Integrated services for multiscale modelling of materials using the UNICORE middleware

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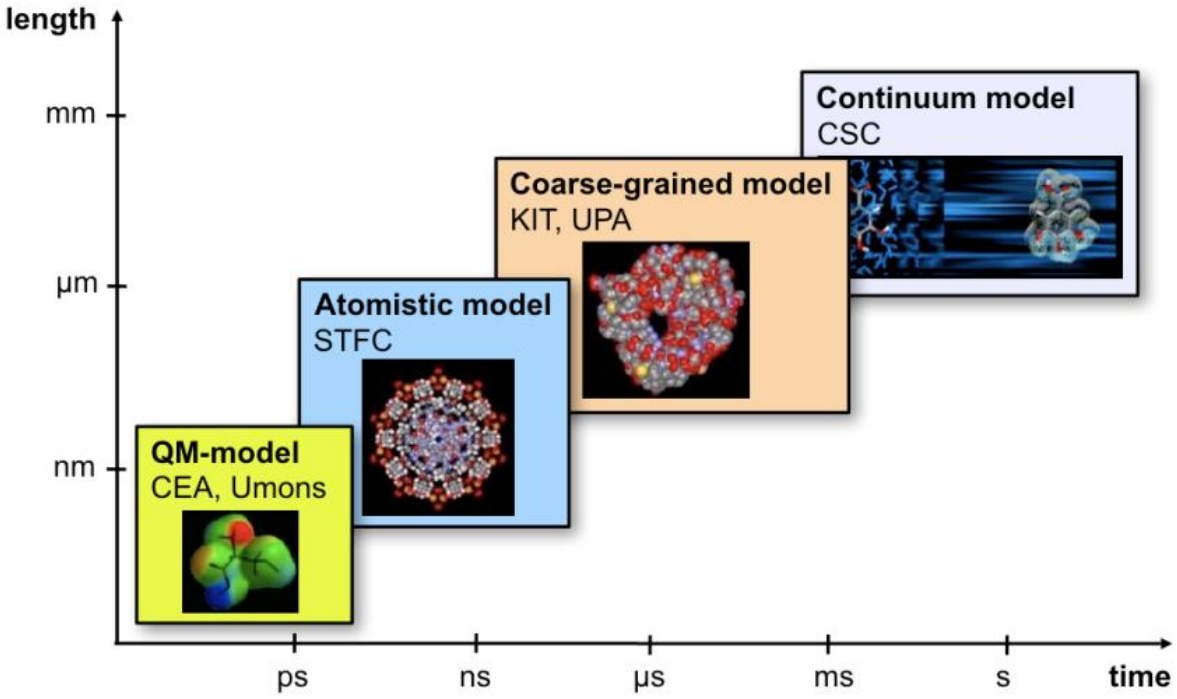
Outline

- Motivation
- Project MMM@HPC overview
- Approach based on UNICORE middleware
  - GridBeans
  - Workflows
  - Data flow management
  - License management
- Prroof of Principle:
  Simulation of Organic Light Emitting Diodes (OLEDs)
- Conclusions and outlook

The challenges



- Integration on different size and time scales to address real-life problems in nano-materials science
- Community and e-infrastructures with both industry and academia involvement

Reusability

Data complexity

Solution for licensing issues

Security & Reliability

Capacity & Capability

MMM@HPC project overview

- 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

Our approach

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

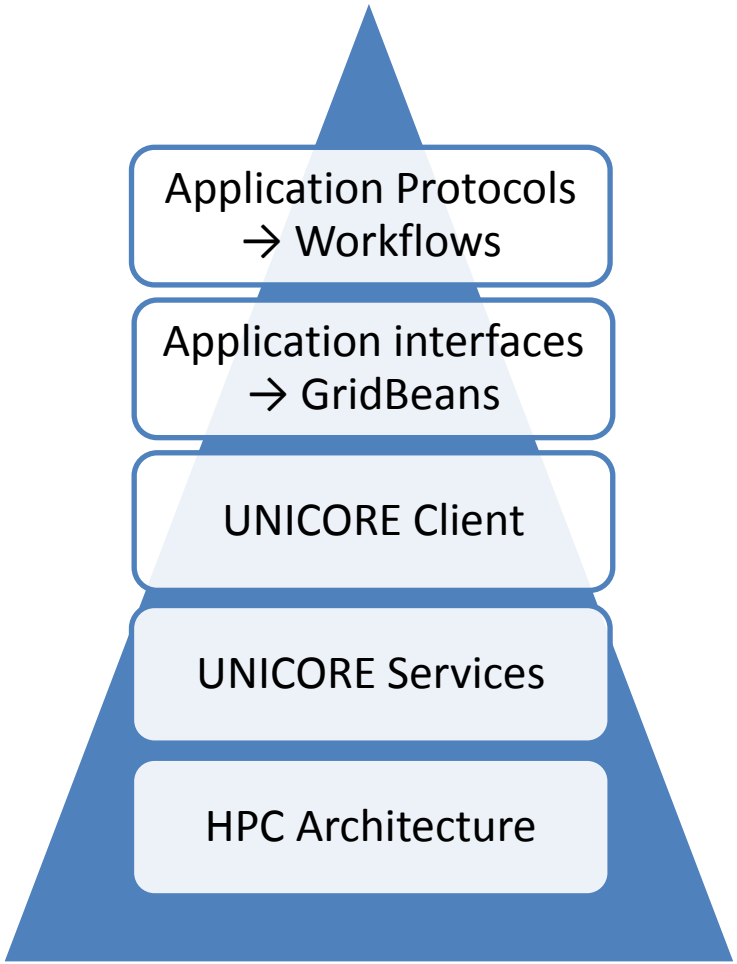
What is UNICORE?

- UNICORE: UNiform Interface to COmputing Resources
- Grid computing technology (grid middleware)
- Seamless, secure, and intuitive access to distributed grid resources
  - Supercomputers
  - Cluster systems
  - Databases
- 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) .

Integration Concept: UNICORE

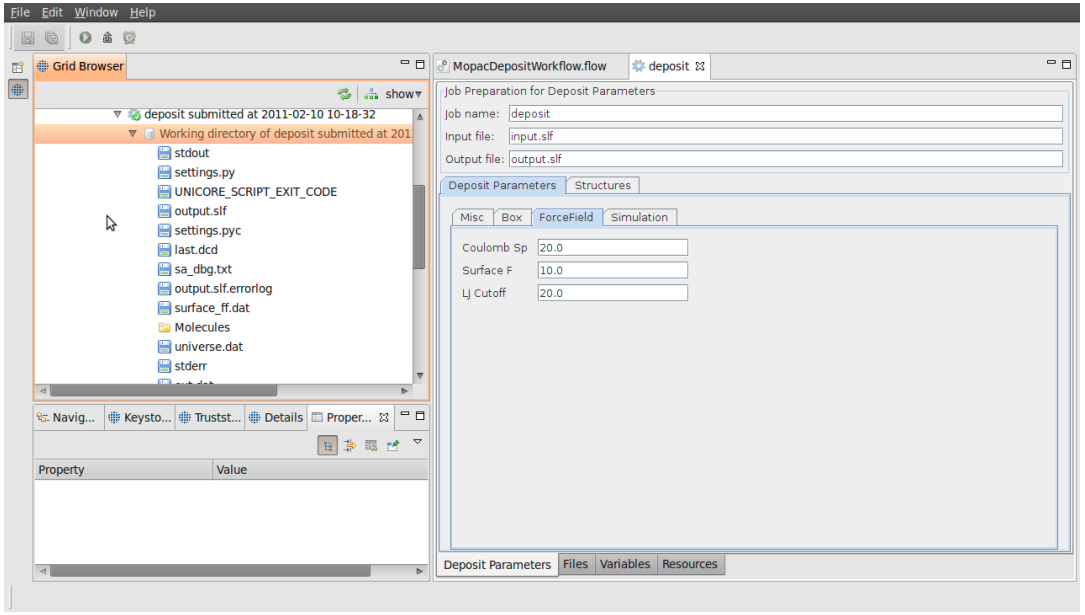
- Provision of simulation tools and services that can be combined in many different application workflows
- Adaptable, reusable and extendable interfaces & workflows based on UNICORE
- Access to distributed HPC resources via UNICORE services



Reusable application interfaces: GridBeans

- GridBeans are designed to decouple scientific applications from the underlying (changing) grid protocols
- Once implemented GridBeans can be used as plug-ins with the UNICORE Rich Client
- Different simulation workflows can re-use the same GridBean
- Different GridBeans can be employed for the same workflow step

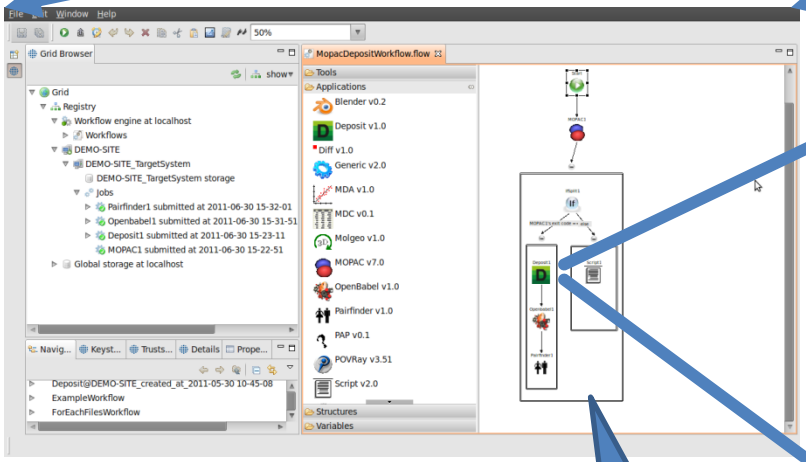
R. Ratering et al., "GridBeans: Support e-Science and Grid Applications", Proceedings of the Second IEEE International Conference on e-Science and Grid Computing (e-Science'06), p. 45, IEEE 2006



The GUI of DEPOSIT GridBean developed in MMM@HPC

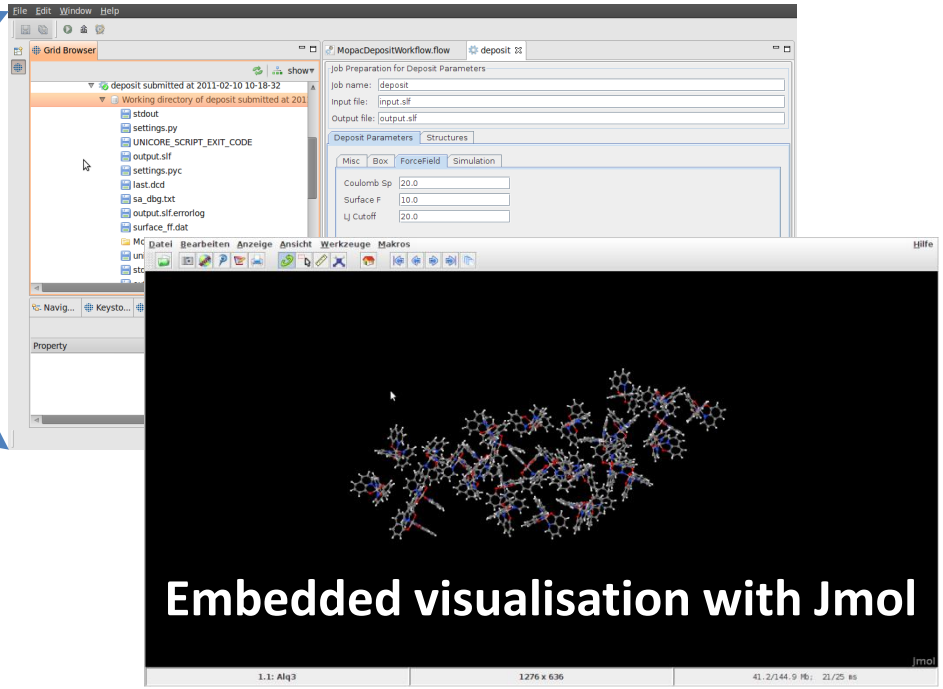
Application protocols: UNICORE workflows

UNICORE Client layer



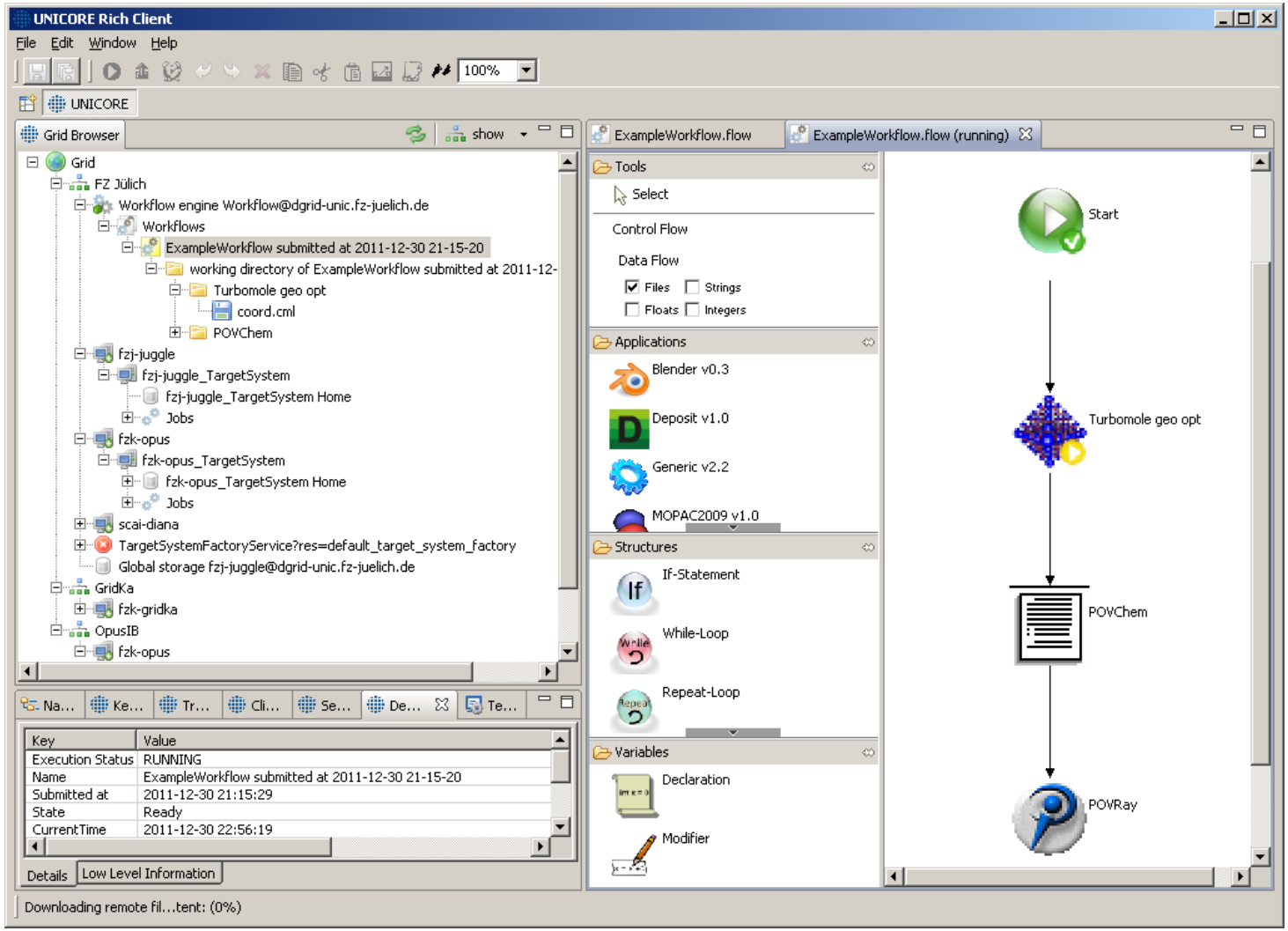
UNICORE Rich Client

DEPOSIT GridBean GUI

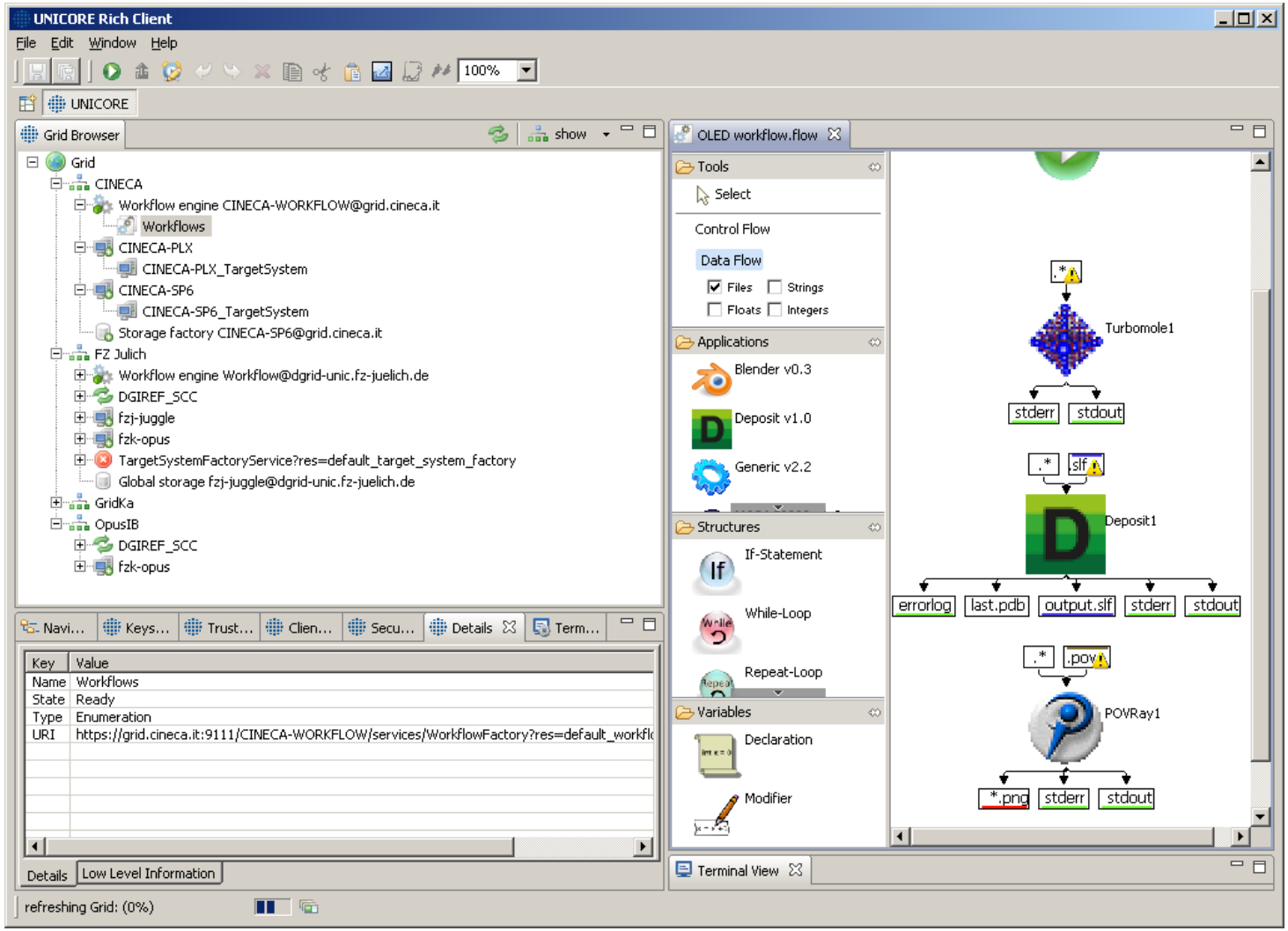


Workflow

Control flow: Example



Data Flow: Example



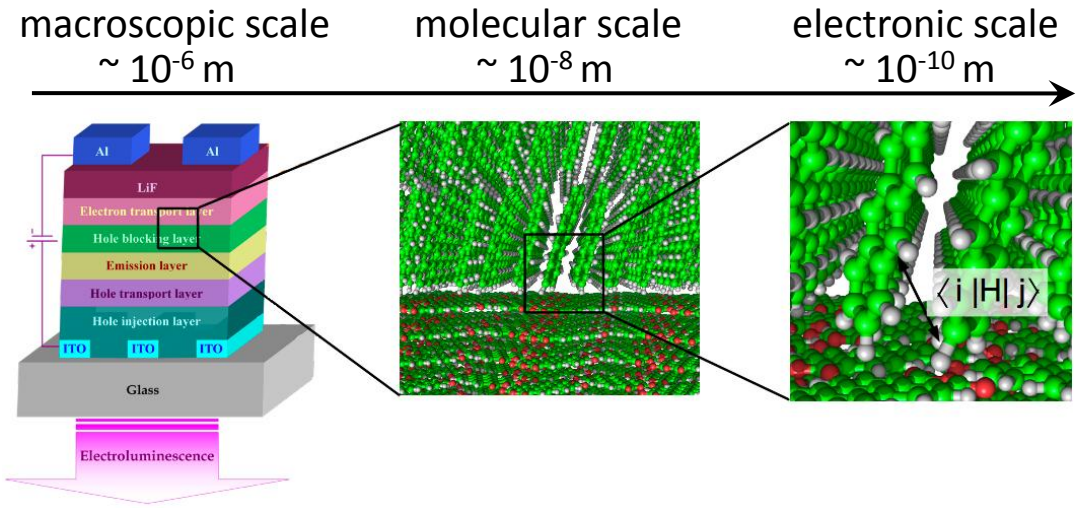
Data exchange and licensing issues

- Data standards
  - Pursue to employ 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).
  - Provides client and server components for UNICORE
  - Currently supports different applications and formats
  - Extensible for further formats
- Further data models are being evaluated
  - MEMOPS (UML based) R. Fogh et al., J. Integr. Bioinf. 7, 123 (2010).
- License management
  - Complex authorization matrix
  - VOMS with UNICORE (UVOS and SAML) is being evaluated

OLED: Simulation protocol

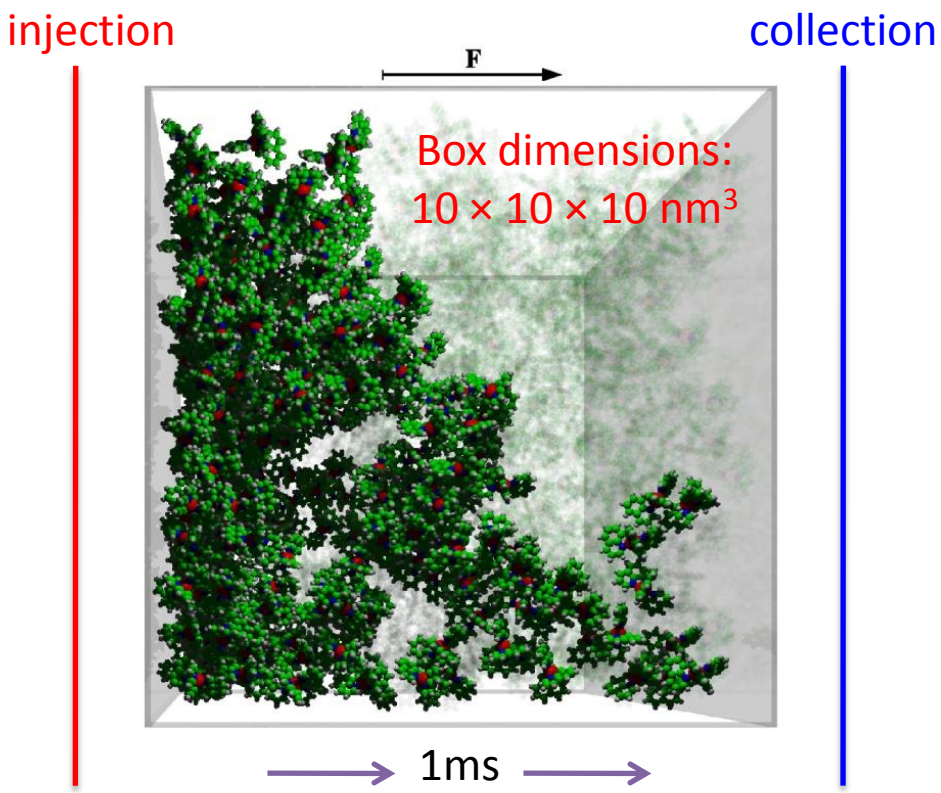
OLED Simulations

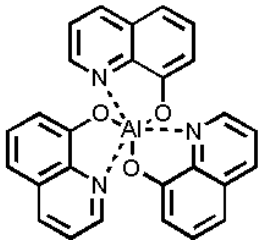
- QM/MM interface simple: no covalent bond breaking
- MM/KMC interface complex, but conceptually simple
- KMC/FEA interface necessary to simulate whole device



Continuum scale	Coarse-grained scale	MM scale	QM scale
Elmer	ToFeT (KMC)	DEPOSIT	MOPAC
FEAP	End-bridging MC	LAMMPS	TURBOMOLE
	Transporter	DL_POLY	BigDFT

Charge transport in Alq3 disordered films

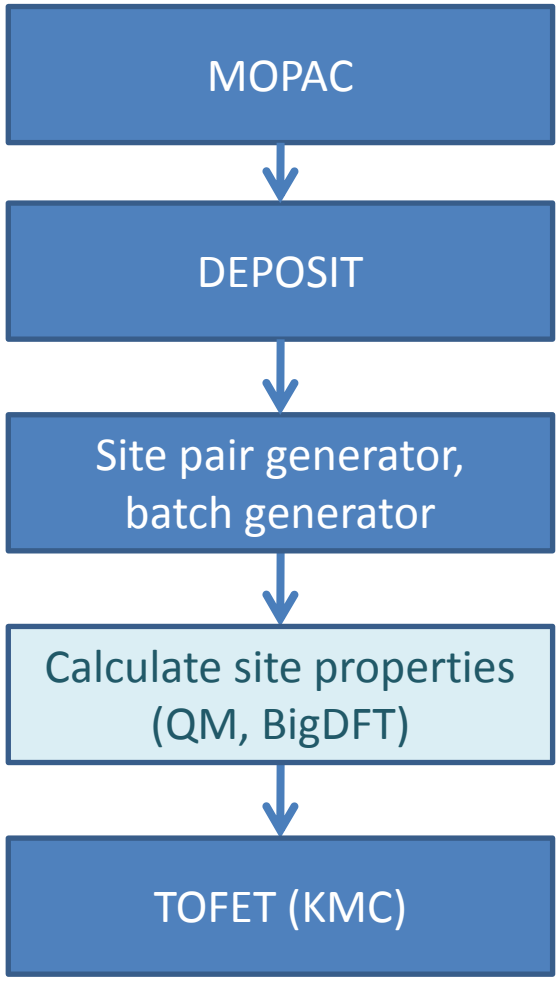


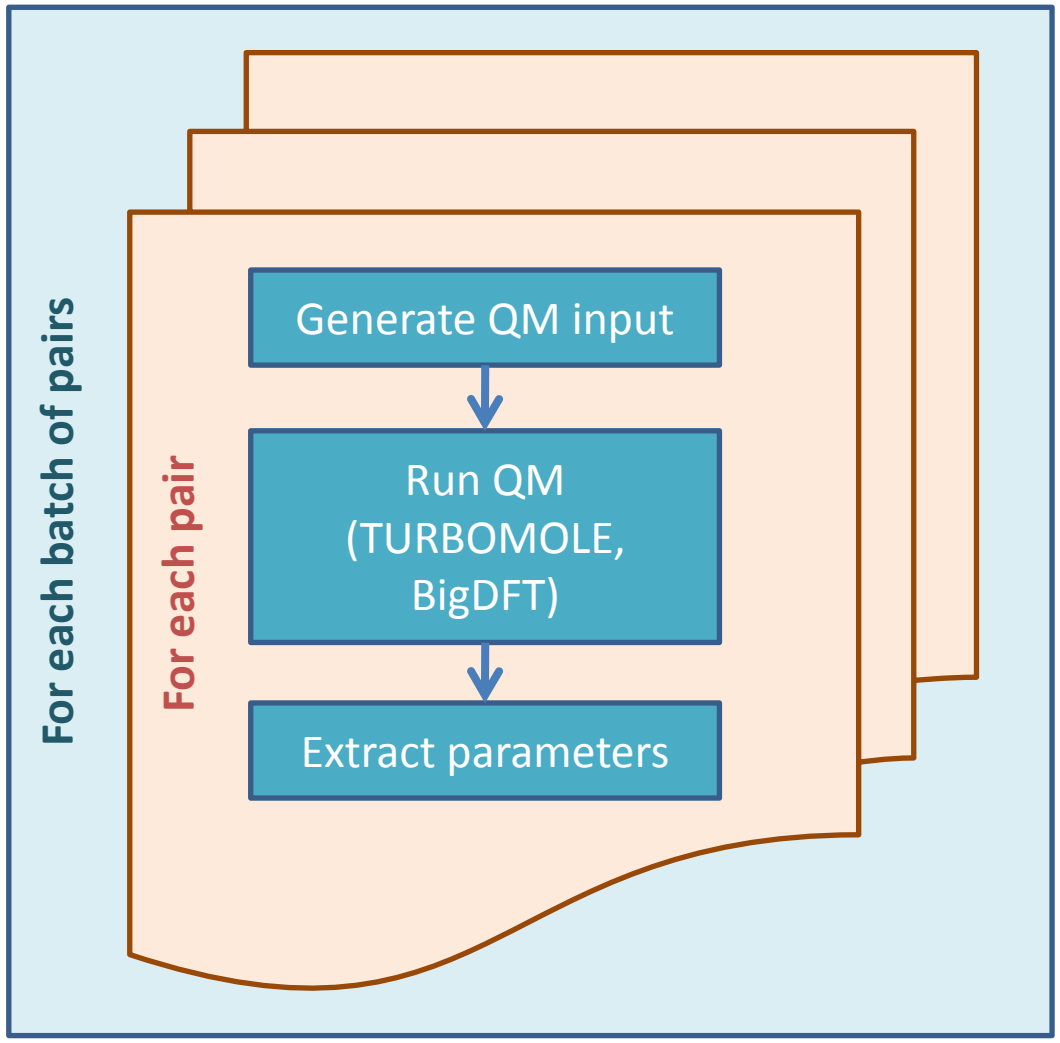


J. J. Kwiatkowski, J. Nelson, H. Li, J. L. Bredas, W. Wenzel, and C. Lennartz, Phys. Chem. Chem. Phys., 2008, 10, 1852–1858.

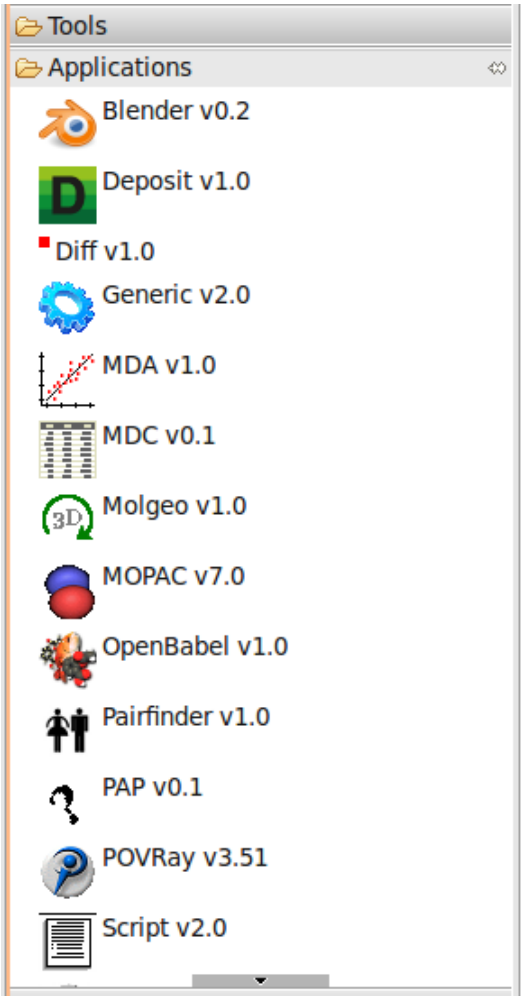
- Film deposition (or MD)
  - Generate disordered film morphologies
  - Optimization via Metropolis & simulated annealing
- QM calculations of hopping sites
  - Calculate HOMO, LUMO, LUMO+1 etc energies.
  - Electronic couplings reorganization energies
  - Calculate charge hopping rates
- Kinetic Monte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

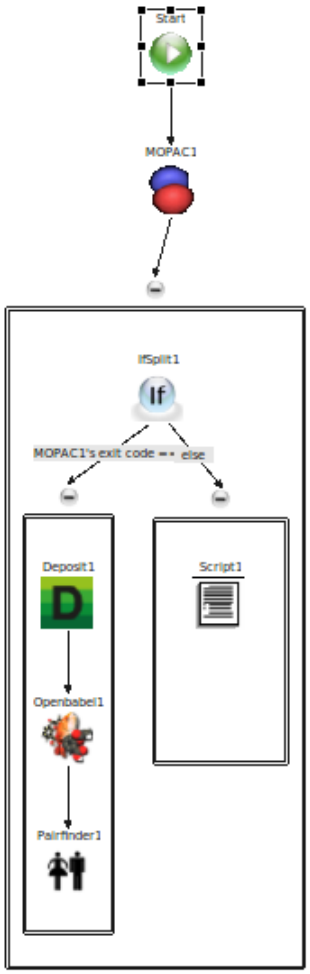
The workflow





Realization: GridBeans and Workflow





Reused GridBeans:

- MOPAC
- Gaussian
- Amber

Newly developed GridBeans:

- DEPOSIT
- TURBOMOLE
- OpenBabel
- PairFinder

Kondov, I. et al., UNICORE-Based Integrated Application Services for Multiscale Materials Modelling , In: Romberg, M. et al. *(Eds.) „UNICORE Summit 2011 Proceedings, 7–8 July 2011, Torun, Poland“, IAS Series,* vol. 9 (2011), pp. 1-10, FZJ Jülich.

Conclusions and Outlook

- With UNICORE we provide an optimal low-effort/low-cost solution for multiscale modelling
- GridBeans → App Interfaces
- Workflow for simulation of OLEDs

Not shown today

- MMM@HPC Development Toolkit
- VO m3hpc

Current work

- Integration of the FEM step into the OLED workflow
- Elmer and BigDFT GridBeans
- Proof-of-principle 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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