Quantum Chemical Workflows in the MoSGrid Science Gateway

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Motivation

- Sophisticated tools and algorithms available
- Lack of graphical user interfaces
- Complexity of computing infrastructures
- Many end users lack computer science background

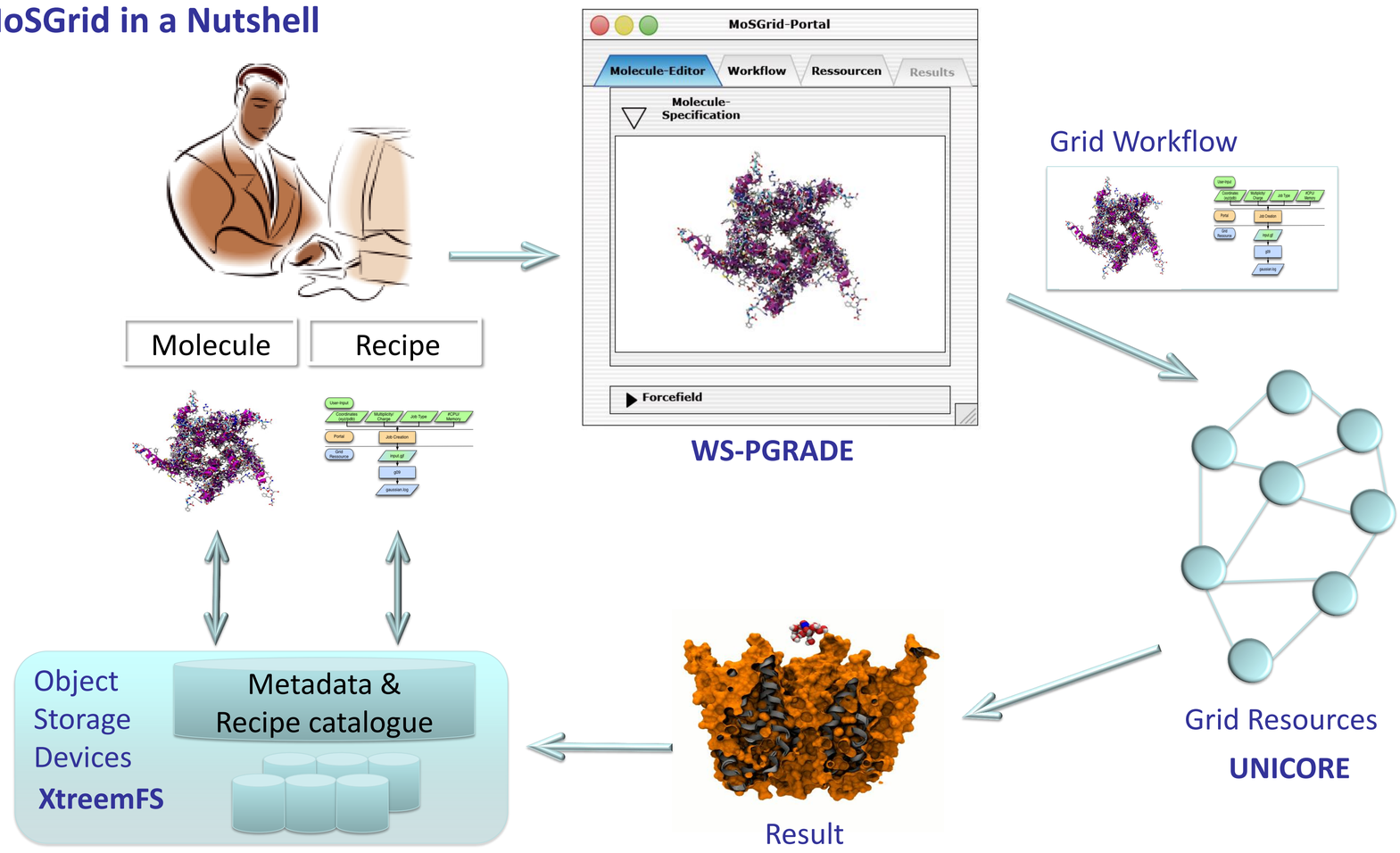
⇒ Need of self-explanatory and intuitive user interfaces
⇒ Portals as ideal tool

MOSGRID-PORTAL:

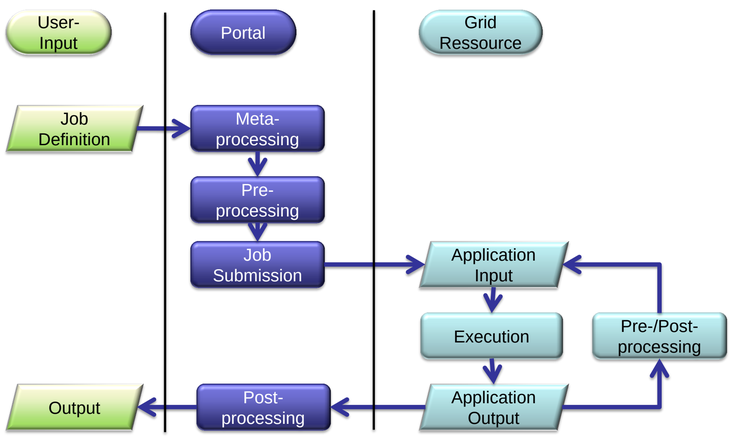
HTTP://WWW.MOSGRID.DE

- Framework for integrating information and applications
- Single point of entry
- Provide each user with a repository of personal information
- Possibility to customize views and tools
- No installation of software on the end-user side
- No firewall issues

MoSGrid in a Nutshell



General Workflow

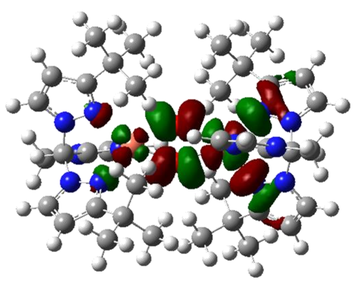


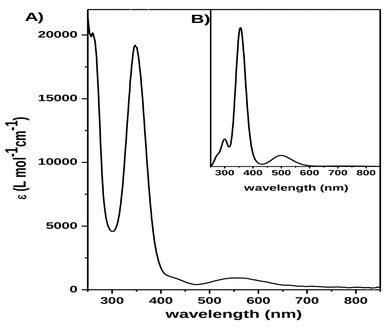
- Definition of atomic workflows
- Combination to meta-workflows via WS-PRADE
- Parsing out data (energies, frequencies)
- Automatic transformation to fchks

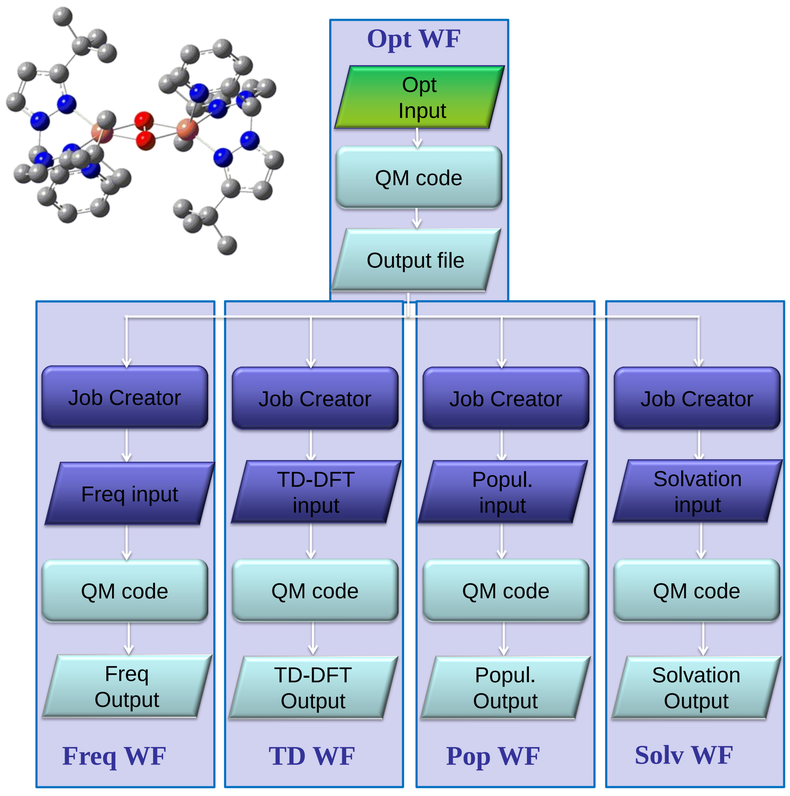
Metaworkflow: Spectroscopic Analysis

Calculation of:

- the optimised structure: Opt WF as basis for all subsequent workflows with automatic input generation
- UV/Vis spectra with TD-DFT: TD WF
- IR frequencies: Freq WF
- population analysis: Pop WF
- solvent effects: Solv WF







Domains and Codes

In General:

Quantum Chemistry:

- ✓ Gaussian09
- ✓ NWChem

Molecular Dynamics:

- ✓ Gromacs 4.5.5
- ✓ eSBMTools

Docking:

- ✓ CADDSuite
- ✓ AutoDockVina
- ✓ FlexX

For expert users:

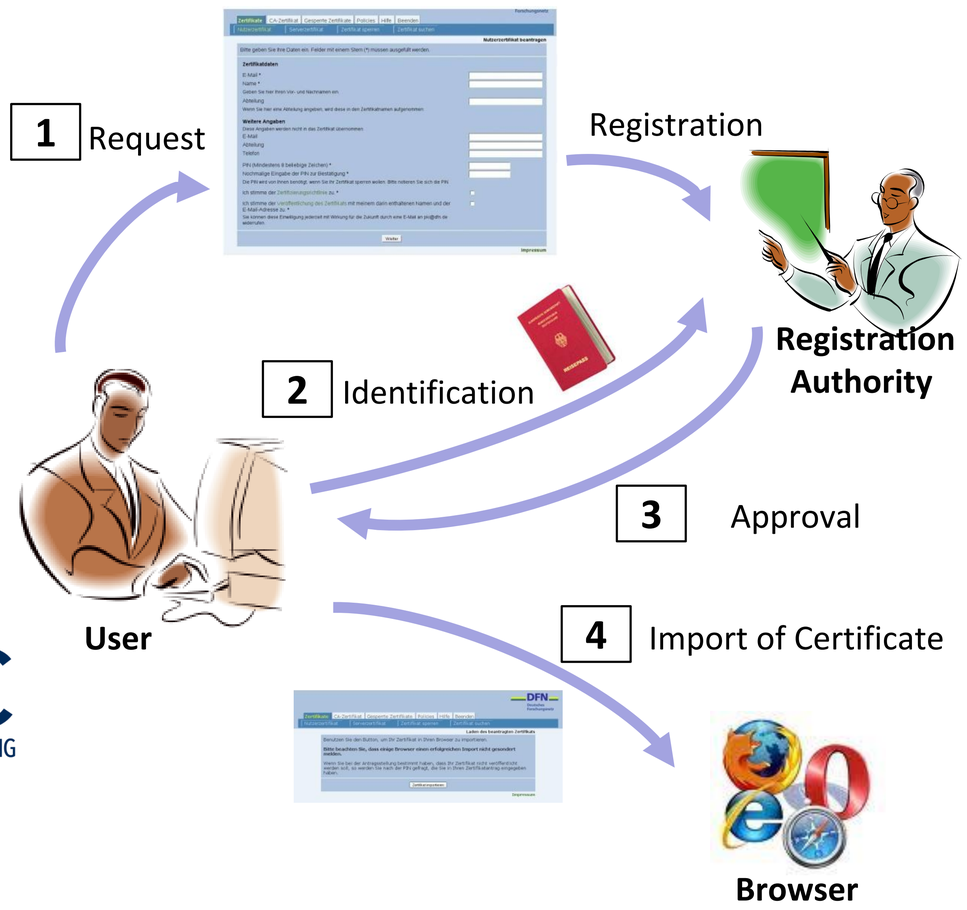
- ✓ Workflow building in a specific portlet possible!
- ✓ Domain-mixing possible

How to access MoSGrid

You need a Grid-certificate!

Via http://www.mosgrid.de you will find:

- **Your registration authority**
- **A concise guide on how to get a certificate and access MoSGrid**



MoSGrid consortium:

Eberhard Karls Universität Tübingen
Technische Universität Dresden
rrzk
Universität zu Köln
CRC Center for Research Computing
RWTH Aachen University
PC² Paderborn Center for Parallel Computing

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