workflow suite
  - Register, search, retrieve & share XML documents
  - User & hierarchical group based authorization
- XBaya
  - GUI based tool to compose & monitor workflows
  - Extensible support for compiler plug-ins like BPEL, Jython, SCUFL
  - Dynamic Workflow Execution support to start, pause, resume, rewind of workflow executions
- Apache ODE Scientific Workflow Extensions
  - XBaya GUI integration for BPEL Generation
  - Asynchronous support for long running workflows
  - Instrumented with fine grained monitoring
- Eventing System
  - Supports both WS-Eventing and WS-Notification Standards
  - Very scalable
  - Persistent Message Box for clients behind firewalls and with intermittent network glitches.

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# User Interactions

**Web Portal**

**XBaya GUI**

**Other Clients**

**Event Bus**

**XBaya Core**

# Middleware Services

**Workflow Engine (ODE)**

**Dynamic Service Creator**

**XRegistry**

**Generic Service Factory**

**Transient Application Services**

**XMCCat Metadata Catalog**

# Compute & Data Resources

**Computational Cloud**

**Computational Grids**

**Local Lab Resources**
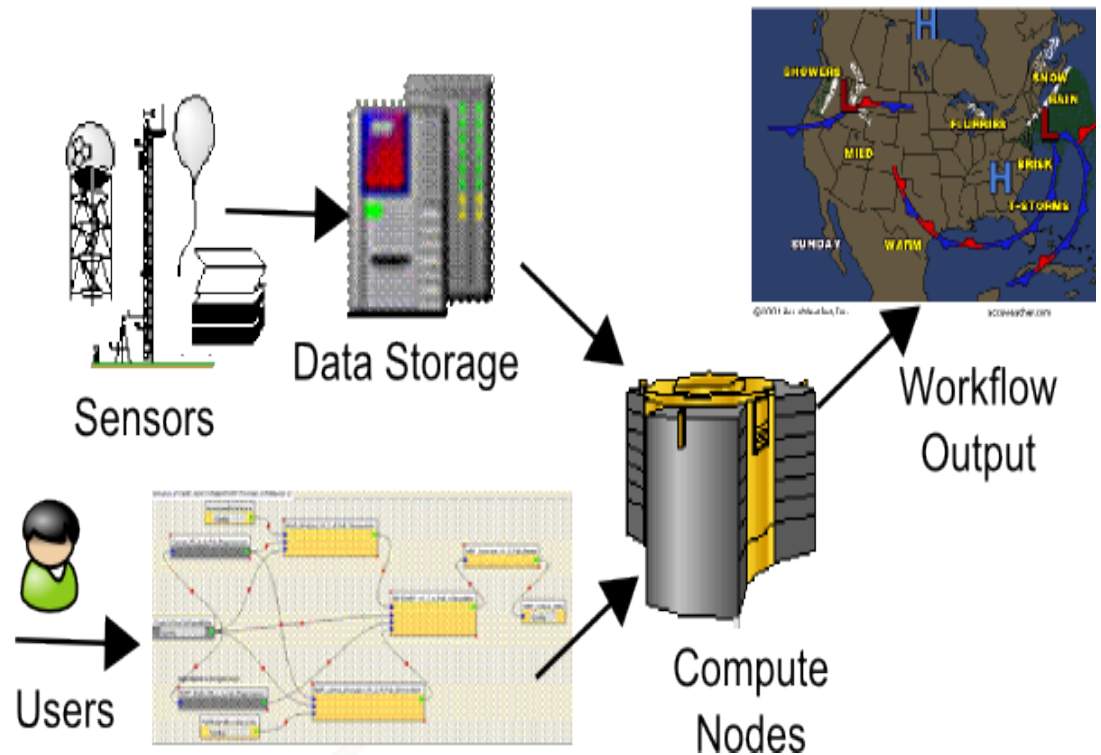
# Generic Application Service Factory

# WS-BPEL

- Business Process Execution Language for Web Services (WS-BPEL)
  - De-facto standard for specifying web service based business processes and service compositions
- Basic activities
  - Invoke, Receive, Assign..
- Structured activities
  - Sequence, Flow, ForEach,..

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# Workflow Composition, Execution & Monitoring

XBaya enables users to construct, share, execute and monitor sequence of tasks executing on their local workstations to high-end compute resources.



Sensors

Data Storage

Users

Compute Nodes

Workflow Output

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# XML Metadata Catalog (XMC Cat)
## Taming Complex Scientific Metadata Schemas

*"A significant need exists in many disciplines for long-term, distributed, and stable data and metadata repositories"*

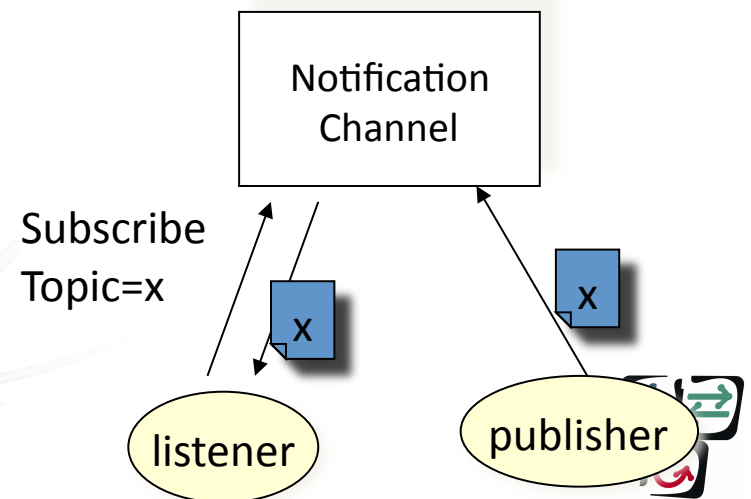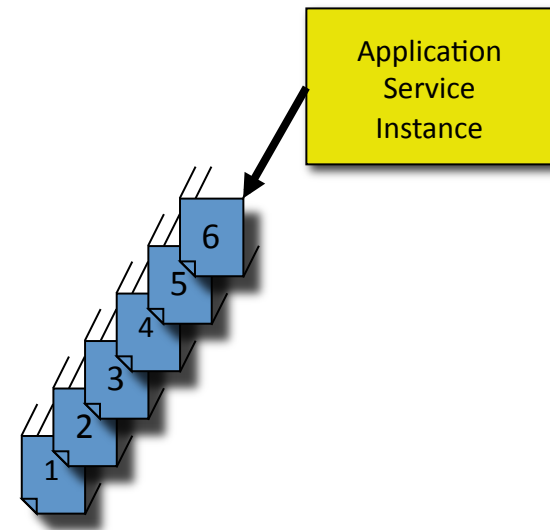– NSF Blue-Ribbon Advisory Panel on Cyberinfrastructure

*"Metadata is key to being able to share results"*

– UK e-Science Core Programme Study



**More Info: Scott Jensen, Beth Plale**

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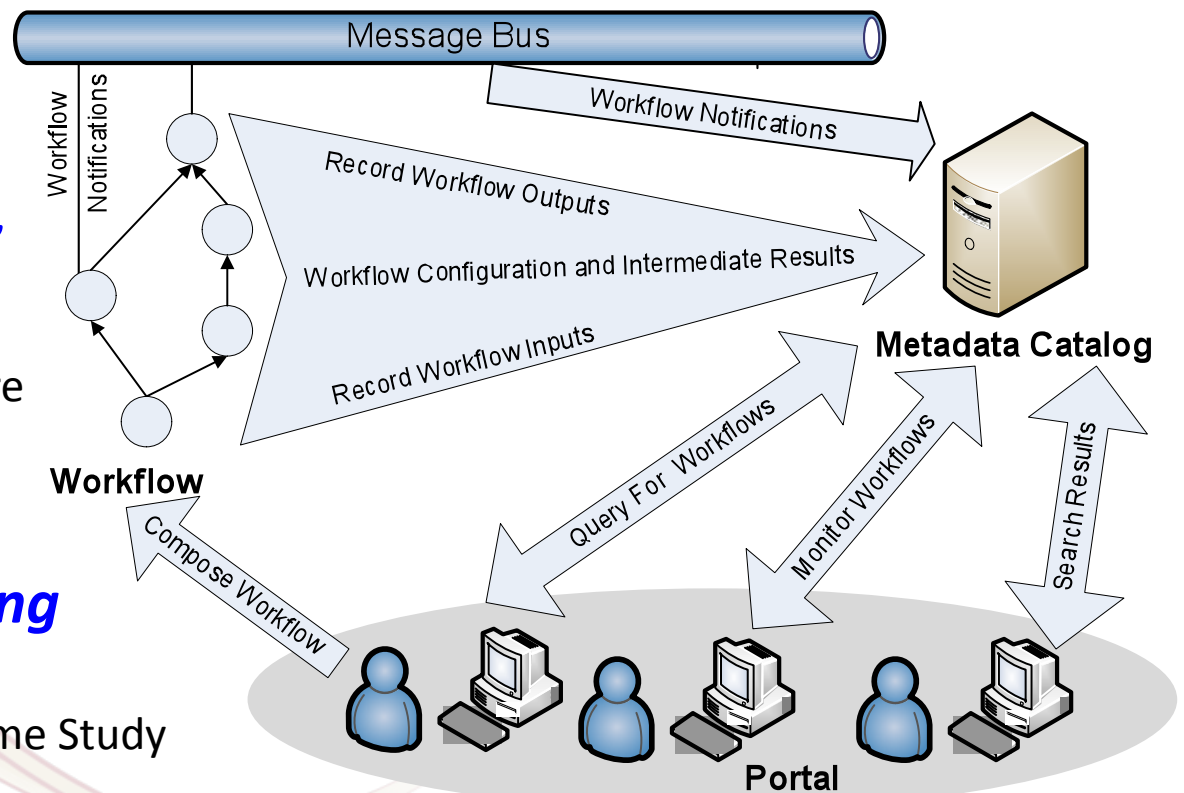
# Service Monitoring via Events

- The service output is a stream of events
  - I am running your request
  - I have started to move your input files.
  - I have all the files
  - I am running your application.
  - The application is finished
  - I am moving the output to you file space
  - I am done.
- These are automatically generated by the service using a distributed event system (WS-Eventing / WS-Notification)
  - Topic based pub-sub system with a well known "channel".

Application Service Instance

6
5
4
3
2
1

Notification Channel

Subscribe Topic=x

x

x

listener

publisher

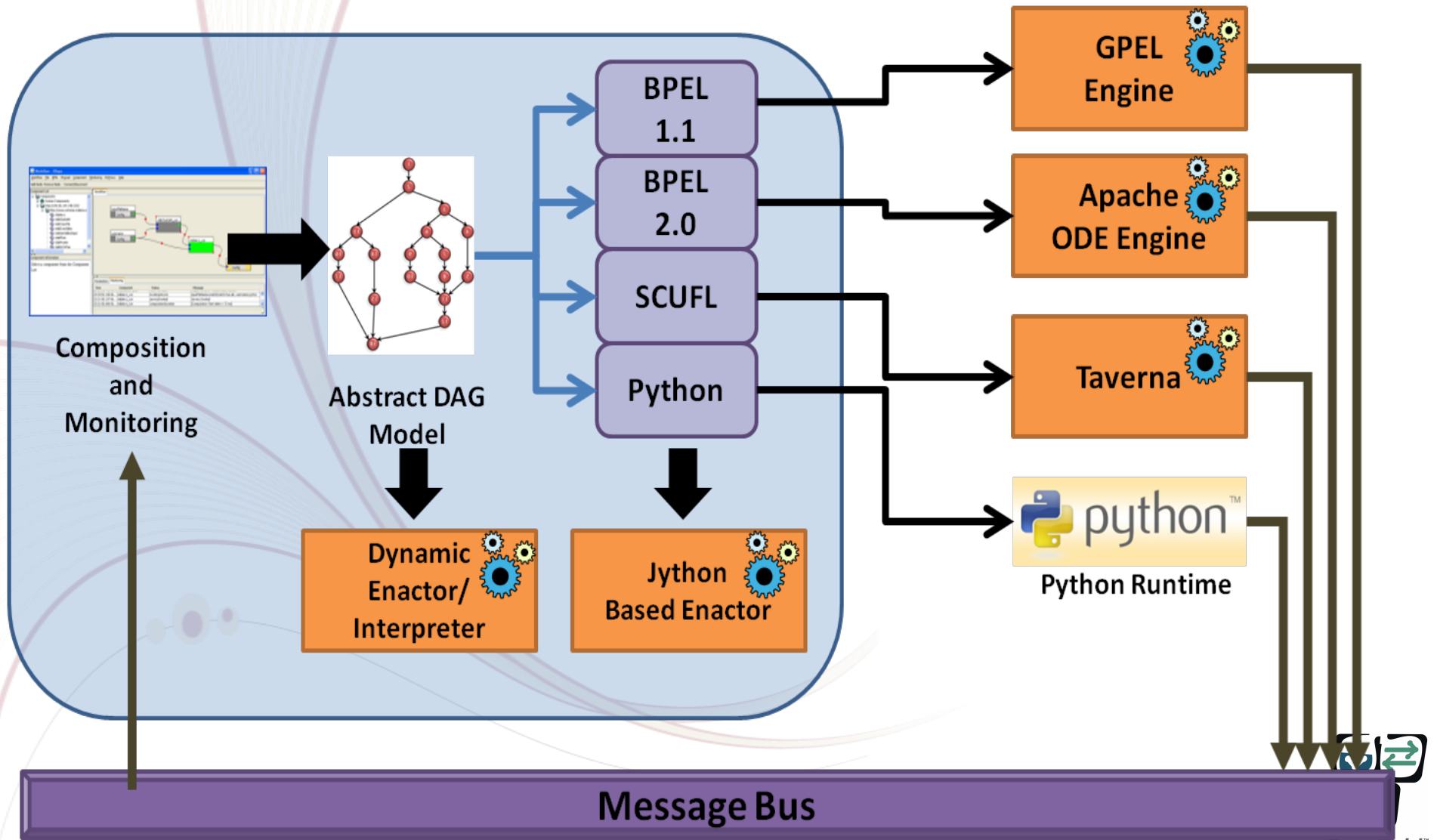# WxChallenge: The National Collegiate Weather Forecast Contest

- Hundreds of graduate and undergraduate students nationwide make daily forecasts for selected US cities
- LEAD was introduced on a trial basis so students could <u>run their own WRF forecasts</u> with fine-scale grids + <u>fine-scale data</u>
  - 7-week pilot study funded by LEAD core
  - 75 students from 10 institutions + faculty sponsors
  - 279 on-demand forecasts made at NCSA, 0.6 TB output produced
  - More than 160 processors reserved on Tungsten 5 days/week, 10 am – 8 pm EDT
  - 78% of workflows completed, subsequent problems fixed
- Significant hands-on experience with models → opportunity for learning about CFD, physics, computing
- Decision Science Opportunity:  How do students decide how, when to run model?
- Huge (but welcome) challenge for TeraGrid
- Good way to identify strengths and weaknesses in ALL components of LEAD
- Formal evaluation conducted

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# Lessons Learned From LEAD

- Large number of users invoking lot of small applications create a surges in load in middleware.
  - Build Reliability into Workflow Infrastructure
- Troubleshooting large scale distributed infrastructure needs coordinated debugging involving multiple experts.
  - Ingest as much as possible fault Tolerance.
- Scientists need Flexibility but too much Flexibility is called Confusion.

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# Workflow Architecture



Composition and Monitoring

Abstract DAG Model

BPEL 1.1

BPEL 2.0

SCUFL

Python

GPEL Engine

Apache ODE Engine

Taverna

python™

Python Runtime

Dynamic Enactor/Interpreter

Jython Based Enactor

Message Bus

*TeraGrid*™

# GPEL

- Grid Process Execution Language
  - BPEL4WS based home grown research workflow engine
  - Supports a subset of BPEL4WS 1.1
  - One of the very early adaptations of BPEL efforts
- Specifically designed for eScience Usage
  - Long running workflow support
  - Decoupled client

# Benefits of Porting to Apache ODE
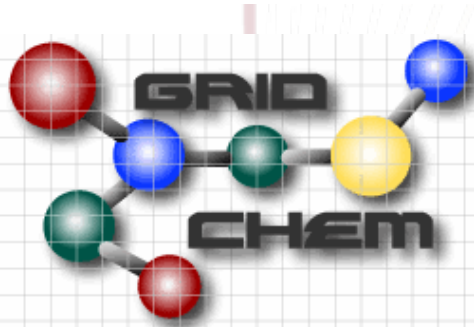
**WS-BPEL 2.0 features**

**Sustainability**
- Well supported run time with minimal custom changes

**Improved Scalability & performance**

**Minimize changes to legacy components**

**Portability & avoid lock in**
- Adhering to widely used open standards
- Avoid using runtime specific

# Molecular Chemistry Gateway

- Challenges:

– Some apps have rich Client Gui's, a challenge with asynchronous long running workflows

– Workflow Verification Service

– Parametric sweep scheduling, monitoring iteration steps, graphical composition

– Human Interaction into Workflows
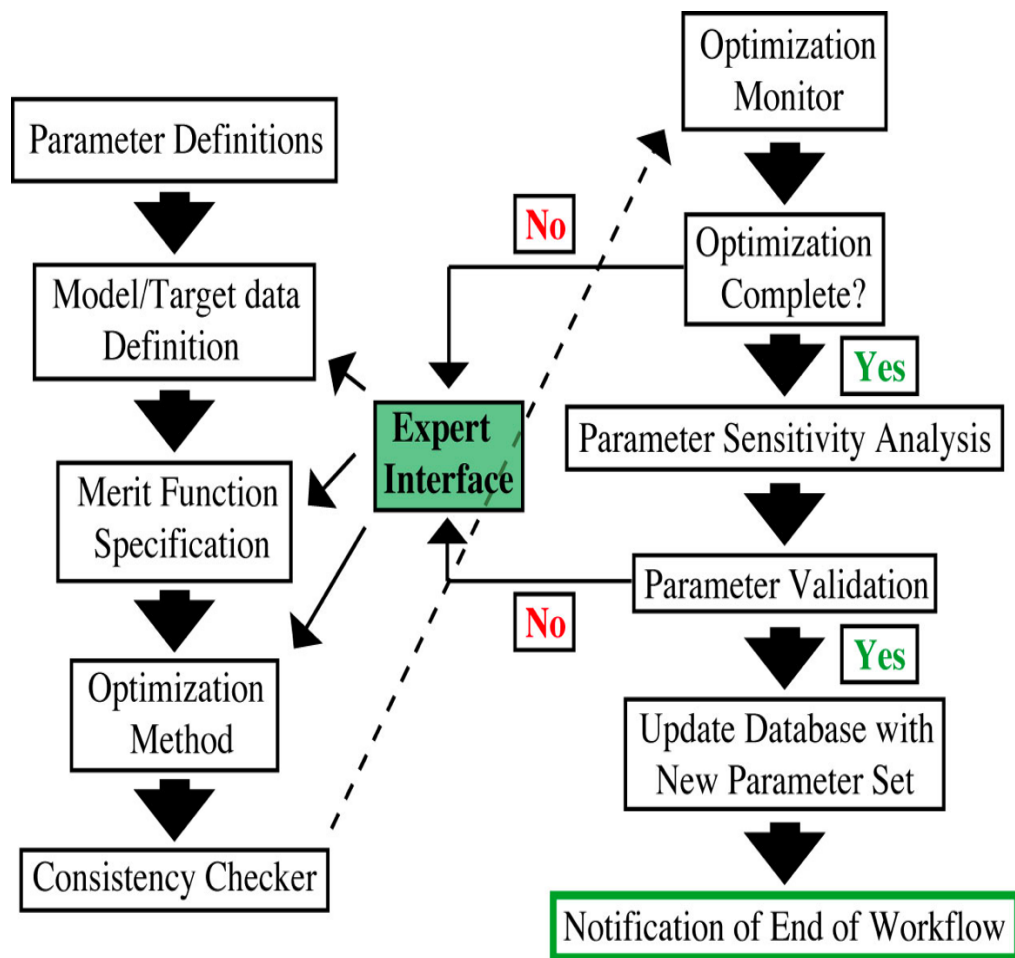
# UltraScan Advanced Support

- Enhance Job Management

- Integrate Information Services

- Improve Fault Tolerance

- Integrate with Unicore and other European Grids

- Enable Workflows for Future

# Packaged, Downloadable Software

- http://www.collab-ogce.org/ogce/index.php/Main_Page

# Live Demo & Questions?

# XBaya Usage Flow

1. Scientist/Application provider registers application description with Registry Service.

2. Workflow Author constructs the workflow with multiple wrapped application services.

3. Workflow is compiled and deployed to the ODE workflow Engine.

4. Workflow inputs are captured by XBaya and workflow is launched to ODE.

5. Workflow system and possibly some services publish notifications to the Message bus reporting the progress of the workflow.

6. XBaya monitoring system listens to notifications and color the workflow components to present workflow progress.

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