User-friendly workflows in quantum chemistry

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Motivation

• Excellent simulation codes available for all chemical domains

• Huge amount of computational resources

• Time consuming access even for experienced users

• Impassable obstacle for beginners
Aims of MoSGrid

• Enabling easier access to HPC (high-performance computing) facilities
• Allowing inexperienced scientists to run molecular simulations on DCIs
• Offering an intuitive user interface (gateway)
• Enabling easy access to recipes, workflows, data repositories
Molecular Simulation Grid

The MoSGrid portal

One goal of the interdisciplinary project MoSGrid (Molecular Simulation Grid) is to offer molecular simulation tools and docking tools via a portal. MoSGrid portal is designed as workflow-enabled grid portal developed on top of the library version of WS-PGRADE. WS-PGRADE is a usable, highly-flexible graphical user interface for the grid User Support Environment (gUSE) developed by MTA SZTAKI.

User interface
WS-PGRADE

High-level middleware service layer
gUSE

Grid resources middleware layer
UNICORE 6

Workflow storage
Application repository
Information system
Workflow engine
Submitters
Logging
MoSGrid Science Gateway

• Portal framework: Liferay
  • Versatile configuration possibilities
  • Allows to provide a user-friendly portal
• Certificate Portlet
  • Easy Management of access to DCIs
• Submission of chemical calculations via gUSE
• High-level middleware: WS-PGRADE
• Middleware: UNICORE
• Resources: Wide range of German D-Grid resources (in the future also European DCIs)
Molecular Simulation Grid

- Start in 2008: 50 associated chemical work groups
- October 2010: Mailing list with 100 addressees as MoSGrid Community
- December 2011: after the community meeting increase to 120 interested chemists from all three domains
- Community serves as pool for requirements analyses.
- Today: 20 real expert users
  40 standard users
Use of Workflows in Domains

• Domains
  • Quantum chemistry
  • Molecular dynamics
  • Docking

• Identifying standard recipes
  • Modelling of suited workflows

• Goals:
  • For Power Users
    • Possibility to design own Workflows
  • For Novices
    • Offer standard workflows
Use of Workflows in Domains

- Quantum Chemical Calculations
  - based on approximated solutions of the Schrödinger equation
  - Average scalability
  - Gaussian, NWChem, Turbomole, ...

- Molecular Dynamics
  - based on forcefields describing molecular interactions
  - Good scalability
  - Gromacs, NWChem, Amber, ...

- Docking
  - Based on simplified forcefields
  - Excellent scalability
  - CADDSuite, FlexX, ...
Basic Workflow

User-Input → Portal → Grid Resource

Job Definition → Meta-processing → Application Input

Job Submission → Execution → Application Output

Output → Post-processing
- Specialised interface for quantum chemistry software (Gaussian, Turbomole, NWChem)
- Basic workflows
- Easy Generation or Uploading of Input Files
- Parsing of result files
Example: Parameter Sweep

- Parameter Sweep
  - Scan of a potential energy surface (PES)
  - Change of one parameters crucial for theoretical analysis
  - Reaction path analysis
  - Pre-defined steps

- Input
  - Molecular structure
  - Parameter
  - Parameter range

- First step
  - automatic generation of Inputfiles

- Second step
  - Submission into the Grid

- Third step
  - Plotting of obtained energies against the chosen parameter
Example: High Throughput

• Native X-ray format needs to be converted into a computational readable mol file.

• Time-consuming process of manual conversion can be transferred into the portlet.

• **Input**
  • X-ray data

• **First step**
  • Conversion into mol file

• **Second step**
  • Conversion into job file with pre-defined job parameters (functional, basis set)

• **Third step**
  • Submission into the Grid
Example: Transition State Analysis

- Zinc complex reacting with lactide
Example: Transition State Analysis

- **Input**
  - Transition state job file (e.g. QST3 file)

- **First step**
  - Calculation of TS geometry

- **Second step**
  - Conversion into job files for frequency and IRC calculations

- **Third step**
  - Calculation of frequency and reaction path
Example: Spectroscopic Analysis

Structure

Time-dependent DFT for UV/Vis prediction

Orbital analysis (LMCT)
Example: Spectroscopic Analysis

1. Opt Input
2. QM code
3. Output file
4. Job Creator
   - Frequency input
   - TD-DFT input
   - Population input
   - Solvation input
5. QC code
   - Frequency Output
   - TD-DFT Output
   - Population Output
   - Solvation Output
6. Complete spectroscopic analysis
Example: Spectroscopic Analysis
Example: Spectroscopic Analysis

- **Freq** input
- **TD-DFT** input
- **Popul. input**
- **Solvation input**

- **Opt** input
- **QM code**
- **Output file**

- **Freq** input
- **Freq output**
- **QM code**
- **Freq WF**

- **TD-DFT** input
- **TD-DFT output**
- **QM code**
- **TD WF**

- **Popul. input**
- **Popul. output**
- **QM code**
- **Pop WF**

- **Solvation input**
- **Solvation output**
- **QM code**
- **Solv WF**
Example: Spectroscopic Analysis

Meta-Workflow

Opt WF

Freq WF  TD WF  Pop WF  Solv WF
Workflows in Quantum chemistry

Application at the QC codes implemented in MoSGrid:

☑ Gaussian
☑ Turbomole
☑ NWChem

- Great Help for User (via standard recipes in the repository)
- Possibility to generate own complex workflows
- Facilitation of data extraction and postprocessing
- Meta-workflows allow re-use of basic workflows!
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