Workflows for the Simulation of Organic Light-Emitting Diodes

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CAPACITIES

e-infrastructure

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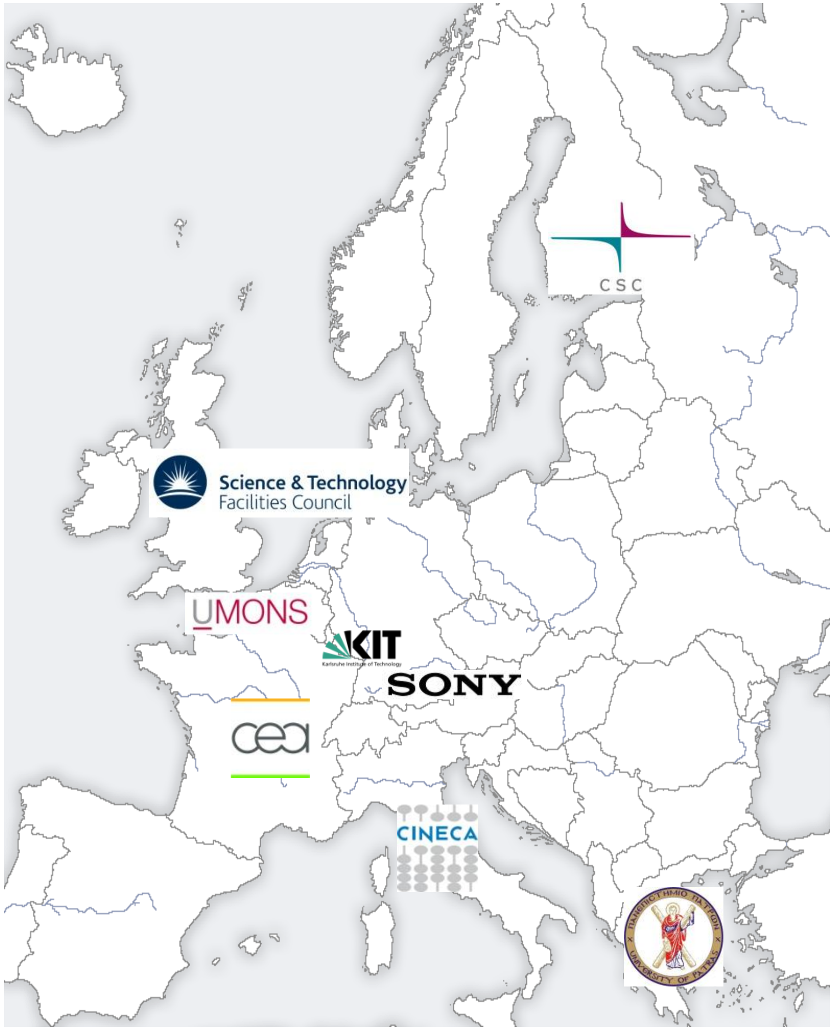
Outline

- Project MMM@HPC overview
- The Challenges
- Approach based on UNICORE middleware
  - GridBeans
  - Workflows
  - Application and data flow
- OpenMolGRID
- Simulation of Organic Light Emitting Diodes (OLEDs)
- OLED workflow architecture
- Conclusions and outlook

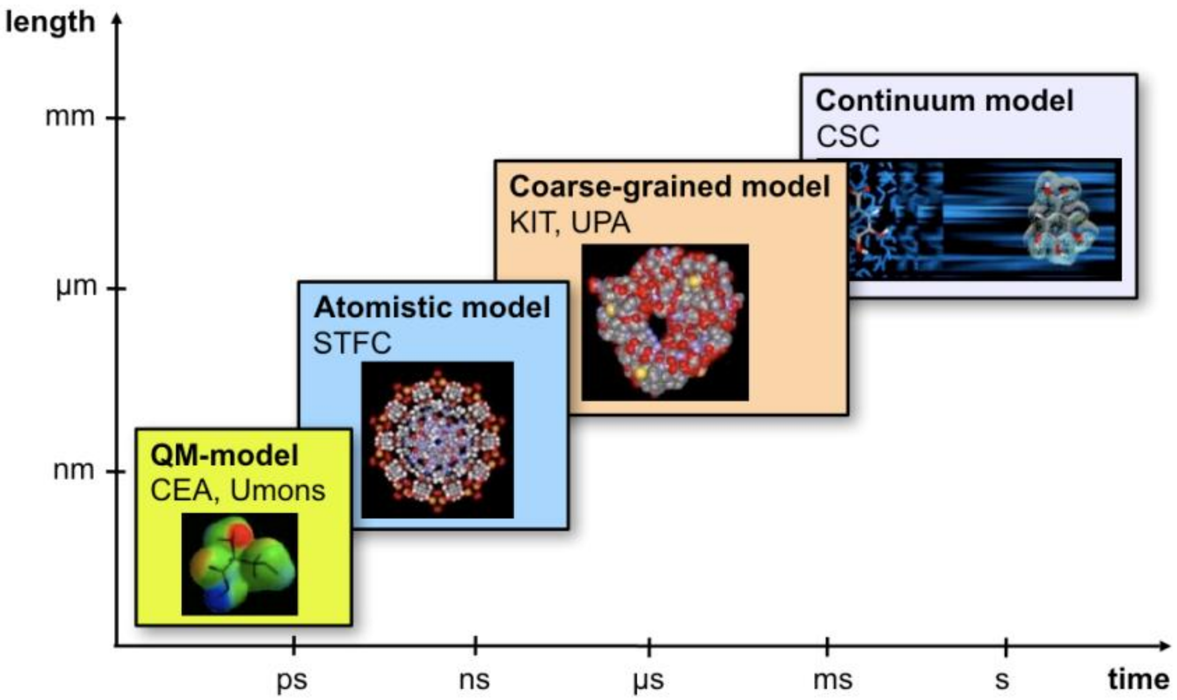
MMM@HPC project overview



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

Can we meet these challenges?

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Challenge	Solution
Reusability	• GridBeans • UNICORE Workflows
Data complexity	• Chemical Mark-up Language (CML) • OpenMolGRID
Solution for licensing issues	• UNICORE: UVOS/SAML/VOMS • Open Source Licenses
Security & Reliability	• UNICORE • Grid Security Infrastructure (GSI)
Capacity & Capability	• High Performance Computing (PRACE) • Distributed resources (D-Grid, EGI)

YES!

What is UNICORE?

- UNICORE: UNiform Interface to COmputing Resources
- Grid computing technology (grid middleware) supported by EMI
- Seamless, secure, and intuitive access to distributed grid resources
- Used in daily production at several supercomputer centres worldwide
- Open source under BSD license
- Implements standards from the Open Grid Forum (OGF)

A. Streit et al., UNICORE 6 - Recent and Future Advancements
Annals of Telecommunications 65 (11-12), 757-762 (2010) .

UNICORE three-layer architecture

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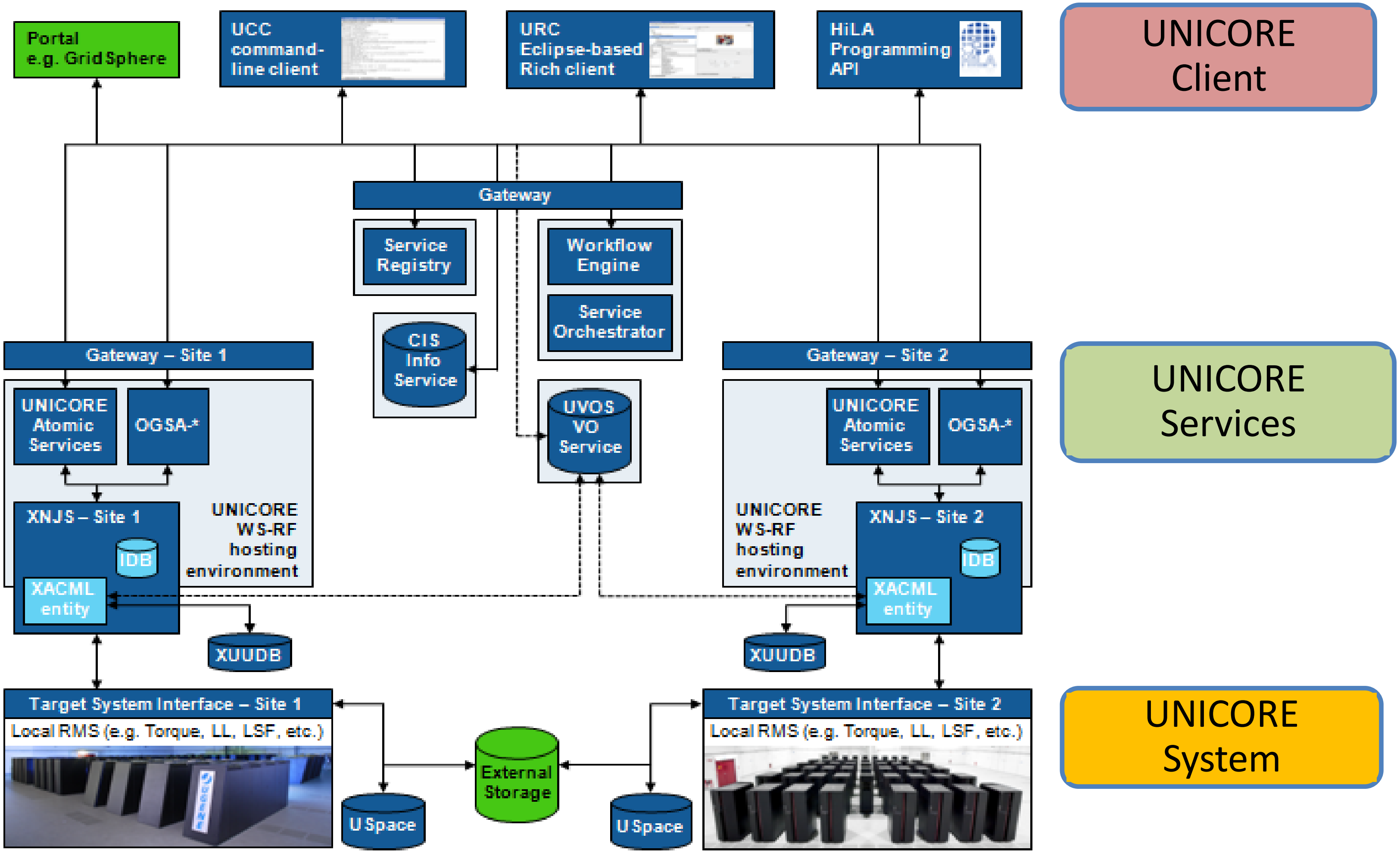
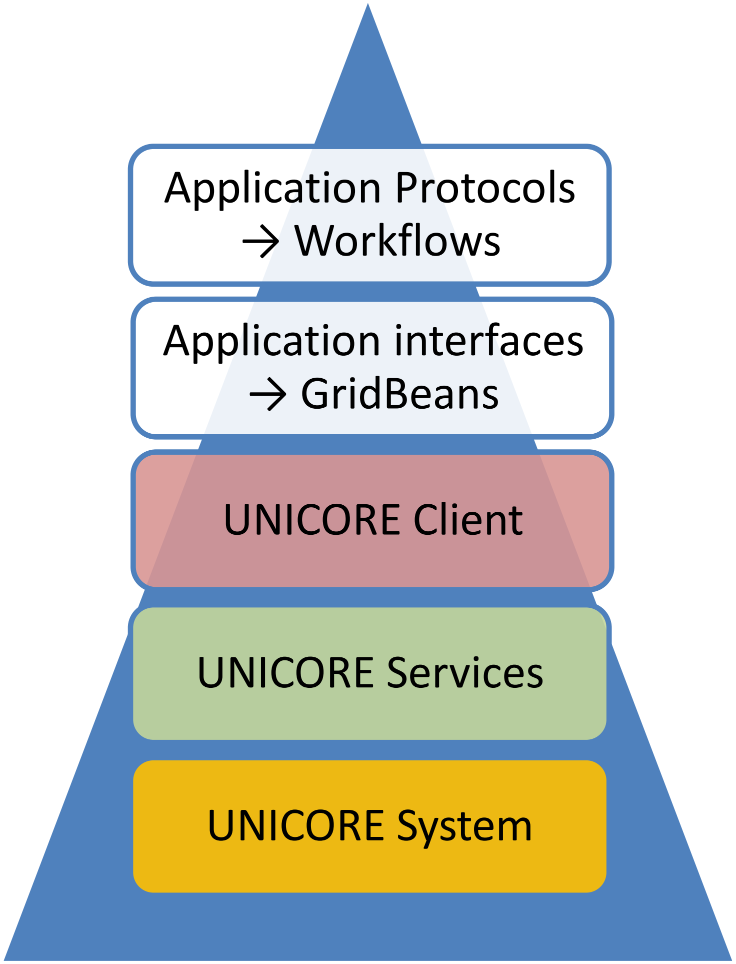


http://www.unicore.eu/unicore/architecture.php

Integration Concept: UNICORE

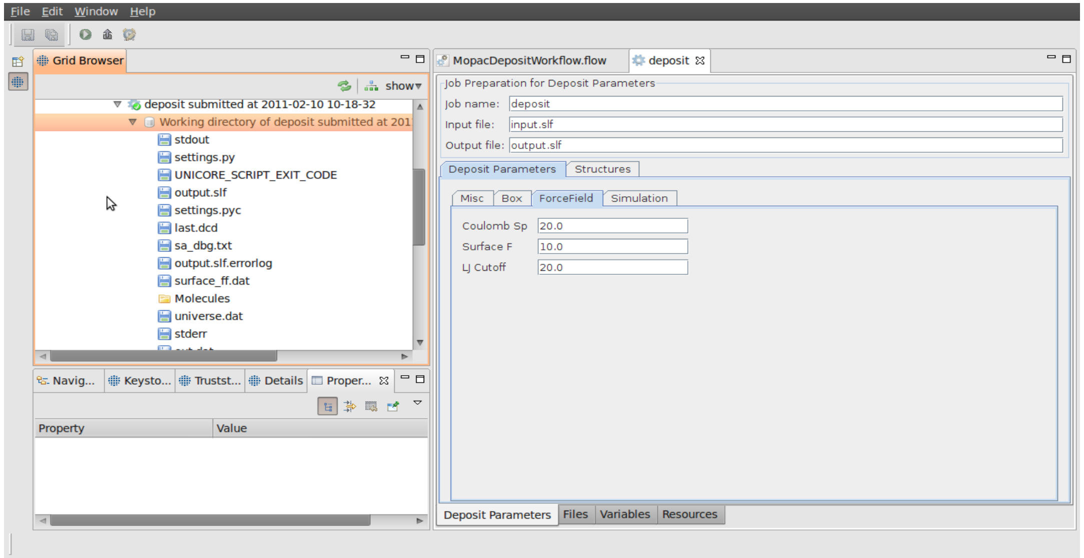
- Provision of simulation tools and services that can be combined in many different application workflows
- Adaptable, reusable and extendable interfaces & workflows based on UNICORE
- Access to distributed HPC/HTC resources via UNICORE services



Application interfaces: GridBeans

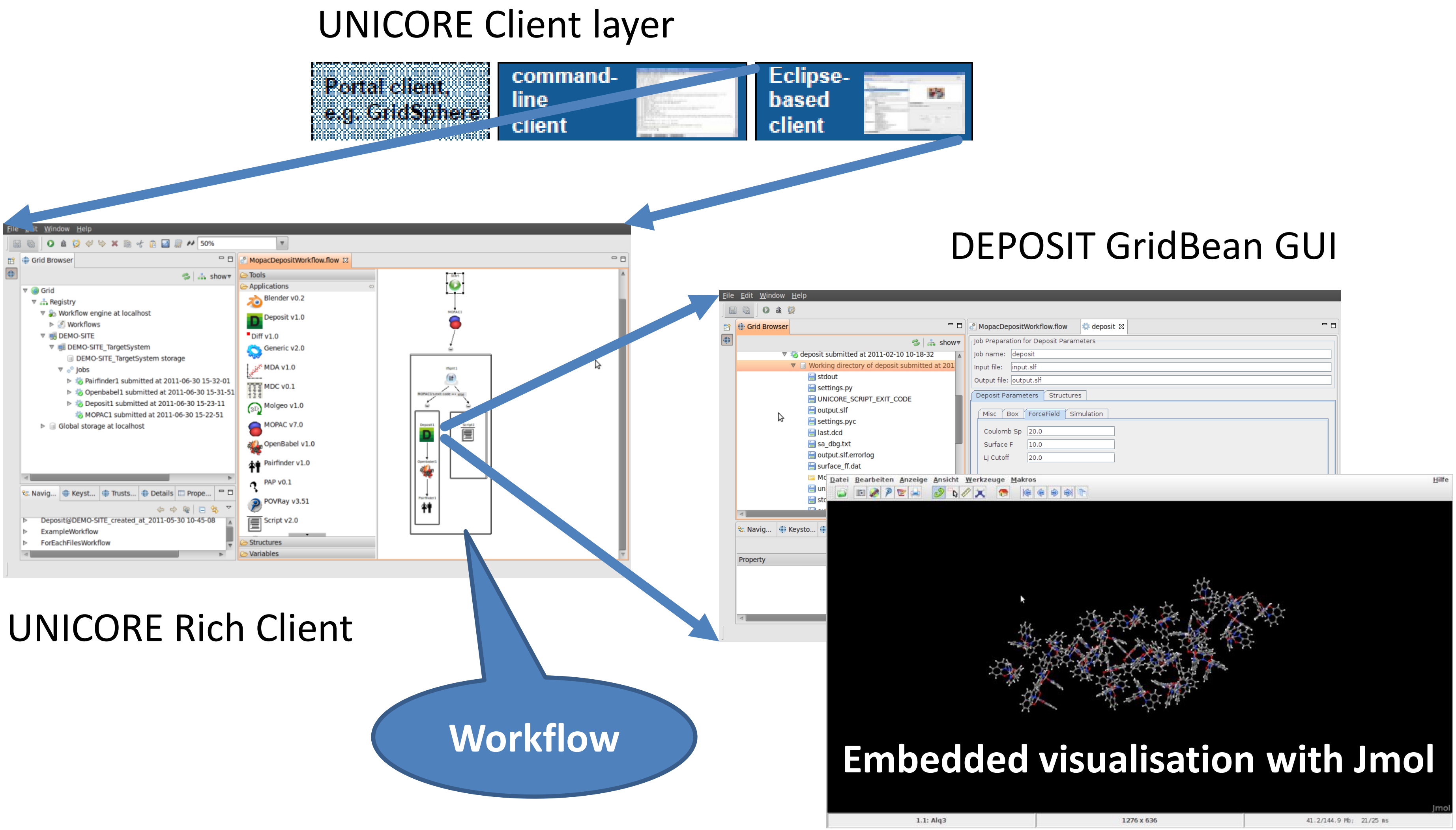
- Provides a way to use scientific application on HPC resources (even by non experts)
- Designed to decouple scientific applications from the underlying (changing) grid protocols (UNICORE, Globus, Portals)
- Different simulation workflows can re-use the same GridBean
- Different GridBeans can be employed for the same workflow step

R. Ratering et al., "GridBeans: Support e-Science and Grid Applications", Proceedings of the Second IEEE International Conference on e-Science and Grid Computing (e-Science'06), p. 45, IEEE 2006

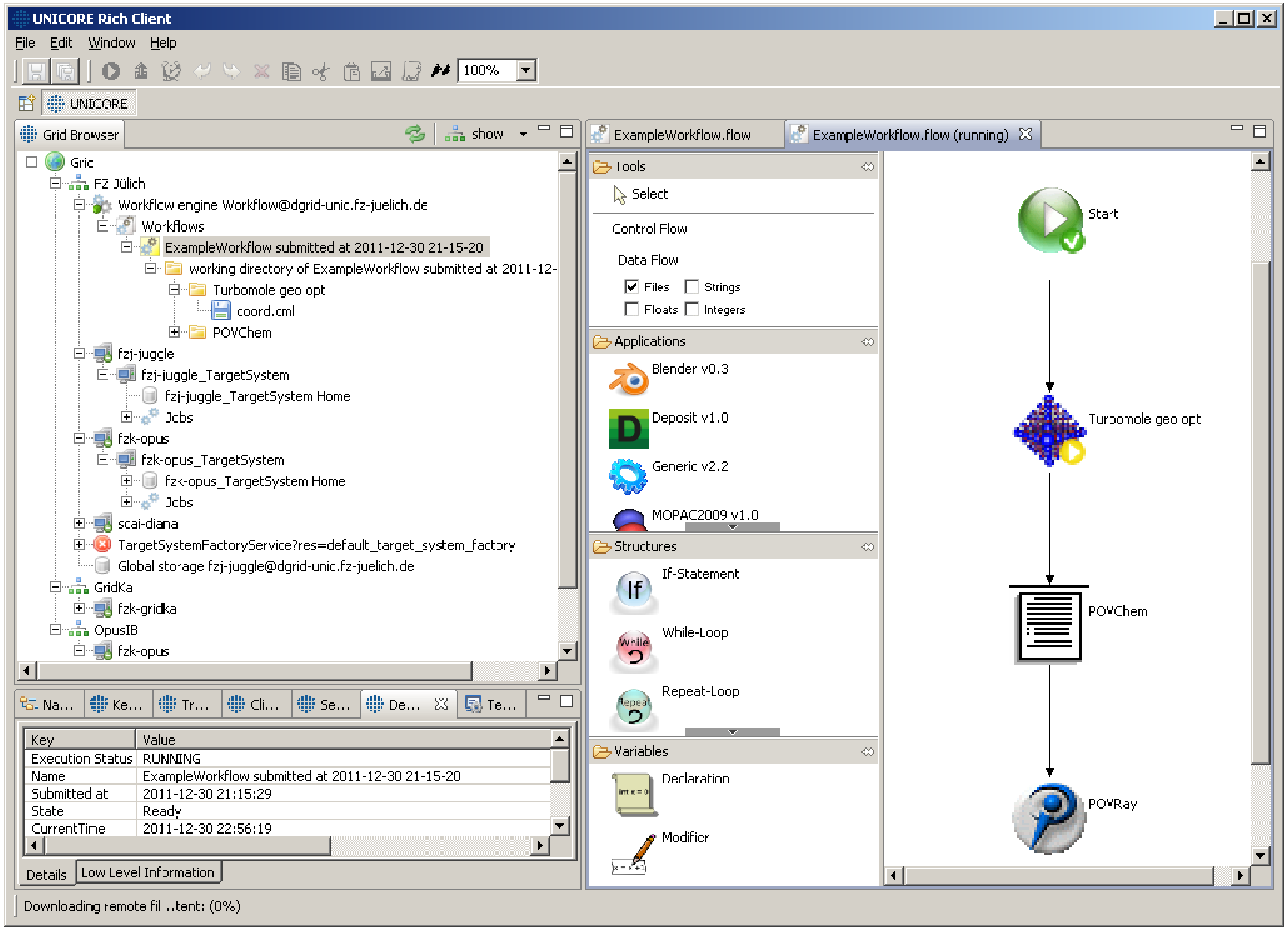


The GUI of DEPOSIT GridBean developed in MMM@HPC

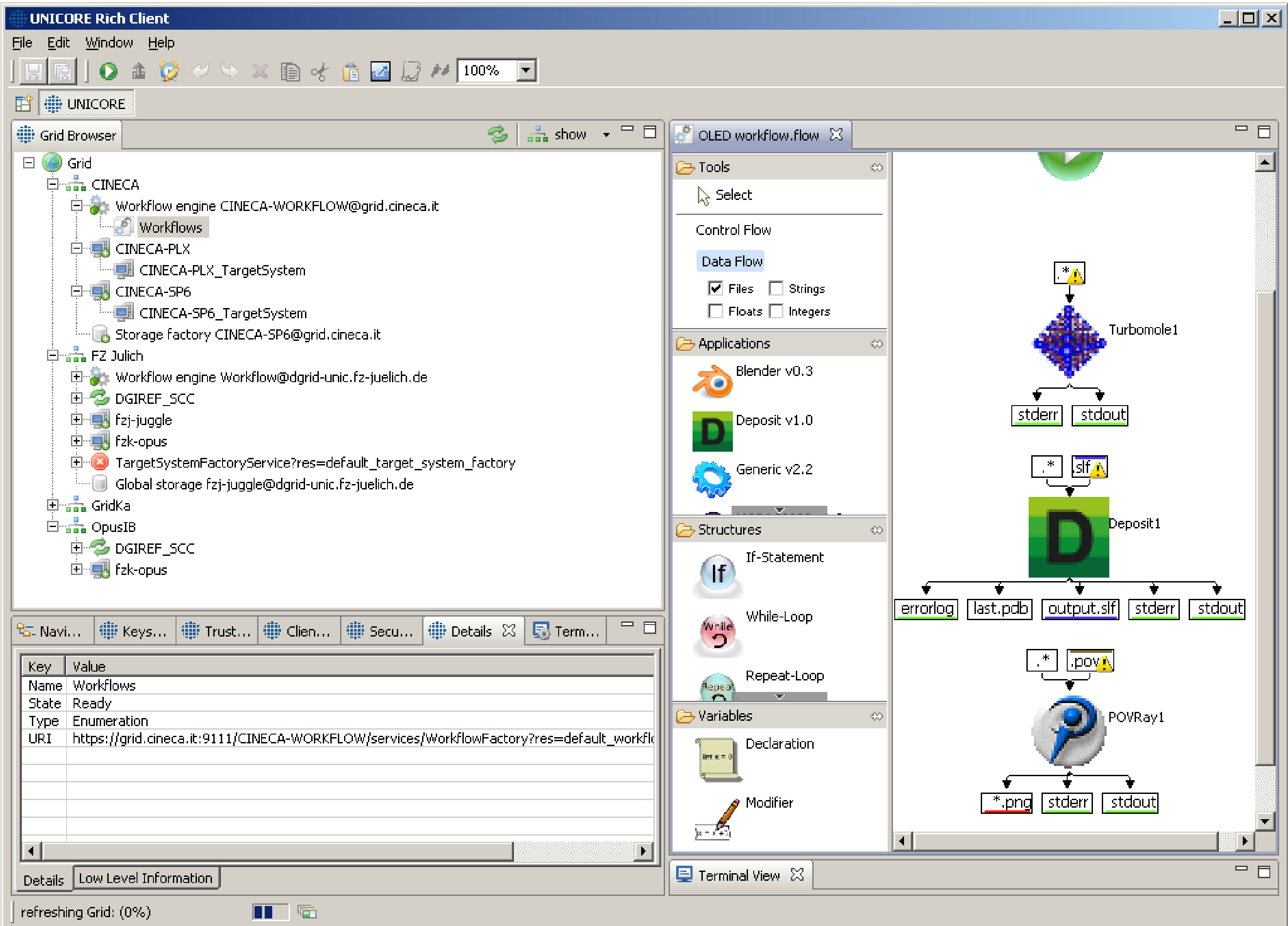
UNICORE Rich Client and Workflows



Application flow: Example



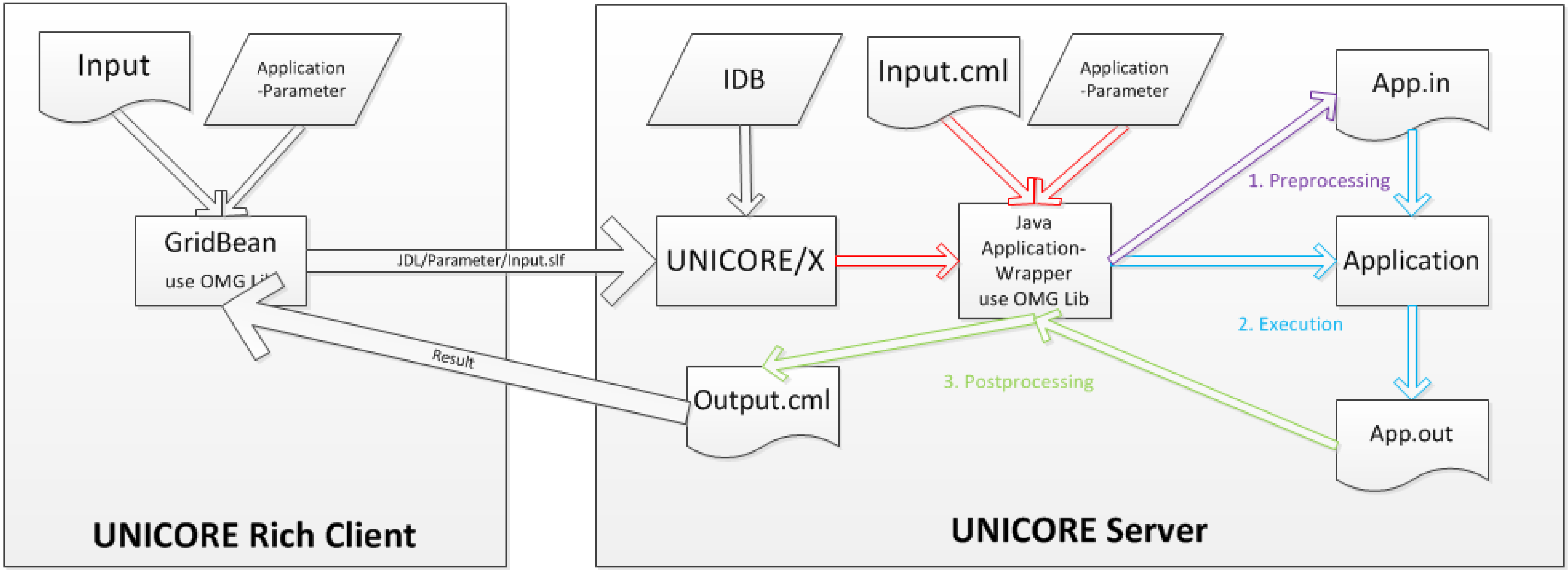
Data flow: Example



Data exchange and licensing issues

- Structure Data exchange format: Chemical Markup Language (CML)
- 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
- License management
  - OpenSource and Commercial applications in simulations
  - VOMS with UNICORE (UVOS and SAML) is being evaluated

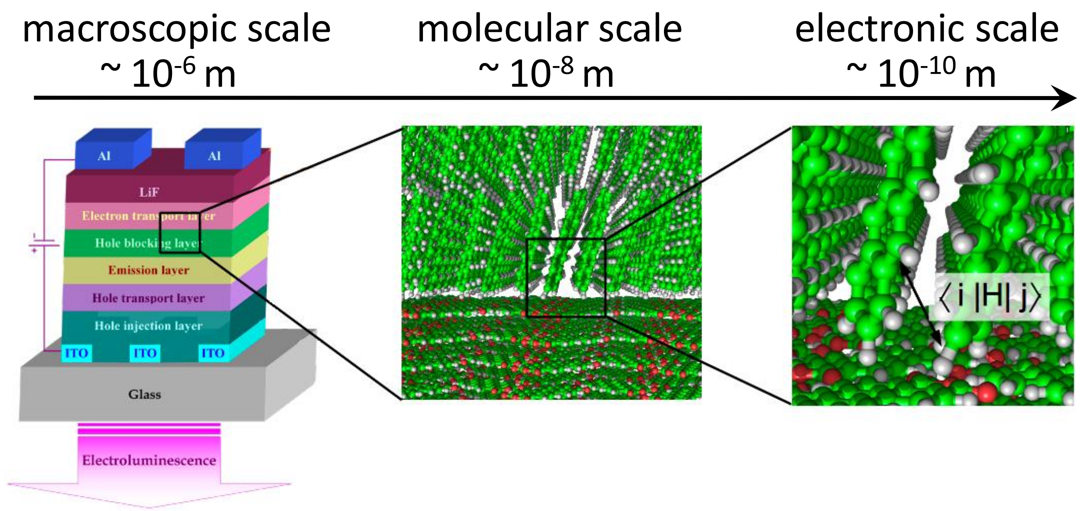
Application Wrapper: OpenMolGRID



Application Wrapper Lifecycle

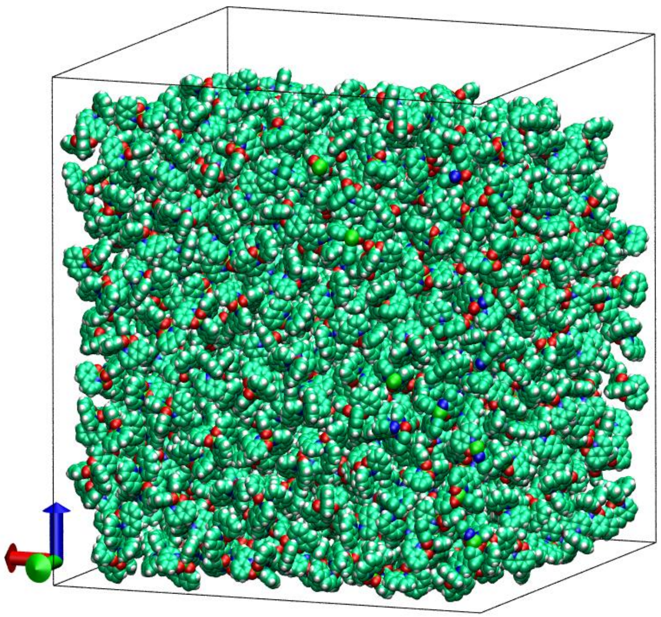
1. Preprocessing: Validation of App. Parameter, Generation of App. specific Input Files
2. Execution: Run App(s) in seperate Process(es), Monitoring of stdout/stderr (allows interaction with the application)
3. Postprocessing: Error Handling, Parsing App Output, Creation of Workflow Data

OLED: Simulation protocol



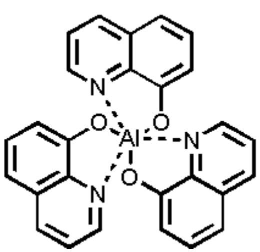
continuum model (FEA)	coarse-grained model (CG)	Atomistic model (MM)	QM model (QM)
Elmer	ToFeT (KMC)	DEPOSIT	MOPAC
FEAP	End-bridging MC	LAMMPS	TURBOMOLE
	Transporter	DL_POLY	BigDFT

OLED: charge transport in Alq3 disordered films



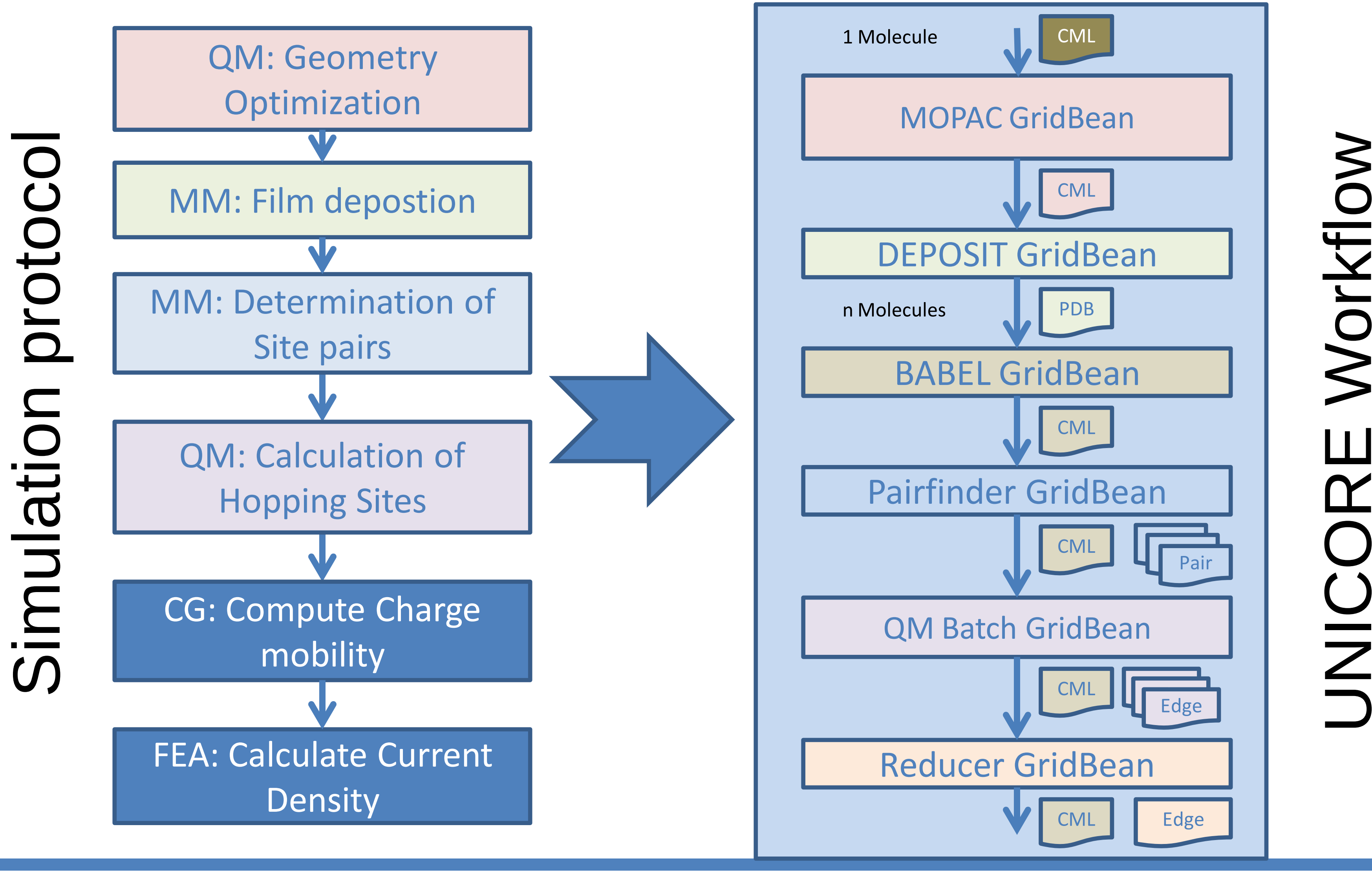
- Film deposition (or MD)
  - Generate disordered film morphologies
- QM calculations of hopping sites
  - Calculate HOMO, LUMO, LUMO+1 etc energies.
  - Electronic couplings reorganization energies
  - Calculate charge hopping rates
- Kinetic Monte Carlo (KMC)
  - Calculate charge (electron-hole) mobility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

Workflow



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

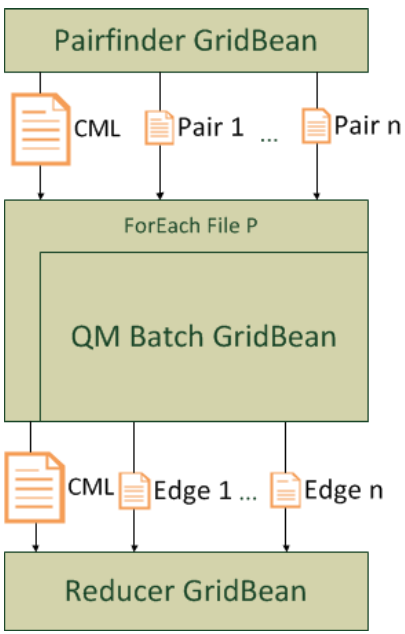
OLED workflow: architecture



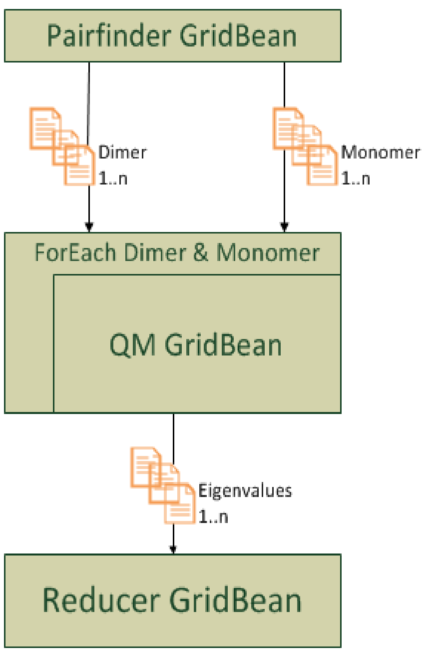
Calculation of Hopping Sites

A deposition film has **1.000 - 100.000** Hopping Site candidates (Site Pairs)
Each Hopping Site needs 3 QM calculations (2 Monomers and 1 Dimer)

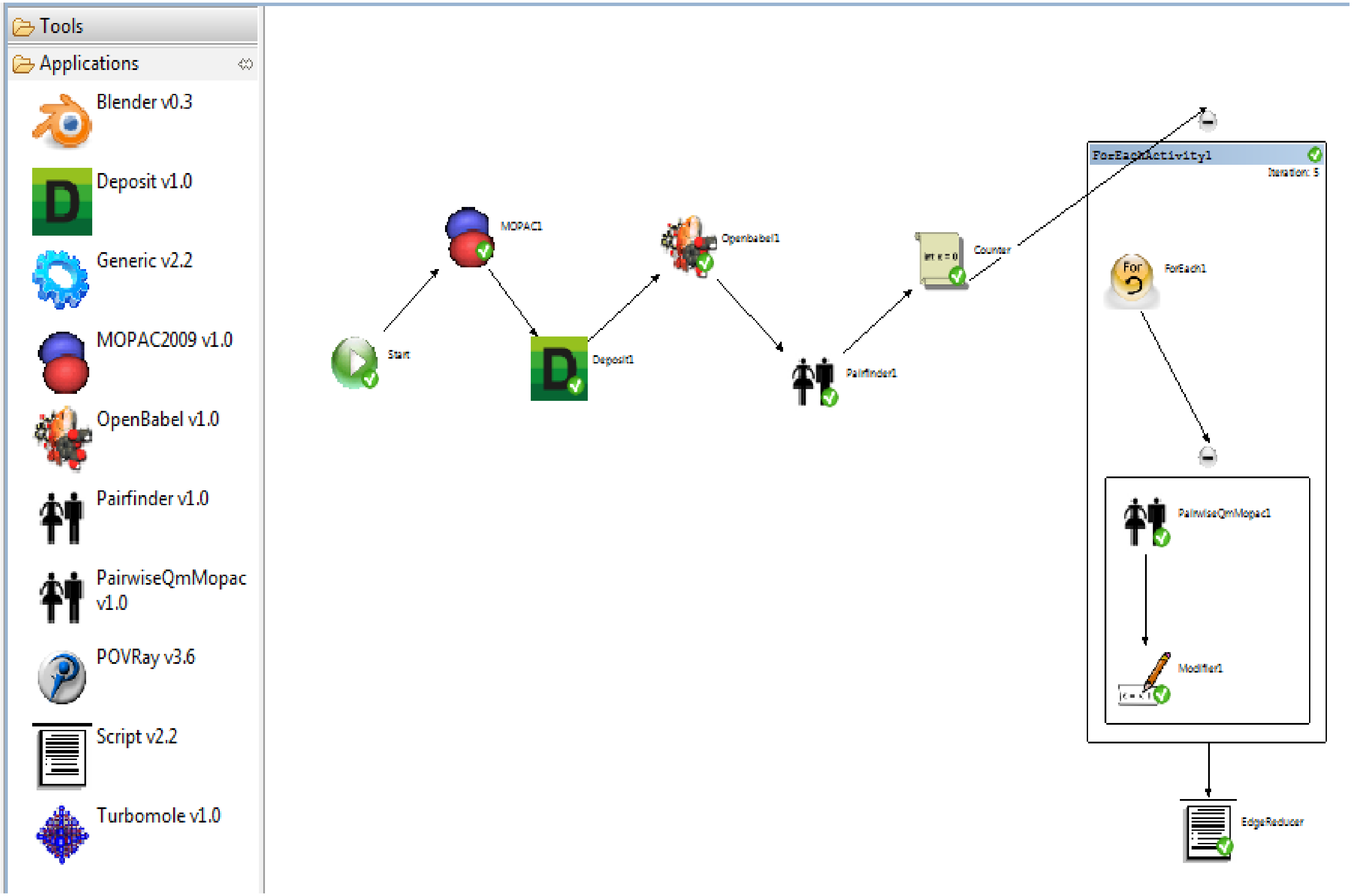
QM-Batch Jobs
- Short QM calculations (~ 0.5 - 5 min)
- Each Job: n * 3 QM calculations
- Less Jobs: Minimize service overhead
- Needs a special GridBean and Wrapper



QM-Single Jobs
- Long QM calculation (30 min +)
- Each Job: one QM calculation
- Many Jobs - > large service overhead
- Needs a special Reducer



Realization: GridBeans and Workflow



Conclusions and Outlook

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- 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 and OpenMolGRID
- Proof of Principle: Workflow for simulation of OLEDs

Current work

- Integration of the CG and FEA steps into the OLED workflow
- Elmer, DL_POLY and BigDFT GridBeans
- Simulation of whole OLED devices
- Deployment and test operation of the workflow

Acknowledgments

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- Funding from the EC

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