UNICORE-based Workflows for the Simulation of Organic Light-Emitting Diodes

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Outline

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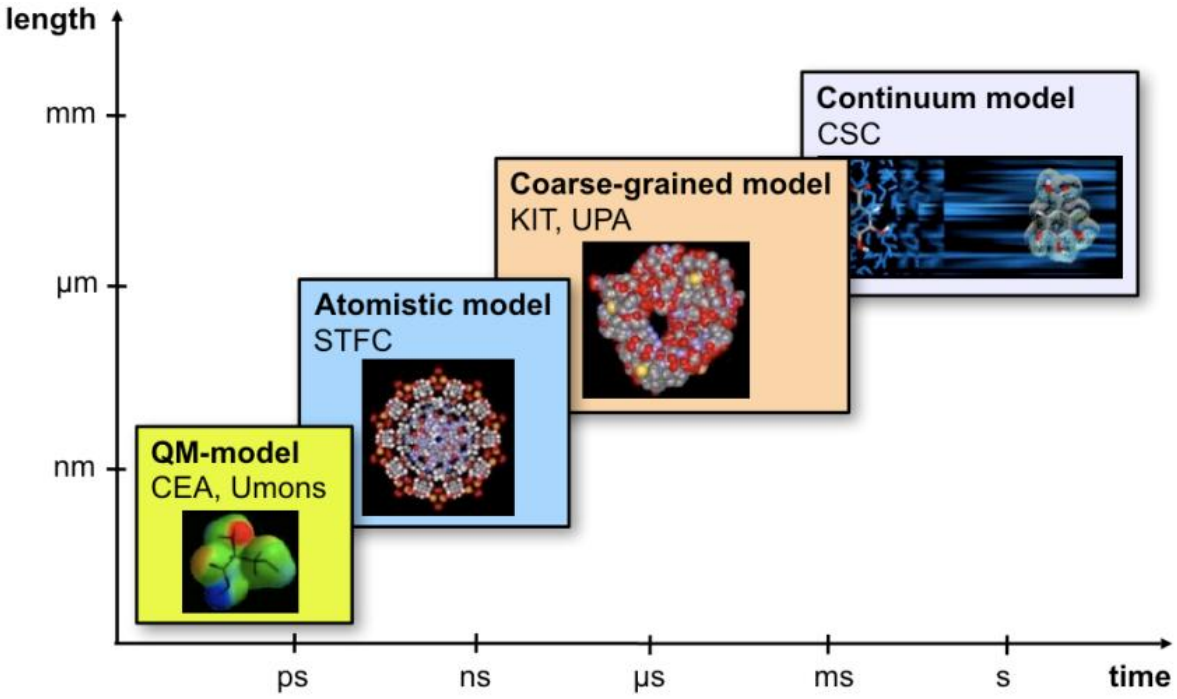
- The Challenges
- Integration concept: UNICORE
- GridBean and UNICORE Workflow
- Simulation of Organic Light Emitting Diodes (OLEDs)
- Data Exchange
- OpenMolGRID
- OLED Workflow
- Sharing the Workflow
- Conclusions and outlook

MMM@HPC project overview

www.multiscale-modelling.eu

- **HPC centres**: CINECA, CSC, KIT and KIST (Korea)
- **Modelling and code developing groups**: University Mons, CEA, CSC, STFC, University Patras, KIT
- **Industrial partners and users**: CEA, SONY, KIT, project MINOTOR
- **Cooperating projects**: PRACE, MINOTOR, D-Grid and NGI-DE

The challenges



- Integration on different size and time scales to address real-life problems in nano-materials science
- Develop an easy to use solution for non-experts: industrial and experimental groups

Reusability

Data complexity

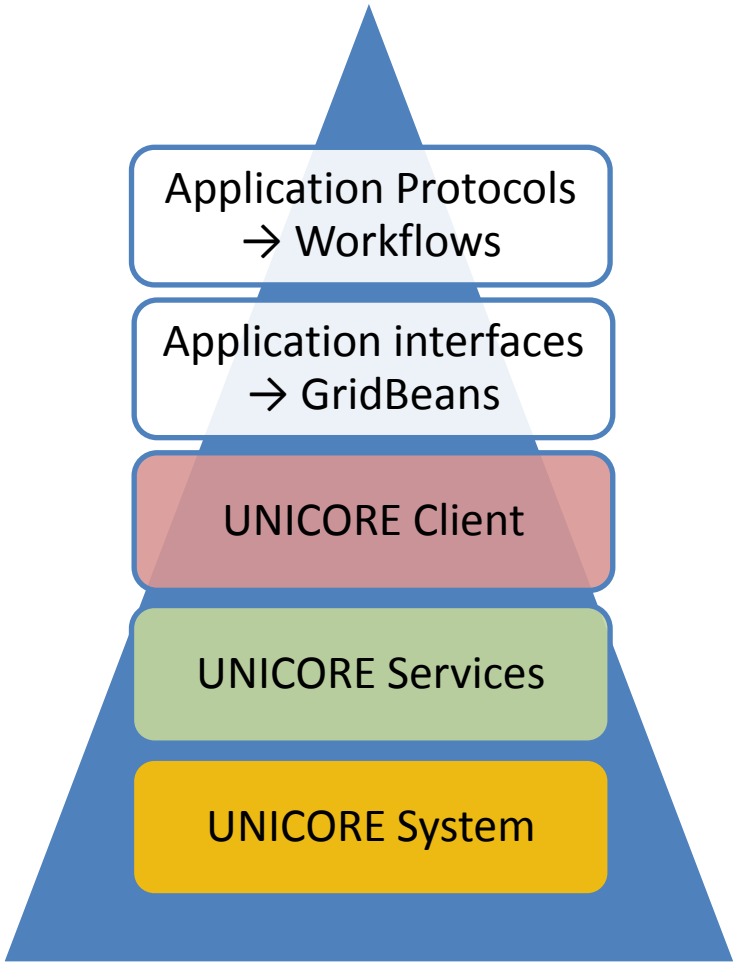
Solution for licensing issues

Security & Reliability

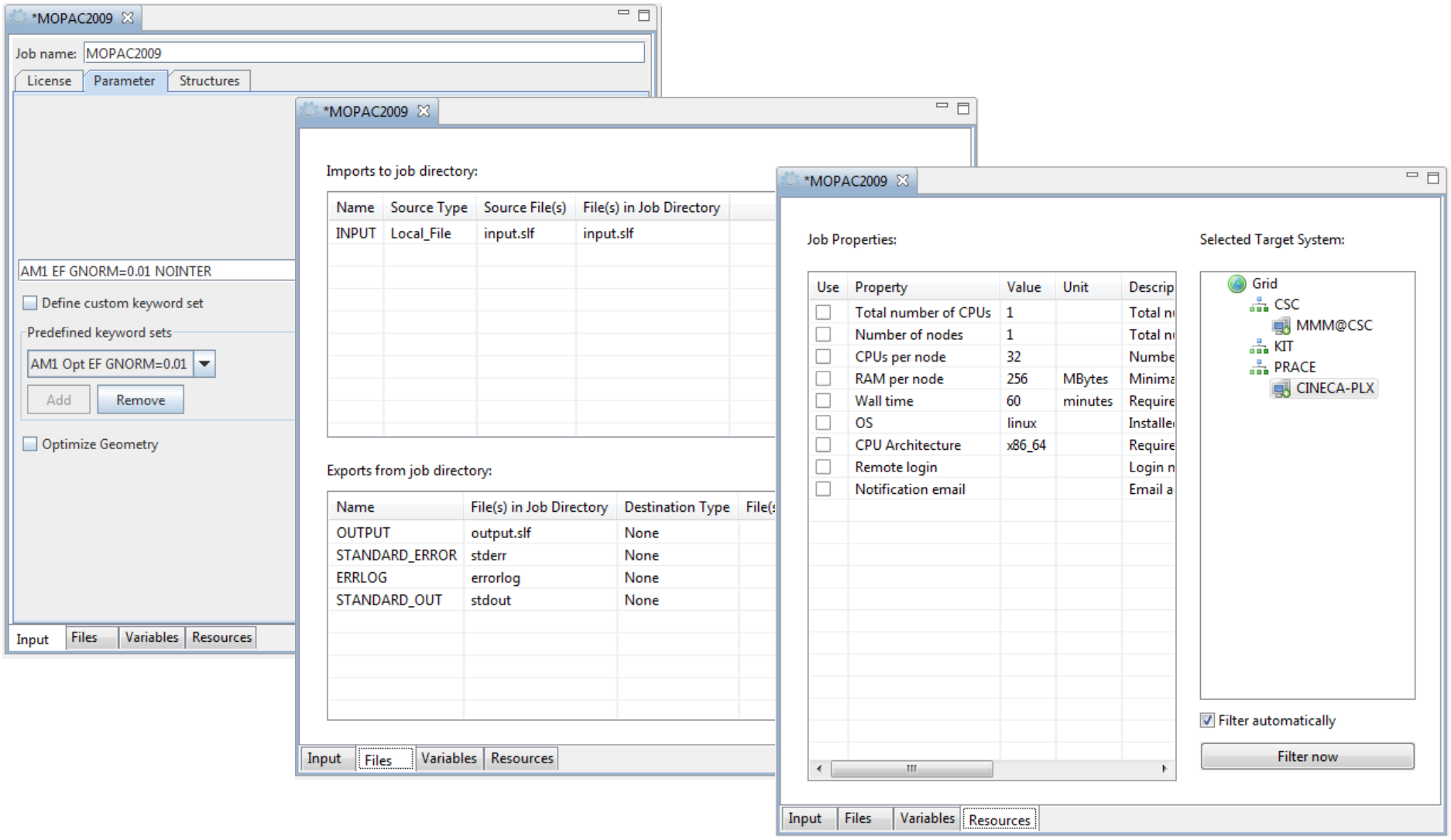
Capacity & Capability

Integration Concept: UNICORE

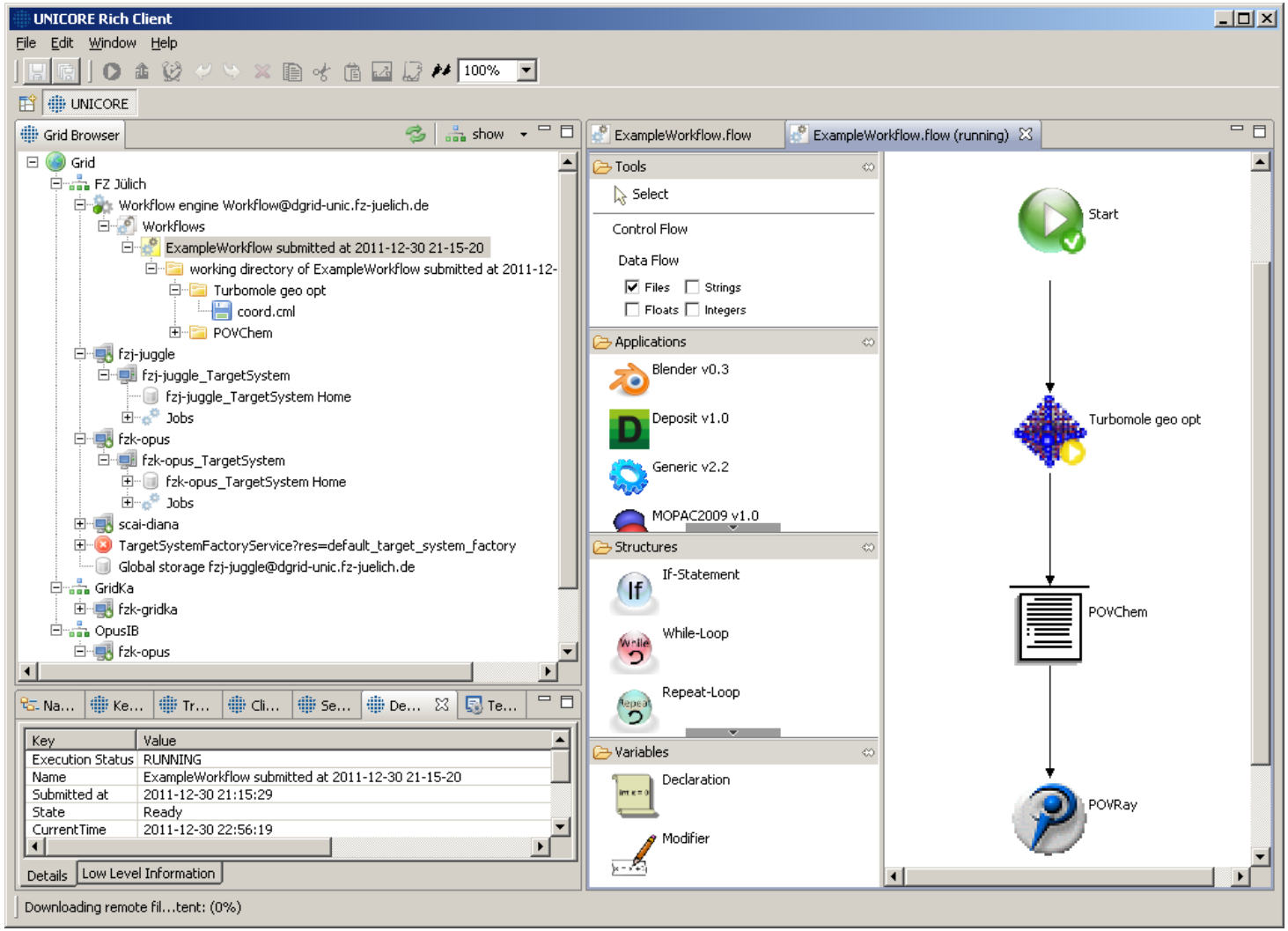
- Provision of simulation tools and services that can be combined in many different application workflows
- Adaptable, reusable and extendable interfaces & workflows based on UNICORE
- Access to distributed HPC/HTC resources via UNICORE services



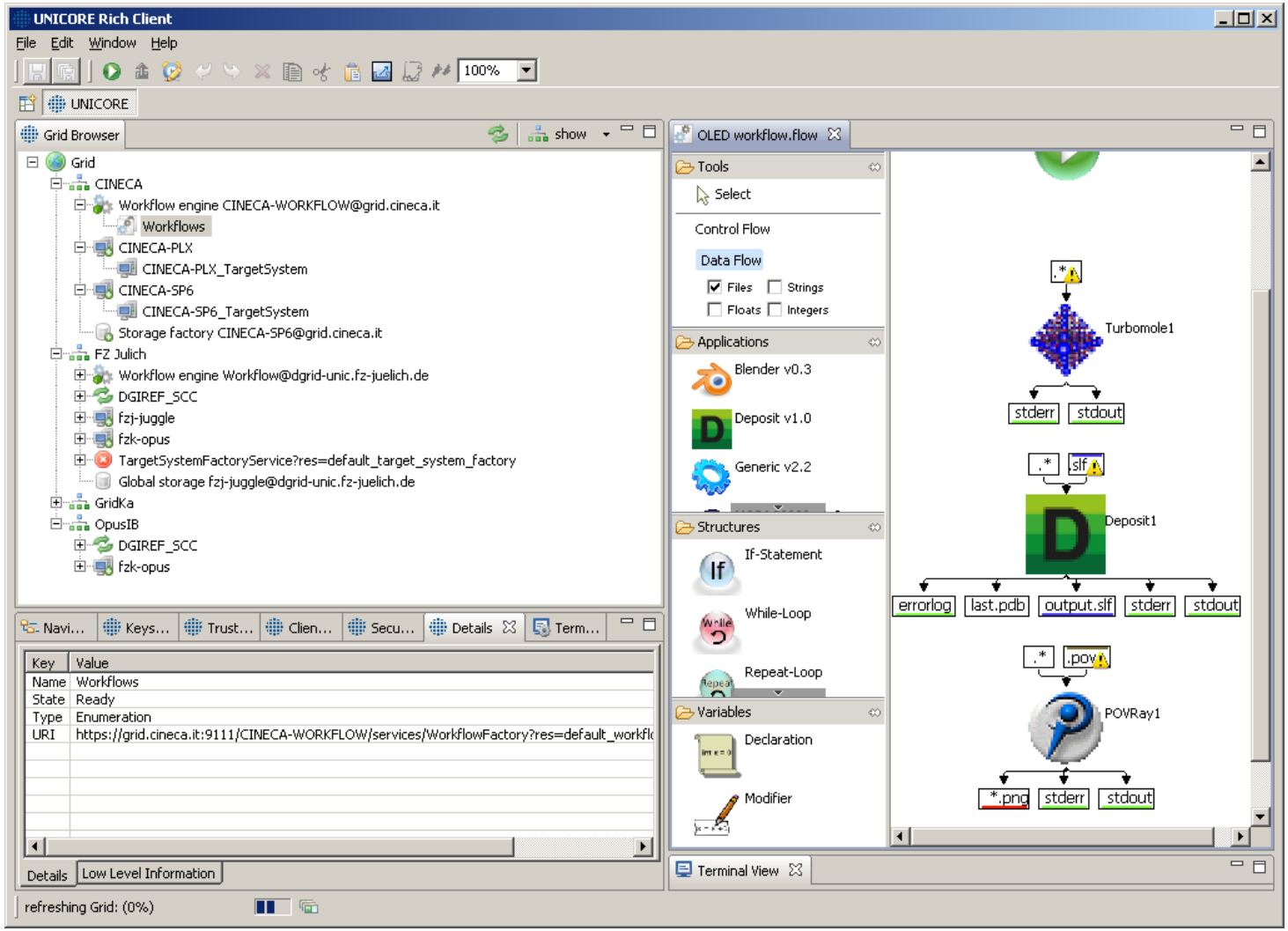
MOPAC GridBean



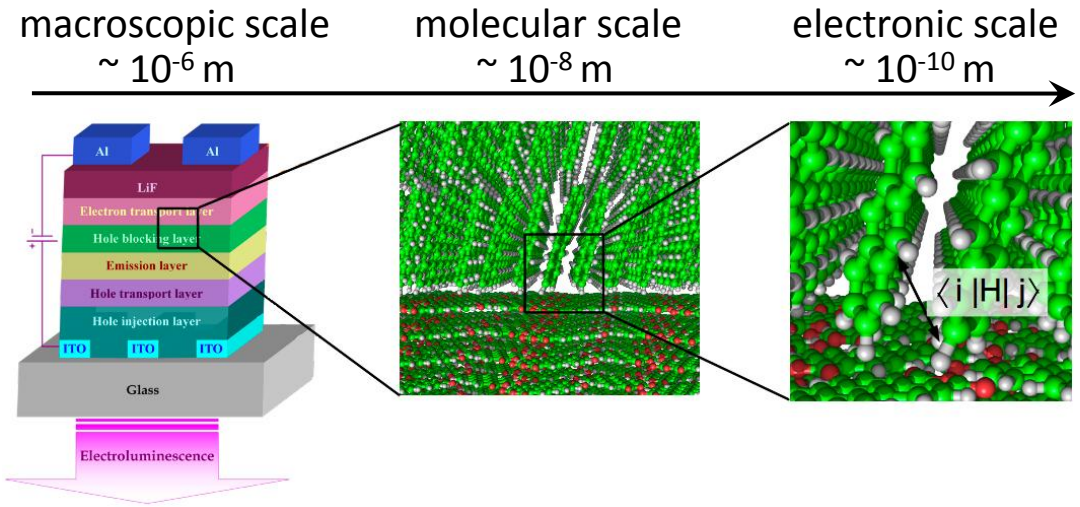
Application flow: Example



Data flow: Example

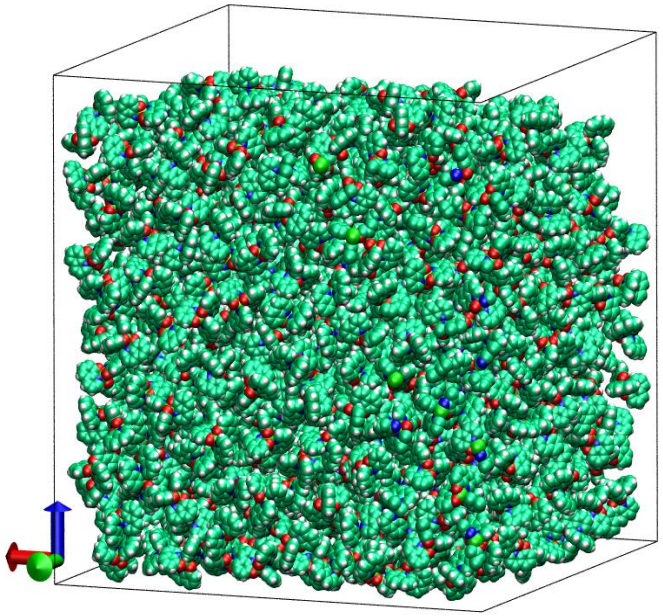


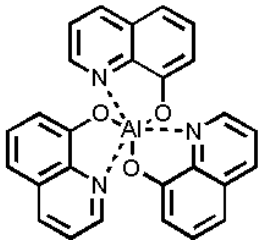
OLED: architecture and modelling tools



continuum model (FEA)	coarse-grained model (CG)	Atomistic model (MM)	QM model (QM)
Elmer	ToFeT (KMC)	DEPOSIT	MOPAC
FEAP	End-bridging MC	LAMMPS	TURBOMOLE
	Transporter	DL_POLY	BigDFT

OLED: simulation protocol for charge transport in Alq3 disordered films

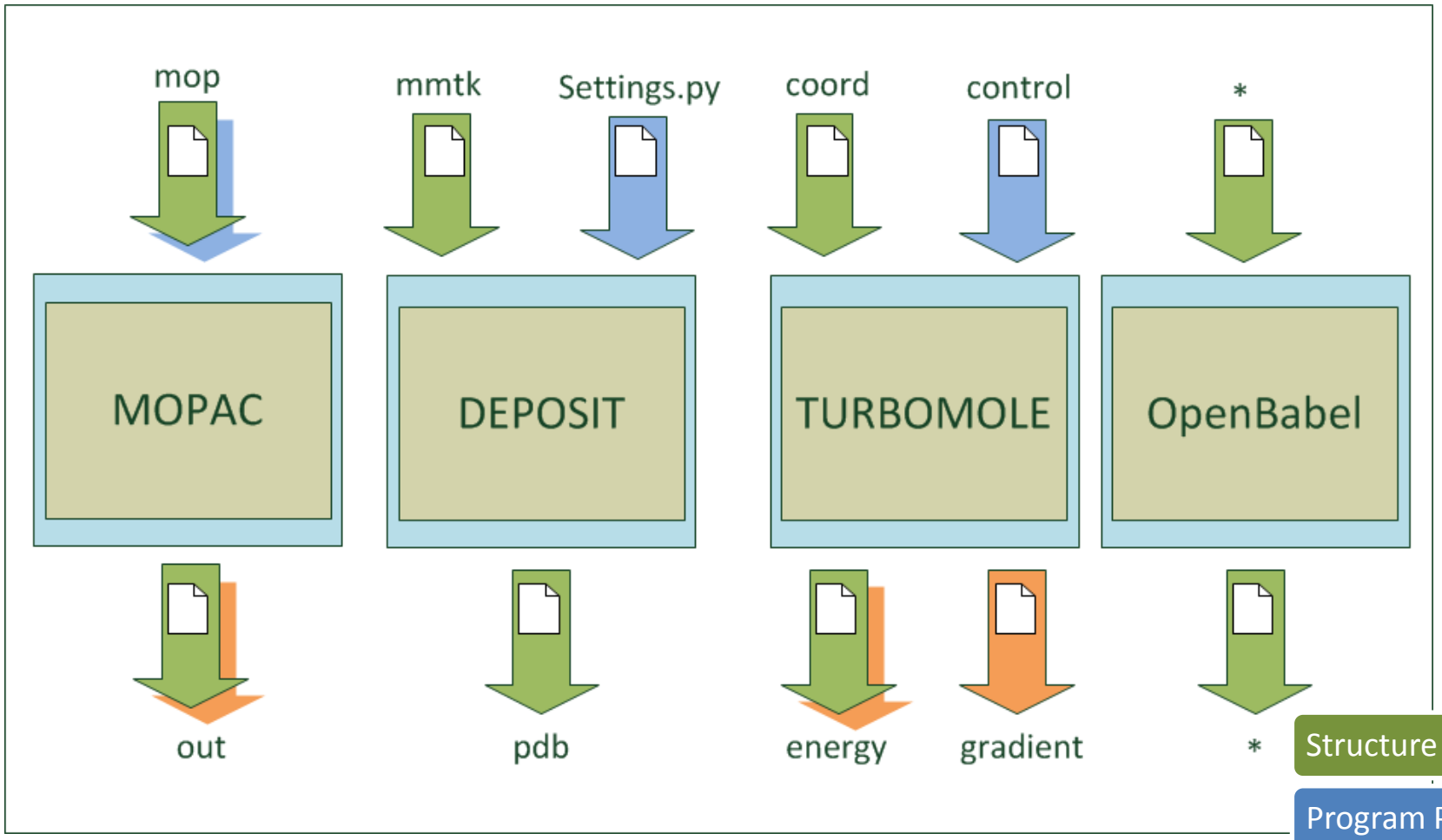




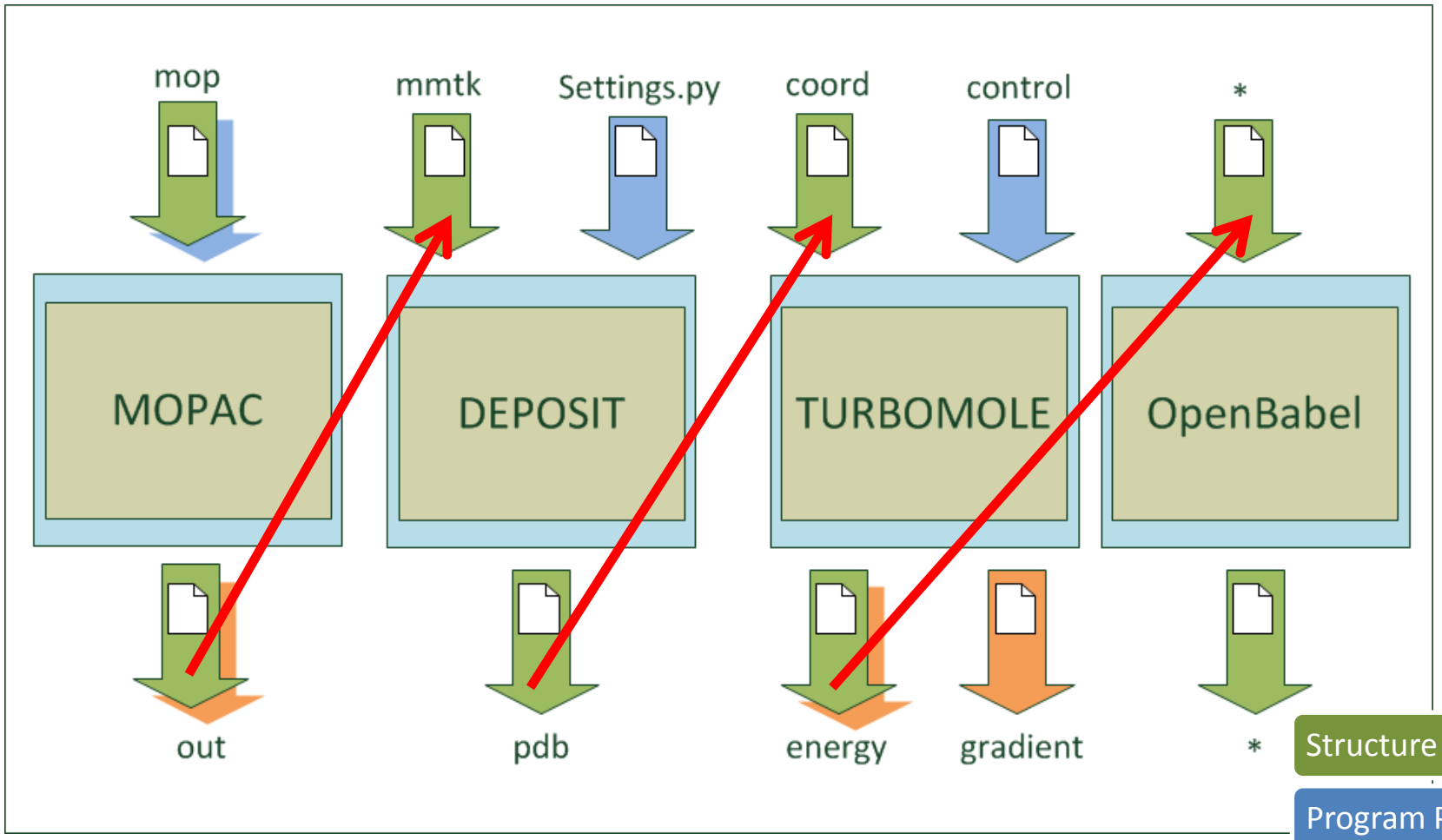
J. J. Kwiatkowski, J. Nelson, H. Li, J. L. Bredas, W. Wenzel, and C. Lennartz, Phys. Chem. Chem. Phys., 2008, 10, 1852–1858.

- Film deposition (or MD)
  - Generate disordered film morphologies
- QM calculations of hopping sites
  - Calculate HOMO, LUMO, LUMO+1 etc energies.
  - Electronic couplings reorganization energies
  - Calculate charge hopping rates
- Kinetic Monte Carlo (KMC)
  - Calculate charge (electron-hole) mobility
  - Calculate current density

Application Input/Output files



Application Input/Output files



How to concatenate these applications?

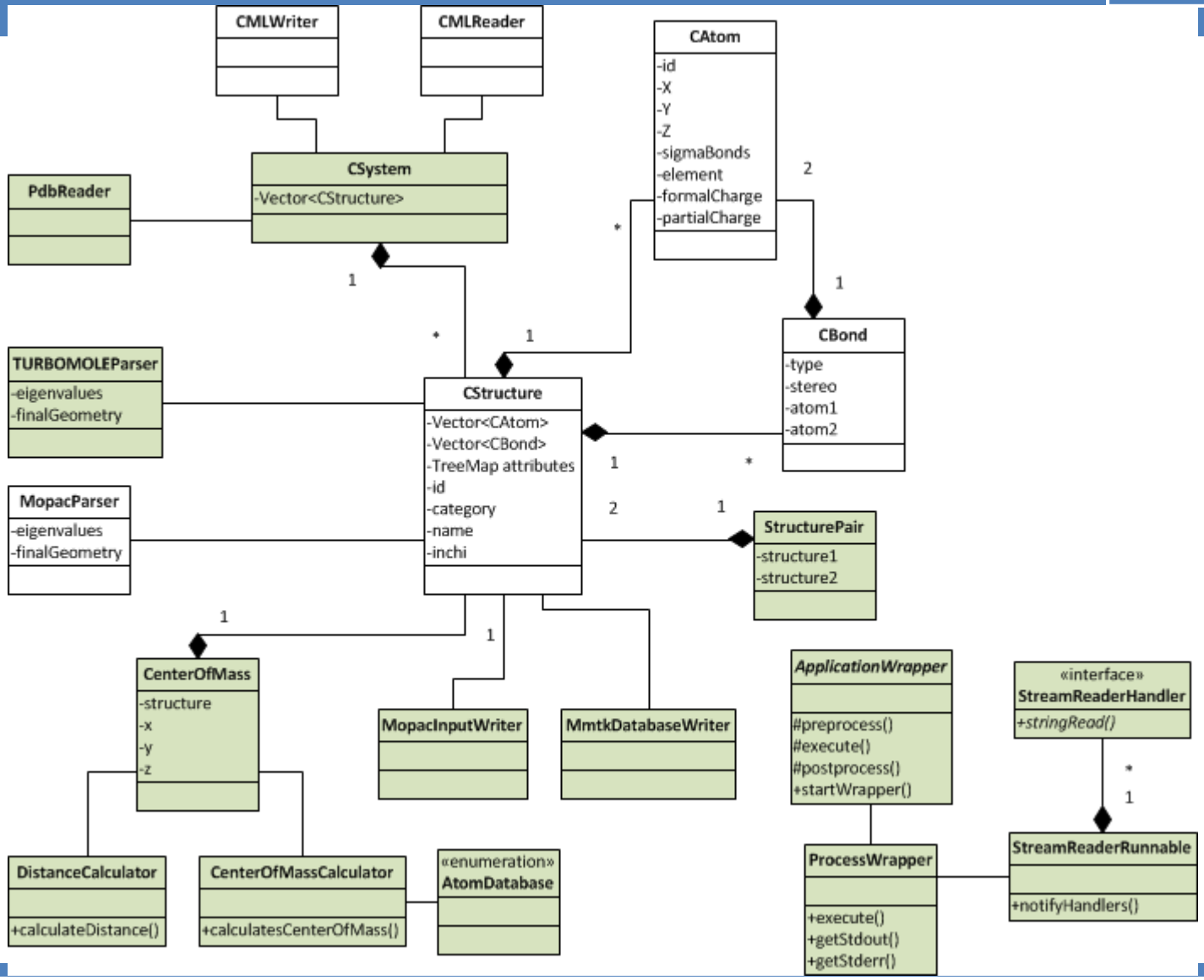
Data exchange between applications

- Structure Data exchange format: Chemical Markup Language (CML)
  - is the *de facto* XML for chemistry
  - Extendable with additional domain specific attributes (charges, temperature, density) in CML dictionaries
- Data flow management with the OpenMolGRID library

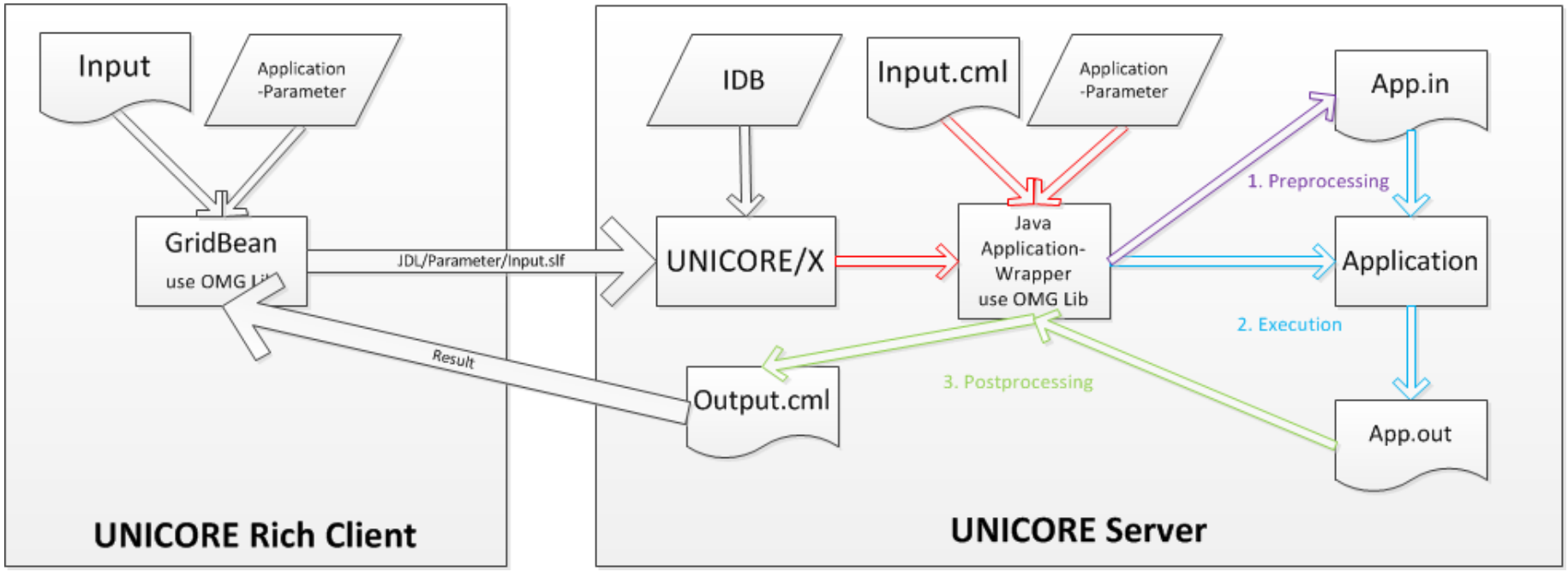
S. Sild et al., LNCS 3470, 464, Springer (2005); S. Sild et al., J. Chem. Inf. Model., 46, 953 (2006).

  - Read, write and convert chemical file format
  - Provides a data model for molecular information
  - Application Wrapper API
- Open Babel
  - Read, write and convert chemical file format

OpenMolGRID



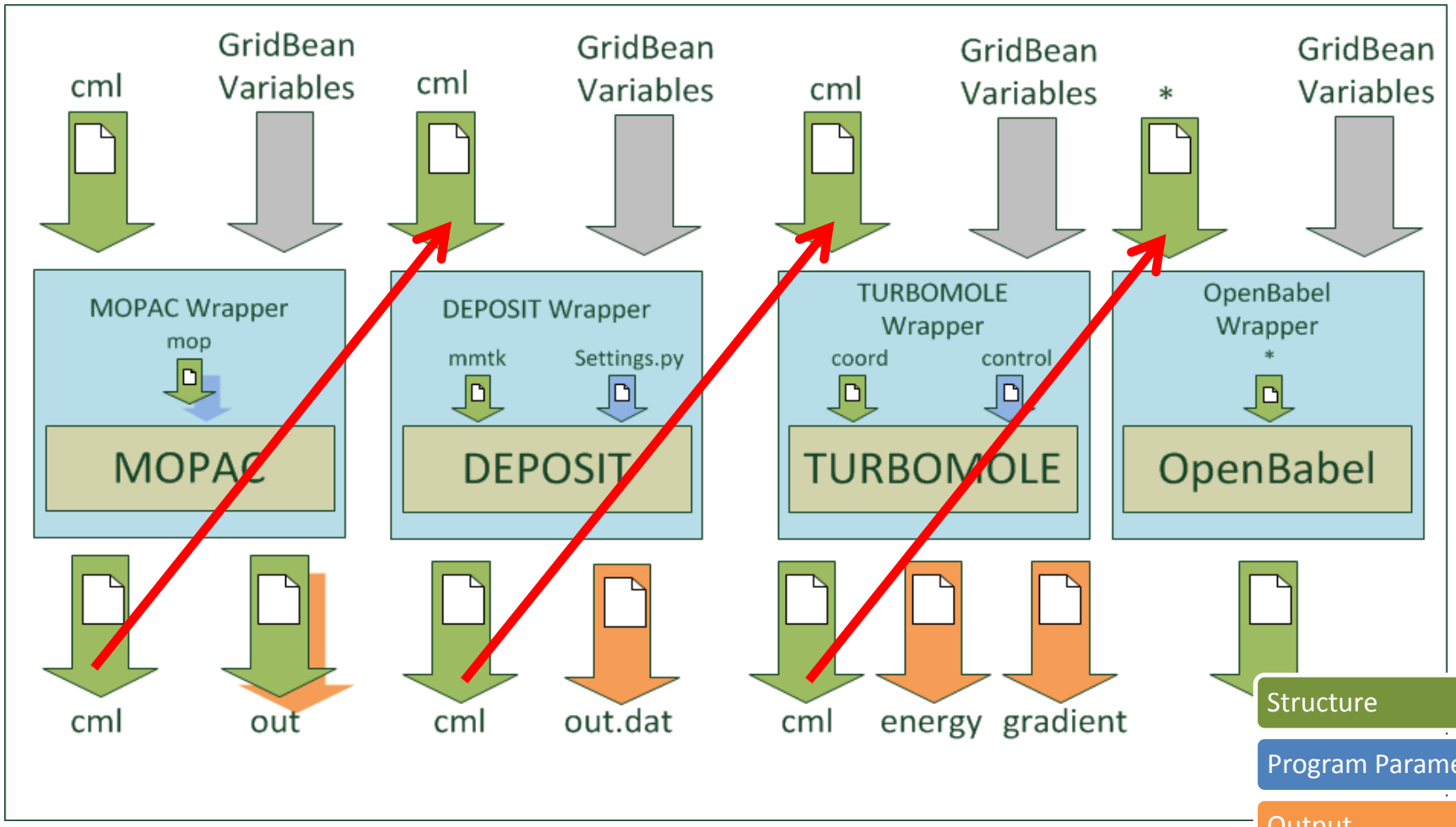
Application Wrapper: OpenMolGRID



Application Wrapper Lifecycle

1. Preprocessing: Validation of App. Parameter, Generation of App. specific Input Files
2. Execution: Run App(s) in seperate Process(es), Monitoring of stdout/stderr (allows interaction with the application)
3. Postprocessing: Error Handling, Parsing App Output, Creation of Workflow Data

Application Wrapper Input/Output files



With CML and Application Wrapper!

OLED Workflow

Simulation protocol

QM: Geometry Optimization

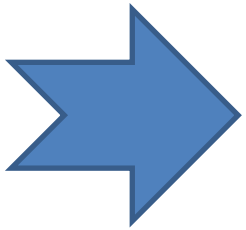
MM: Film depostion

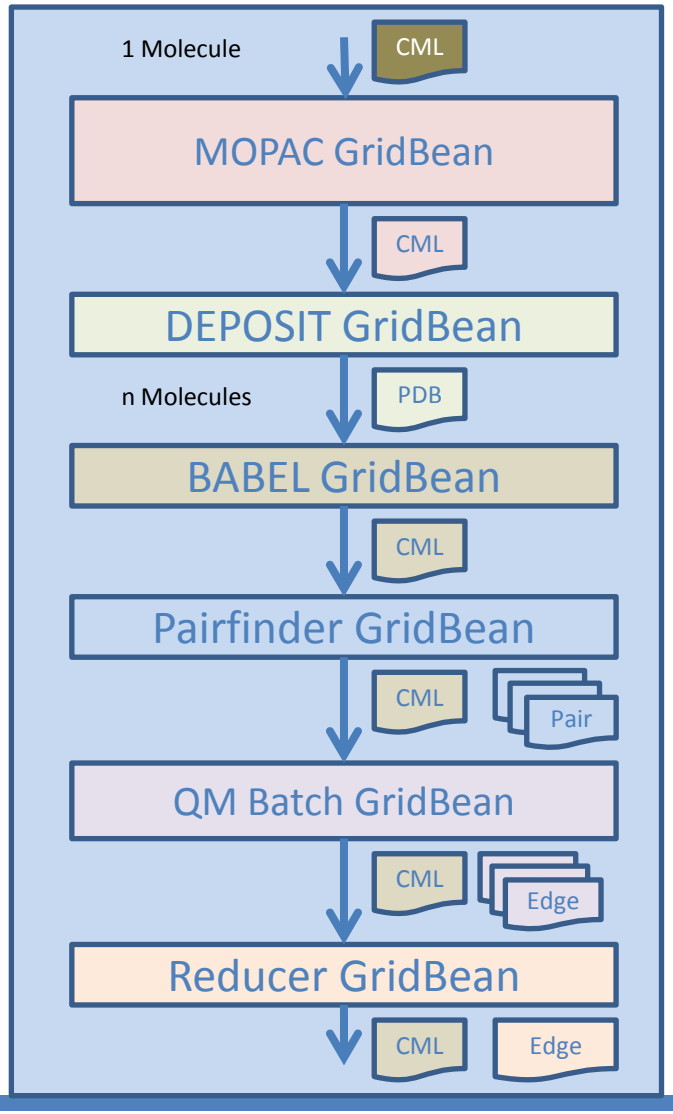
MM: Determination of Site pairs

QM: Calculation of Hopping Sites

CG: Compute Charge mobility

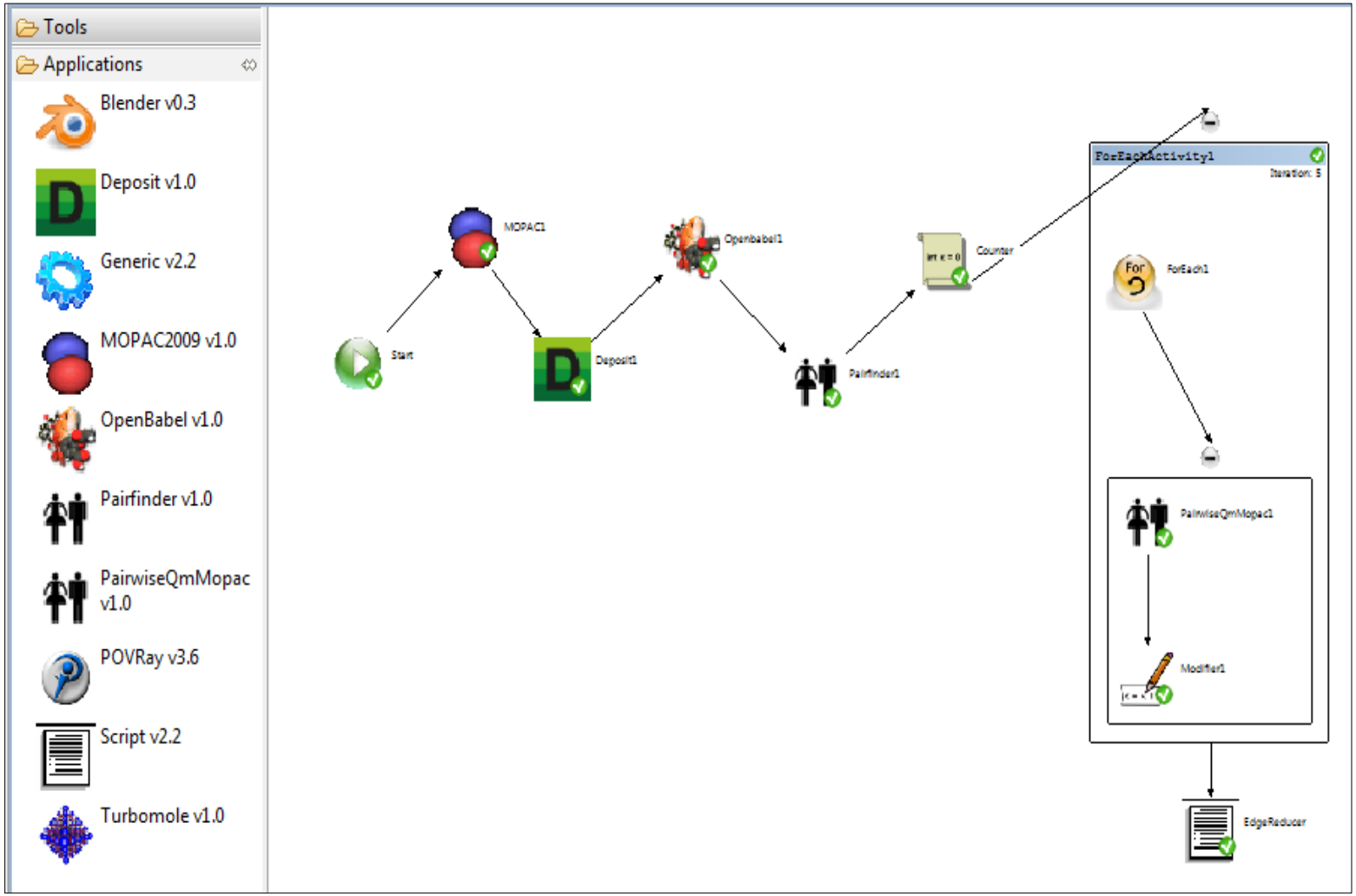
FEA: Calculate Current Density





UNICORE Workflow

UNICORE Workflow



Calculation of Hopping Sites

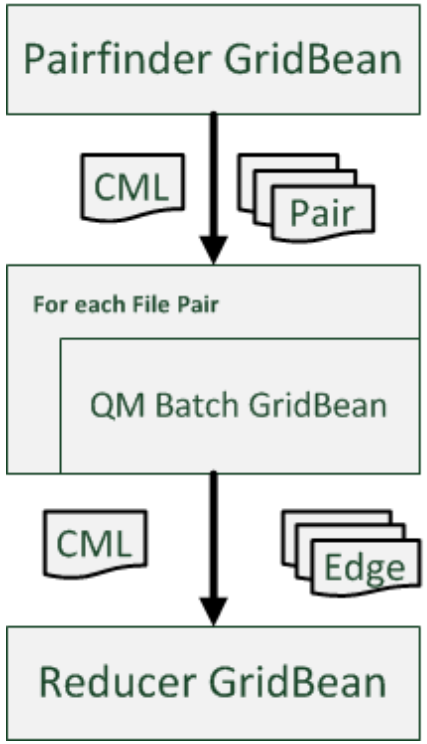
A deposition film has **1.000 – 1.000.000** Hopping Site candidates (Molecule Pairs)
Each Hopping Site needs 3 QM calculations (2 Monomers and 1 Dimer)

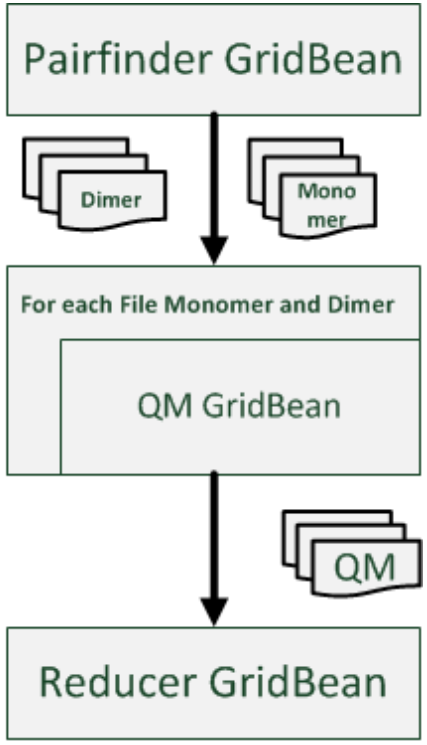
QM-Batch Jobs

- Short QM calculations (~ 0.5 - 5 min)
- Each Pair file: includes n Molecule Pairs
- Each Job: n * 3 QM calculations
- Less Jobs: Minimize service overhead
- Each QM Code needs additional GridBeans & Wrapper

QM-Single Jobs

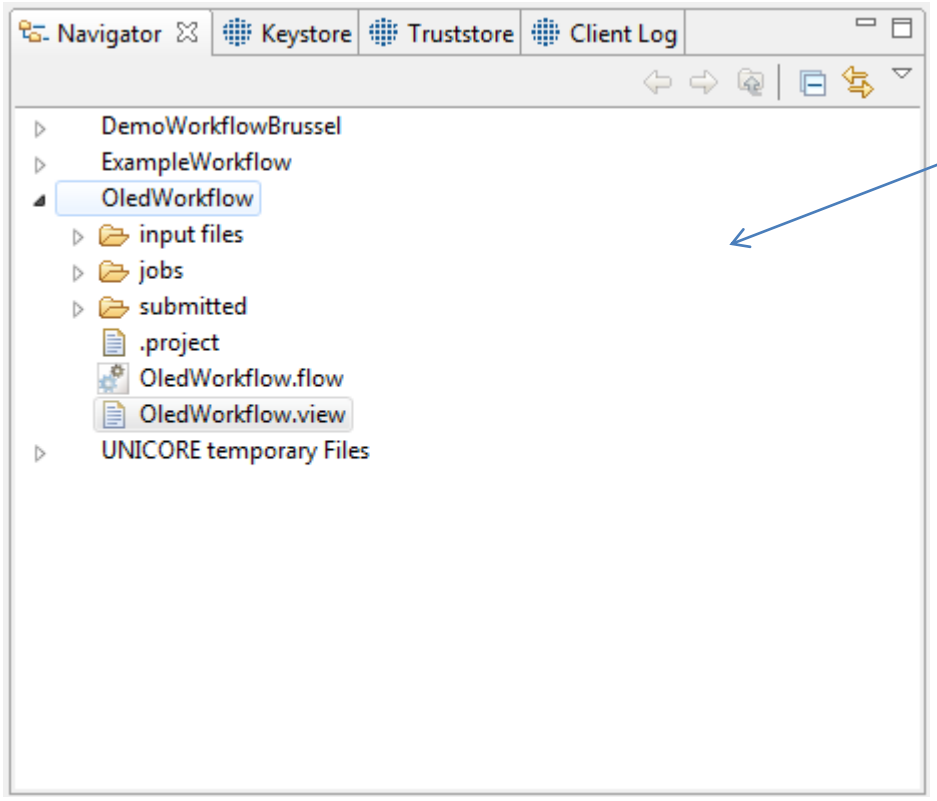
- Long QM calculation (30 min +)
- Each Job: one QM calculation
- Many Jobs & Files
- Reuse of QM GridBeans
- Each QM Code needs a special Reducer

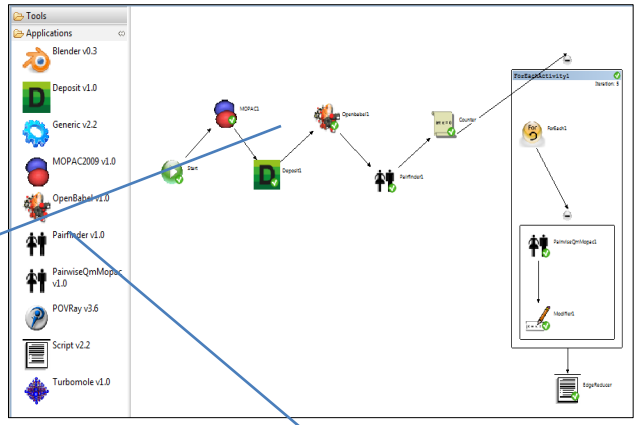




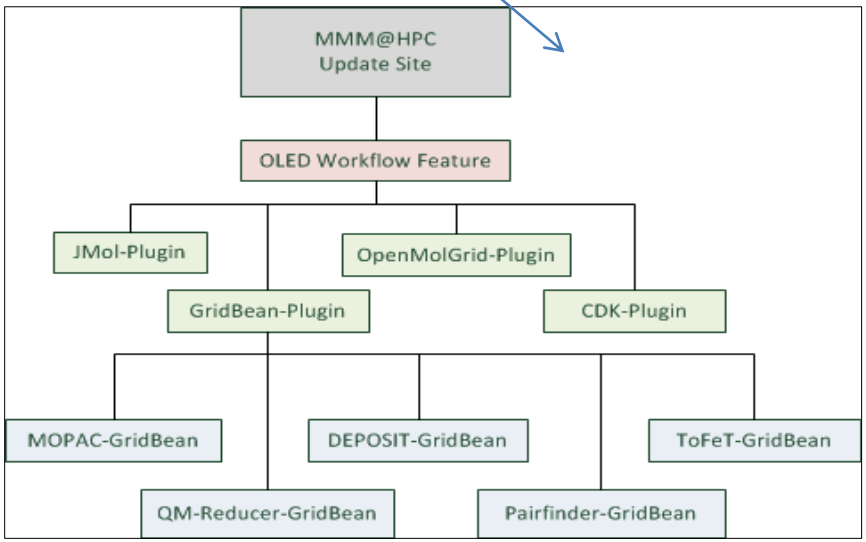
Sharing the Workflow

1) Workflow Project





2. GridBeans in MMM@HPC Update Site



Conclusions and Outlook

- With UNICORE we provide an optimal low-effort/low-cost solution for multiscale modelling
- GridBeans → App Interfaces
- Workflows → Simulation protocol
- Data Exchange in WFs between applications handled with CML, Open Babel and OpenMolGRID
- Different approaches on the calculation of Hopping Sites

Current work

- Integration of the CG and FEA steps into the OLED Workflow
- Elmer, DL_POLY and BigDFT GridBeans
- Simulation of whole OLED devices
- Workflows for Molecular Electronics, Carbon Molecular Devices and Li-Ion Batteries

Acknowledgments

- All consortium partners in MMM@HPC
- Funding from the EC

- Partner projects, supporting infrastructures and software