LMU LUDWIG-MAXIMILIANS-UNIVERSITÄT MÜNCHEN

MoSGrid

User-friendly workflows in quantum chemistry

ER-flow

Prof. Dr. Sonja Herres-Pawlis

Ludwig-Maximilians-Universität München

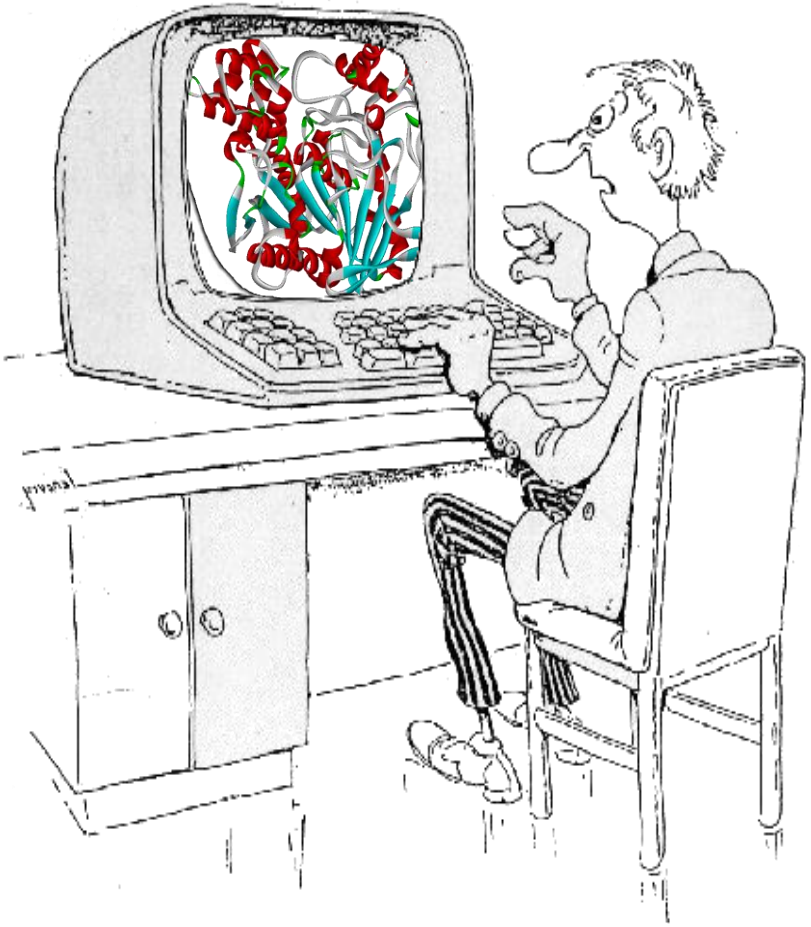
Akos BALASKO, Georg BIRKENHEUER, André BRINKMANN, Sandra GESING, Richard GRUNZKE, Alexander HOFFMANN, Peter KACSUK, Jens KRÜGER, Lars PACKSCHIES, Gabor TERSTYANSKY, and Noam WEINGARTEN

International Workshop on Science Gateways

3.06.2013, Zürich

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



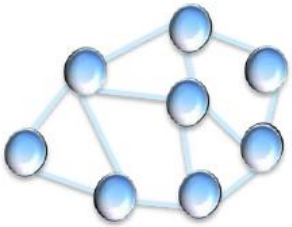
Aims of MoSGrid

- 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

User interface
WS-PGRADE

High-level middleware service layer
gUSE



Grid resources middleware layer
UNICORE 6

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

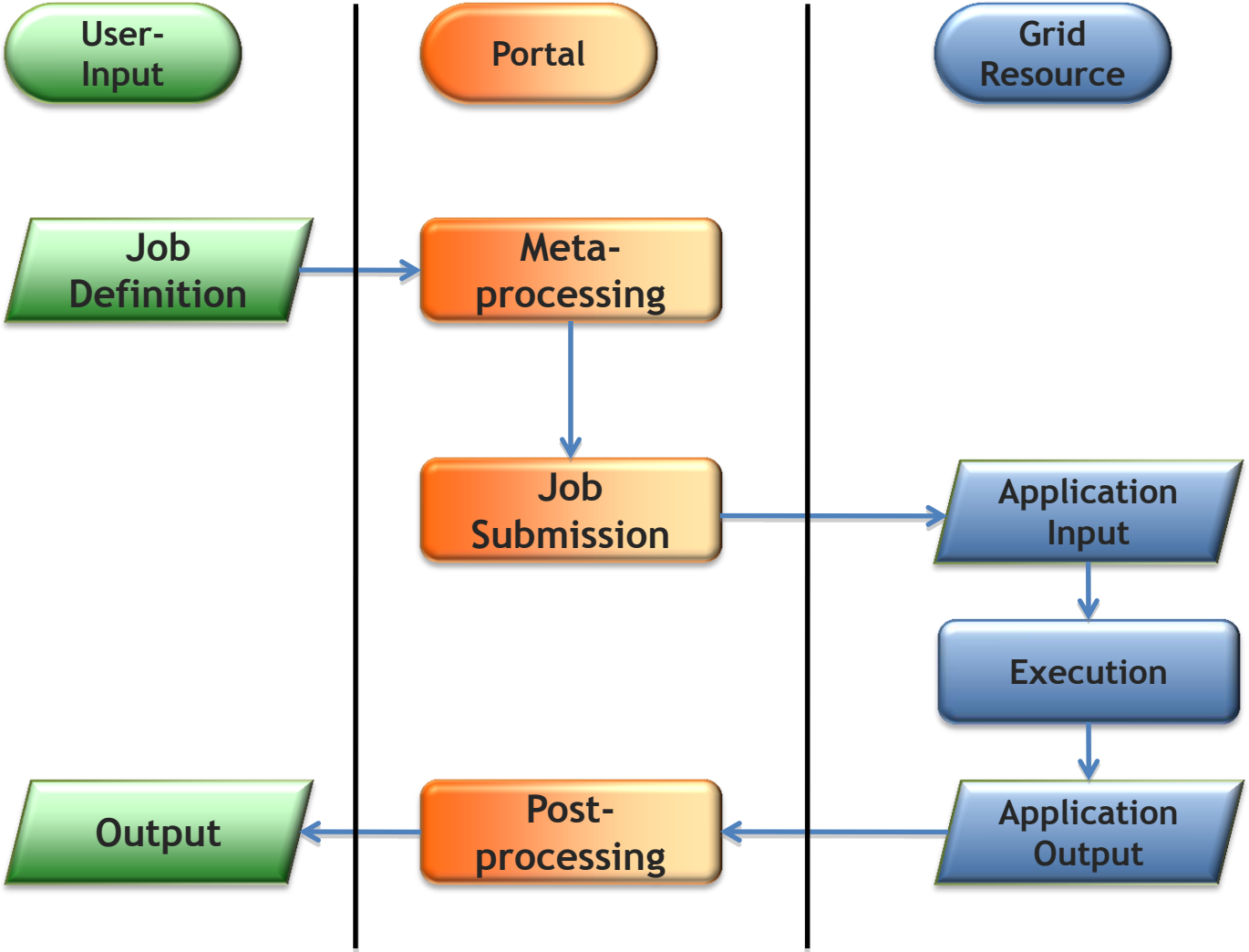
Use of Workflows in Domains

- 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

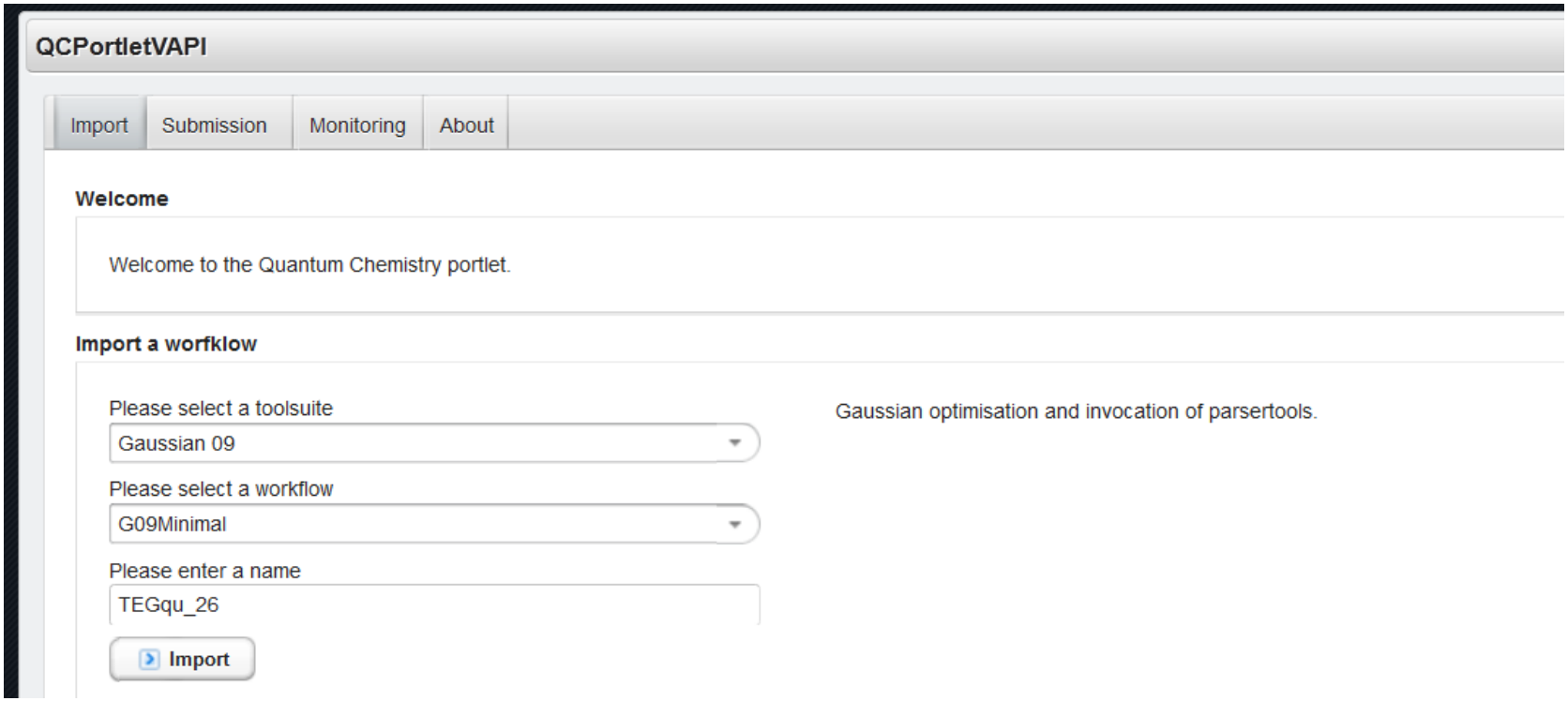
Use of Workflows in Domains

- 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



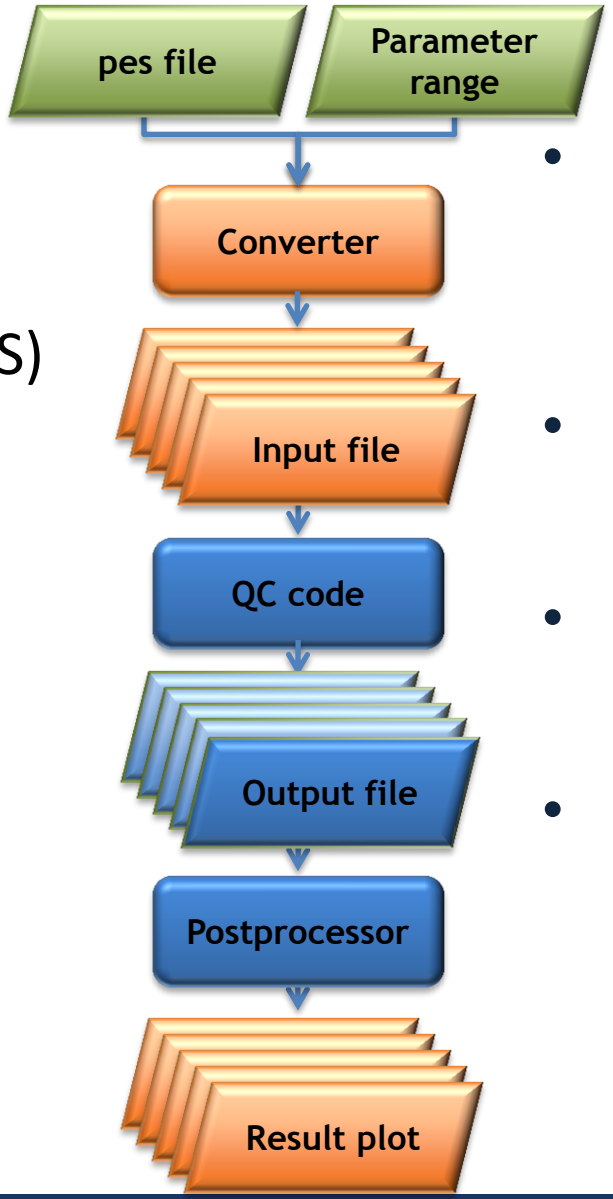
The QC Portlet @ MoSGrid.de



- 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

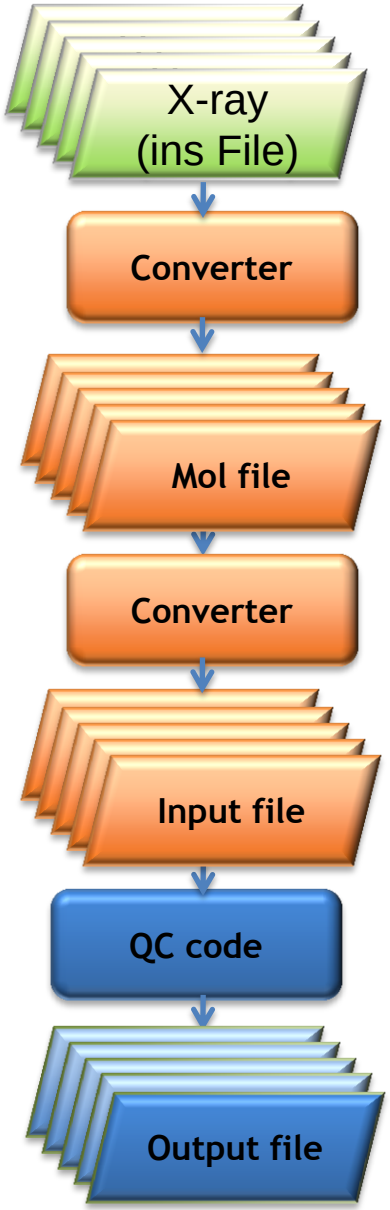
- Parameter Sweep
  - Scan of a potential energy surface (PES)
  - Change of one parameters crucial for theoretical analysis
  - Reaction path analysis
  - Pre-defined steps



- 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

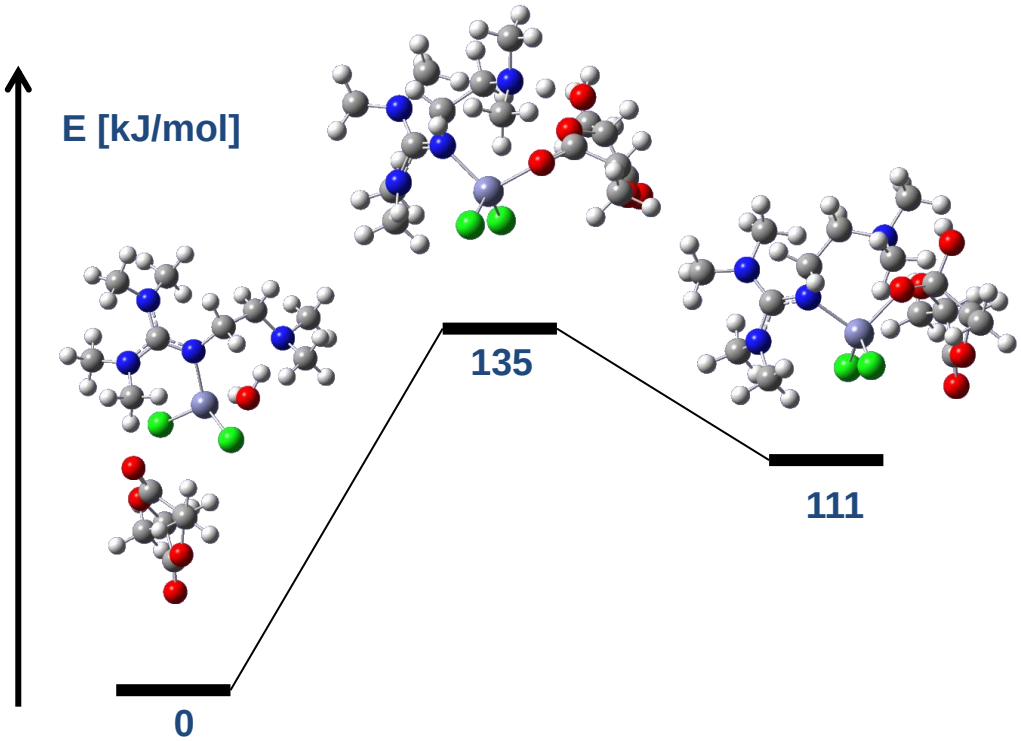
- Native X-ray format needs to be converted into a computational readable mol file.
- Time-consuming process of manual conversion can be transferred into the portlet.

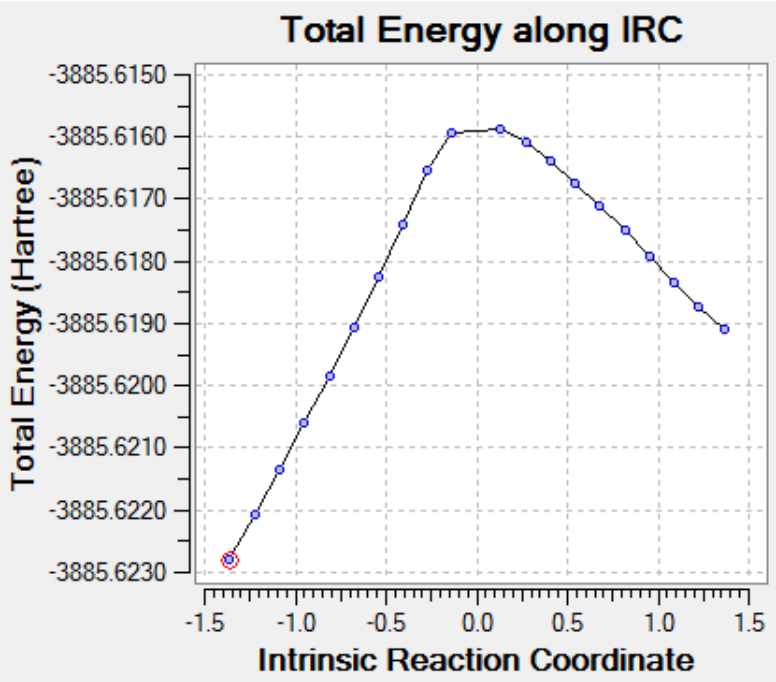


- Input
  - X-ray data
- First step
  - Conversion into mol file
- Second step
  - Conversion into job file with pre-defined job parameters (functional, basis set)
- Third step
  - Submission into the Grid

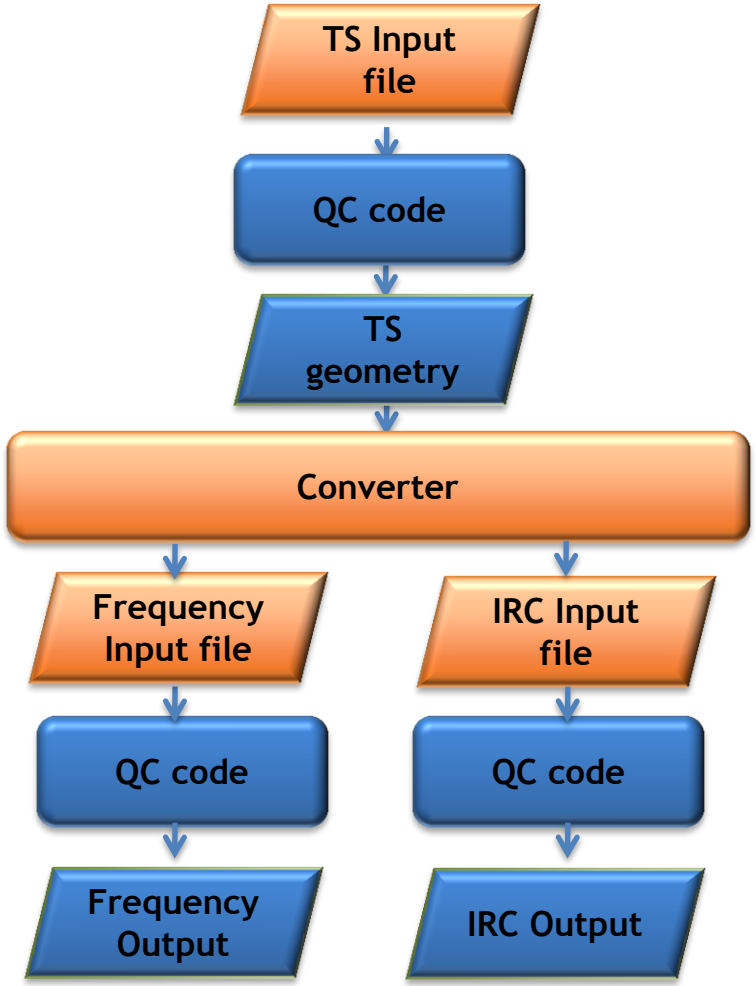
Example: Transition State Analysis

- Zinc complex reacting with lactide





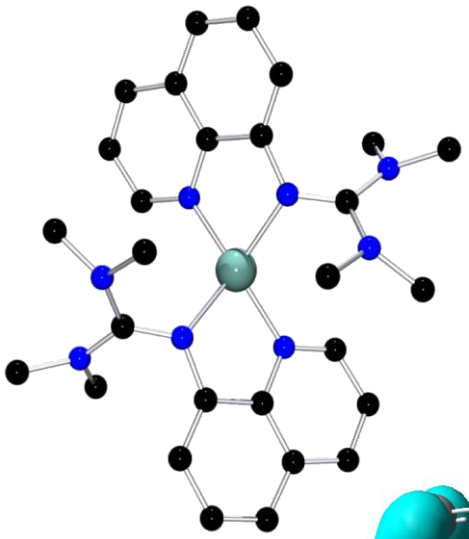
Example: Transition State Analysis



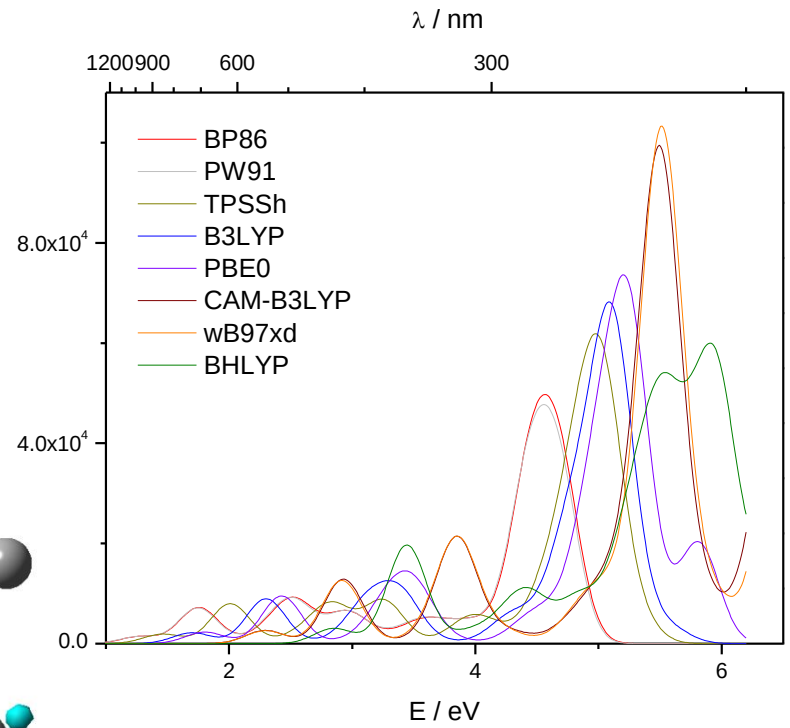
- Input
  - Transition state job file (e.g. QST3 file)
- First step
  - Calculation of TS geometry
- Second step
  - Conversion into job files for frequency and IRC calculations
- Third step
  - Calculation of frequency and reaction path

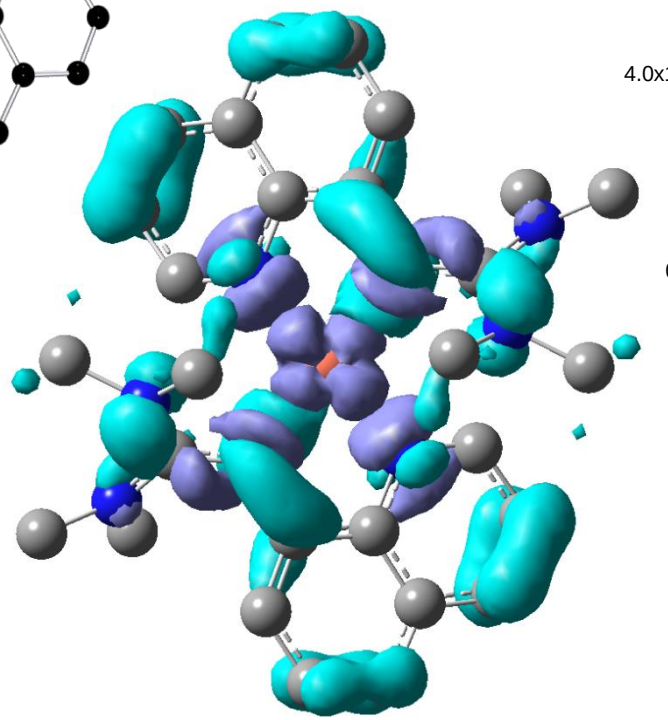
Example: Spectroscopic Analysis

Structure



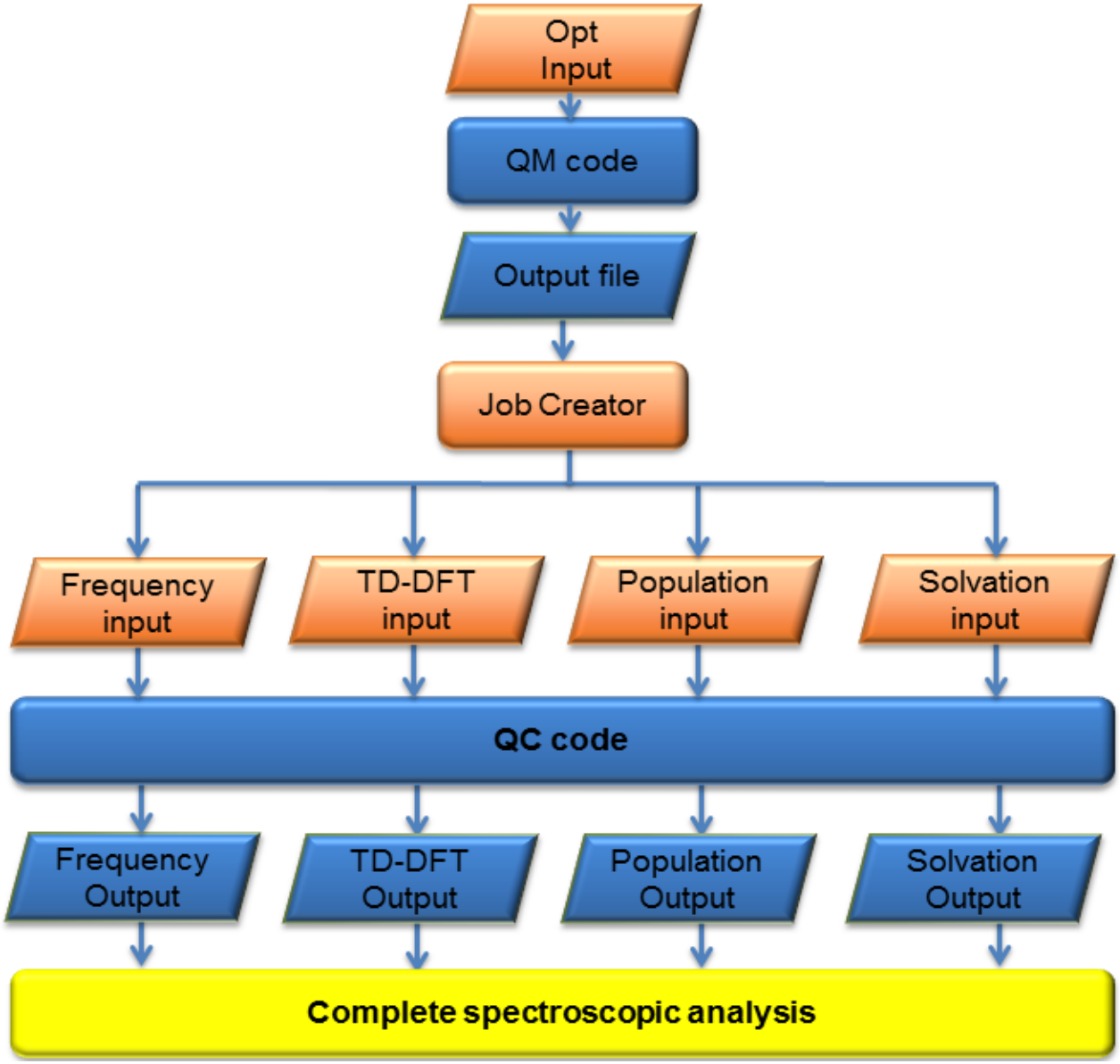
Time-dependent DFT for UV/Vis prediction



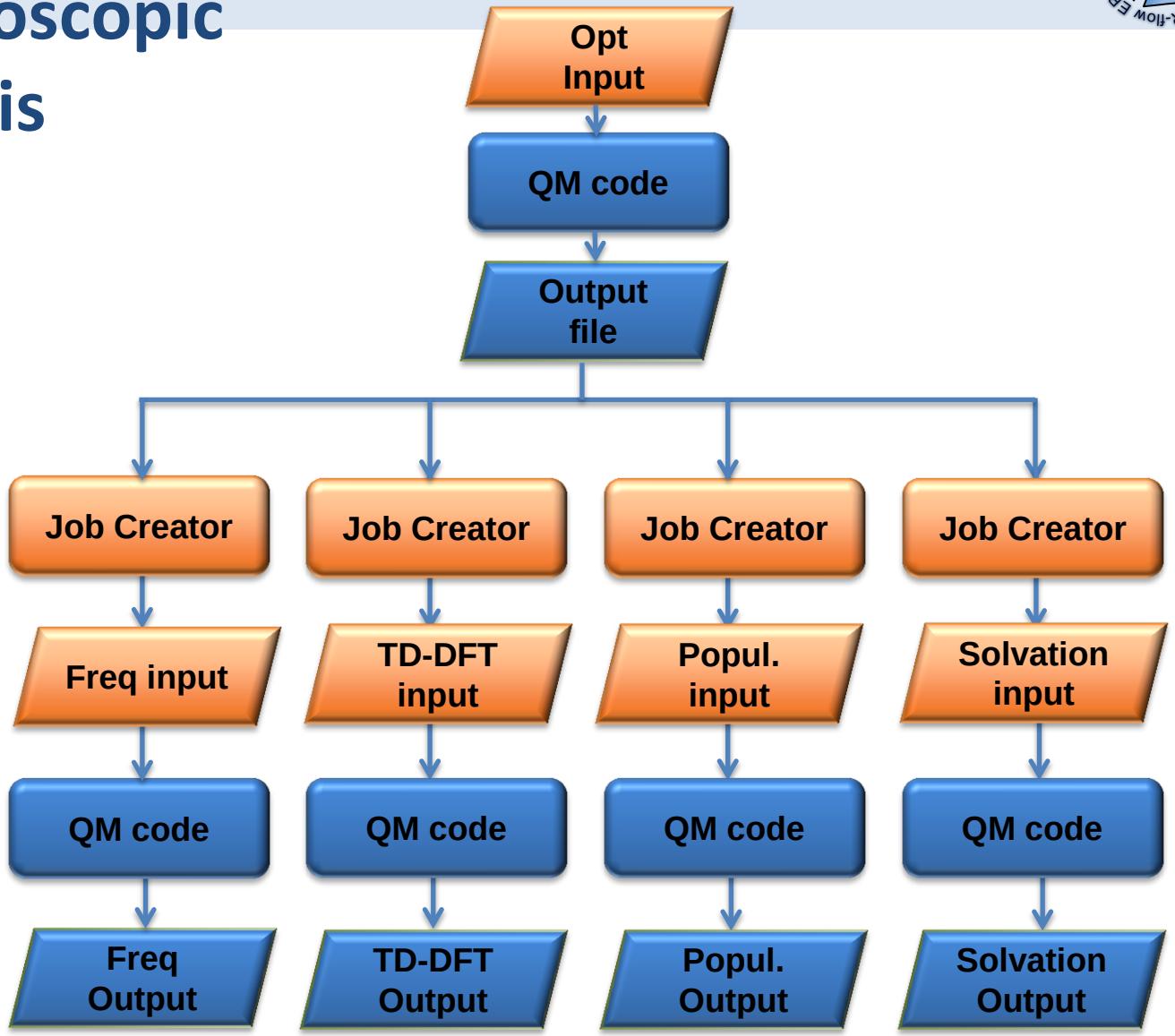


Orbital analysis (LMCT)

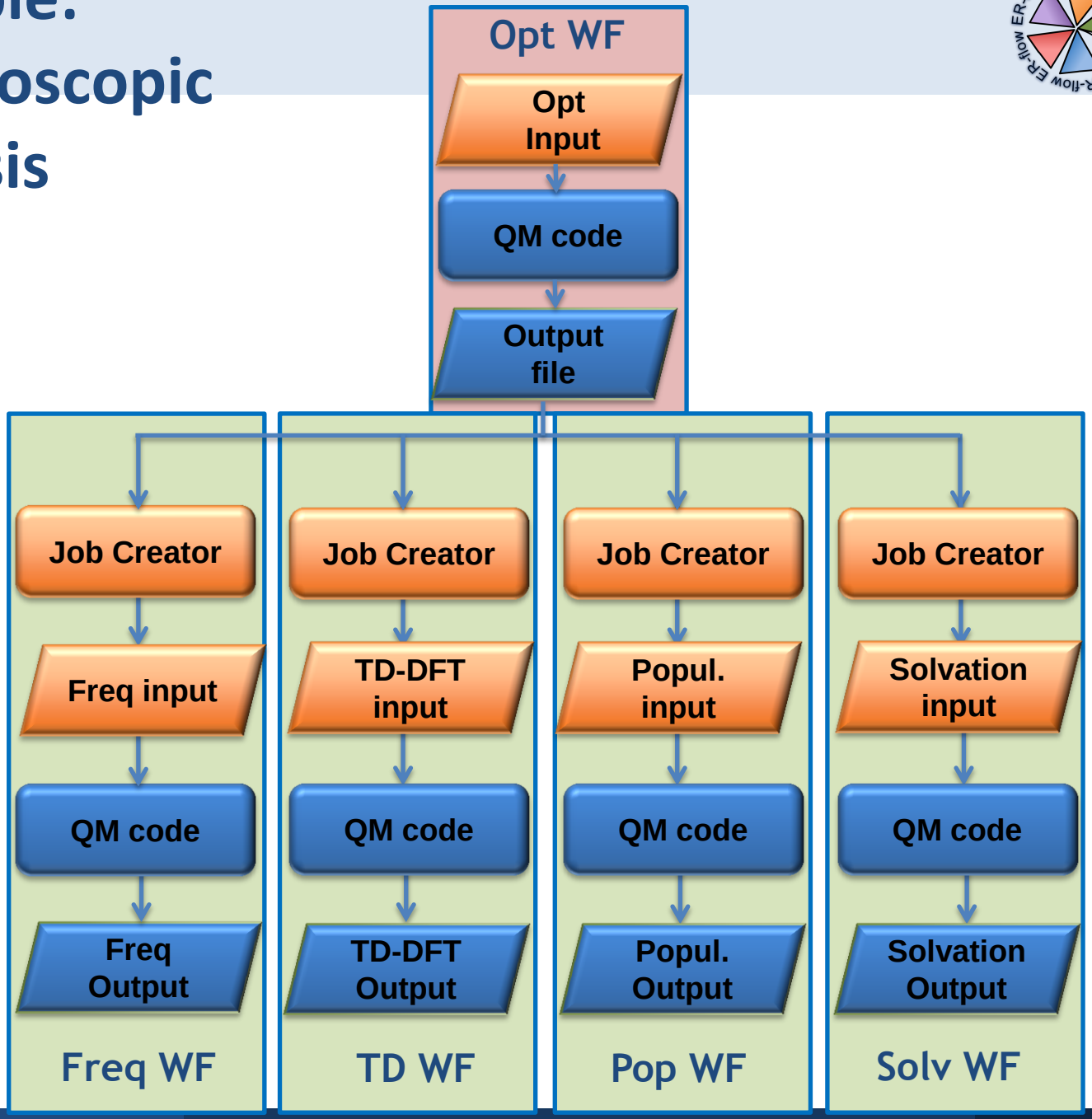
Example: Spectroscopic Analysis



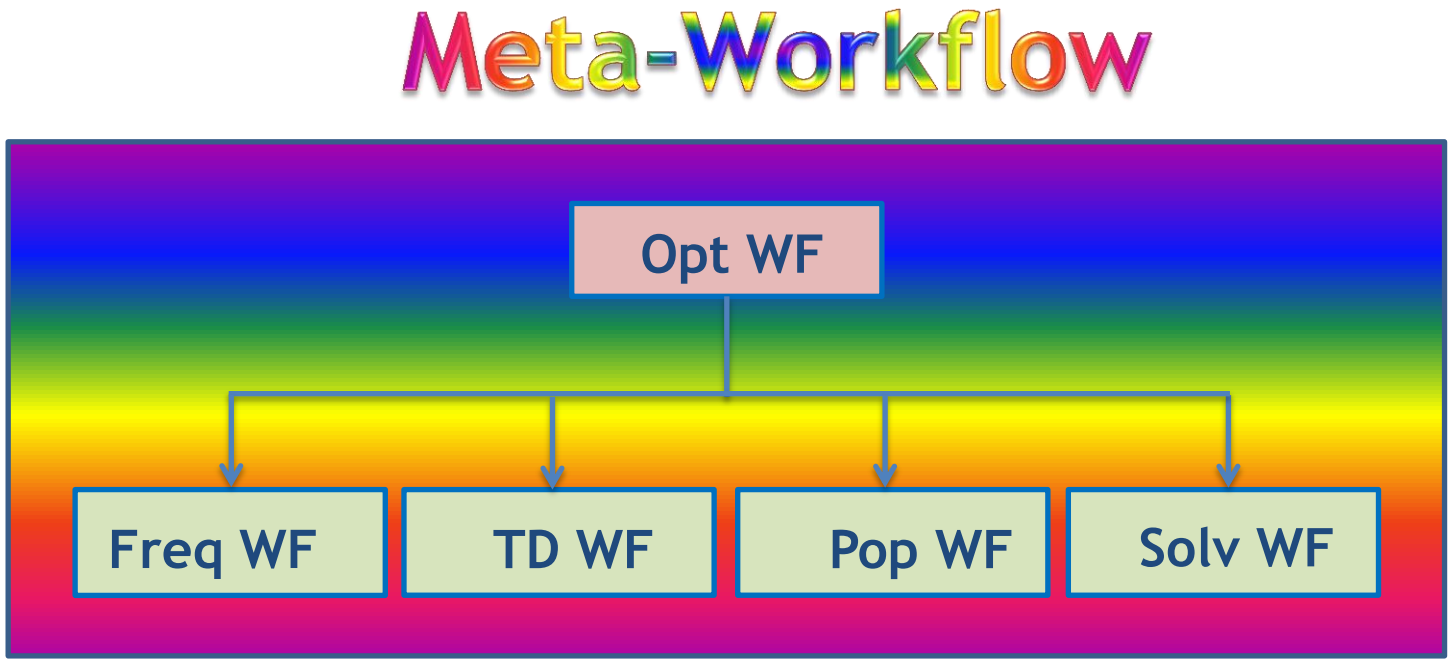
Example: Spectroscopic Analysis



Example: Spectroscopic Analysis



Example: Spectroscopic Analysis



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!

Acknowledgement

Köln, RRZK

- Lars Packschies
- Martin Kruse

Bundesministerium für Bildung und Forschung

Tübingen, Bioinformatics

- Oliver Kohlbacher
- Jens Krüger

Berlin, Zuse Institut

- Thomas Steinke
- Patrick Schäfer

Dresden, ZIH

- Ralf Müller-Pfefferkorn
- Richard Grunzke

MTA SZTAKI, Computer and Automation Research Institute, Budapest

Centre for Parallel Computing, University of Westminster, London