OpenMolGRID: Complex Problem Solving in Molecular Design

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Outline

• The OpenMolGRID Project
• Molecular Design and Engineering
• Grid Architecture
  – Integration of Applications
  – Database Access
  – Workflow Support
• Status and Outlook
OpenMolGRID

• Funded in part by EC: IST-2001-37238
• 01.09.2002- 30.11.2004
• Partners:
  – University of Tartu, EE (Project Coordinator)
  – University of Ulster, UK
  – Mario Negri Institute, IT
  – Forschungszentrum Jülich, DE
  – ComGenex Inc., HU
• www.openmolgrid.org
Project Objectives

• Development of tools for secure and seamless access to distributed information and computational methods relevant to molecular engineering within the UNICORE frame

• Provide a realistic testbed and reference application in life science

• Development of a toxicity prediction model validated with a large experimental set

• Provide design principles for next-generation molecular engineering systems
Work Packages

- **WP1**: Grid Data Warehousing of Molecular Structure -- Property (Activity) Information
- **WP2**: Molecular Descriptor Generation and QSPR Model Building on the Grid
- **WP3**: Computational Molecular Engineering of New Compounds and Materials
- **WP4**: Grid Integration
- **WP5**: Test application of the OpenMolGRID System for Chemical and Pharmaceutical Predictions
Molecular Engineering

Rational design and targeted synthesis of

• new molecules
• new materials
• new chemical reactions
• new technological processes
Molecular Engineering

**STRUCTURE**

![Chemical structure](image)

**PROPERTY**

- PHYSICAL
  - $t_B$, $\nu_{(\text{max})}$
  - $\rho$
- CHEMICAL
  - $\log k$
  - % yield
- BIOMEDICAL
  - $LD_{50}$

Complex Problem Solving in Molecular Design
Basis: UNICORE Infrastructure

Complex Problem Solving in Molecular Design
OpenMolGRID enhances UNICORE

• Plugins for
  – Classes of applications for molecular calculations
  – Workflow support
  – Database access

• Application ‘Database Access Tool’
  – Interface between UNICORE and database
  – Flexible output formats (XML, XSLT)

• Abstraction Layer for software modules
OpenMolGRID Architecture

Automated Workflow Support
UNICORE Client

UNICORE

Abstract Resource Interface
Data Source 1

Abstract Resource Interface
Data Source n

Abstract Resource Interface
Software Package 1

Abstract Resource Interface
Software Package m
Application Specific Support

• Client plugins
  – GUIs for applications and workflow
  – Resource selection
• Resource definition for applications
  – Part of Incarnation DataBase
• Application metadata
  – Description of the application
  – Information for the client plugin
Application Definition in IDB

- **APPLICATION** \( A_{n.m} \) metadata_file
- **INVOCATION** \( A_{n.m} \) [ ....... ]
- Metadata format:
  - Task (name, description)
  - Input [inile (type, use)]*
  - Output [outfile (type, occurs)]*
  - Appspecific information for client plugin
Application layer

Application A

Software Package A

Application Metadata for A

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Database Access Architecture

• Access to a data source is seen as an application
• Structural information is described in the metadata file
• User interface is an application specific interface
Database Access Architecture (cont.)

• General
  – Valid for all types of information
  – Valid for all kinds of databases

• Flexible
  – Metadata file allows for adaptation to db changes

• Extensible
  – Arbitrary output formats can be supported
  – XML Document Type Definition
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Workflow Support

Workflow (XML)

OpenMolGRID MetaPlugin

Server Resources
(Applications, compute resources, storage, ...)

Client Resources
(Plugins, resource management, ...)

User Preferences

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Meta-Plugin

- Plugin able to see all task plugins
- Workflow description (XML) is used to generate UNICORE job tree
- Look for matches between output file / input file specifications of two dependent applications
- Allow for user intervention at predetermined positions in the workflow (hold forever / release)
- Distribute tasks to multiple Vsites
- Select target site(s) and application resource
- Insert transfer and data conversion tasks where necessary
Status

- Data Warehouse (MOLDW) specified
- Application interfaces in progress
- Abstraction layer (DBAT) for relevant Databases available
- Initial version of Meta-Plugin available
- Initial testbed set up
- Workflow specification for selected steps available
Outlook

• Feed MOLDW with data

• Develop abstract resource interfaces for
  – descriptor calculation
  – model development

• Develop resource information provider plugin