UNICORE-Based Integrated Application Services for Multiscale Materials Modeling

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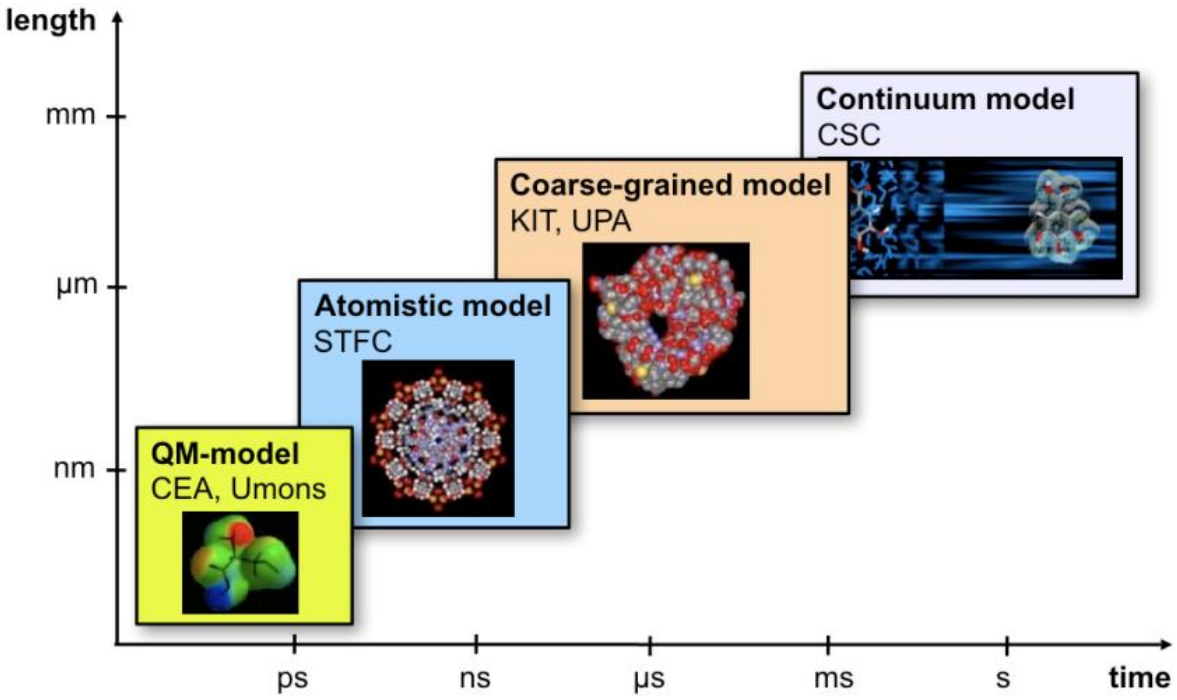
Overview

- Motivation
- Project MMM@HPC overview
- Approach based on UNICORE middleware
  - GridBeans
  - Workflows
  - Data flow management and license management
- Example: 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

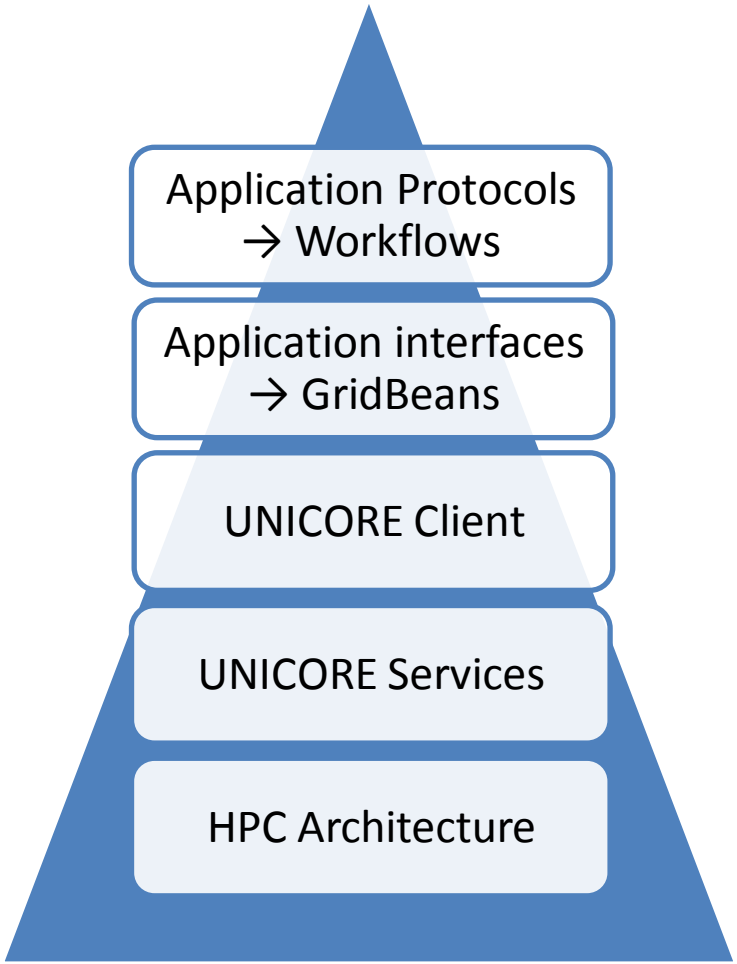
- HPC centres: CINECA, CSC, KIT and KIST (Korea)
- Modelling and code developing groups: University Mons, CEA, CSC, STFC, University Patras, KIT
- Industrial partners and users: CEA, SONY, KIT, project MINOTOR
- Cooperating projects: PRACE, MINOTOR, D-Grid and NGI-DE

Our approach

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

Concept for application integration: UNICORE

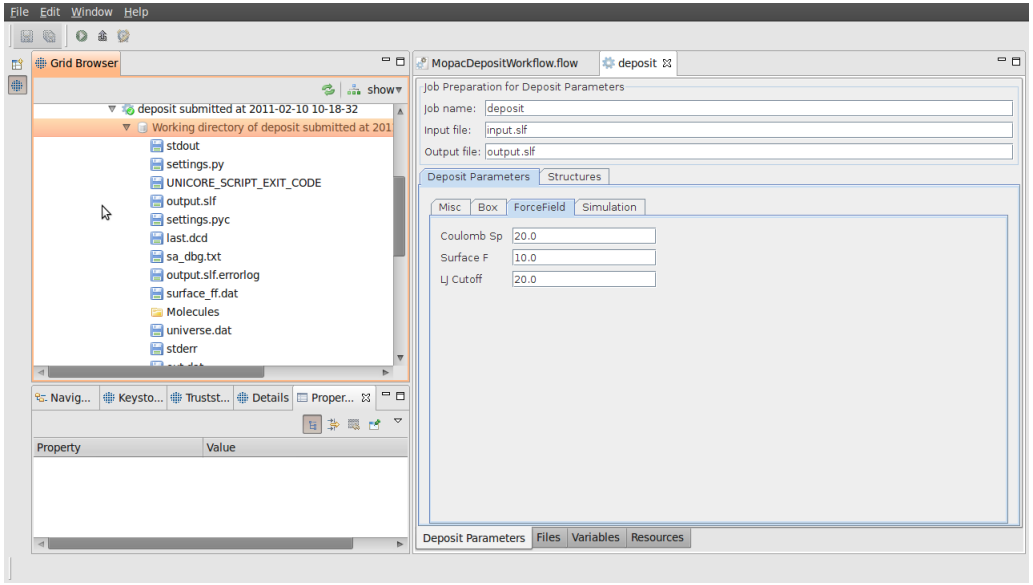
- Provision of simulation tools and services that can be combined in many different application workflows
- Adaptable, reusable and extendable interfaces & workflows based on UNICORE
- Access distributed HPC resources via UNICORE services



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

Reusable application interfaces: GridBeans

- GridBeans are plug-ins designed to decouple scientific applications from the underlying (changing) grid protocols
- Once implemented GridBeans can be used with the UNICORE Rich Client
- Different application workflows can access the same GridBean
- Different GridBeans can be used at the same node of a workflow



The GUI of DEPOSIT GridBean developed in MMM@HPC

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

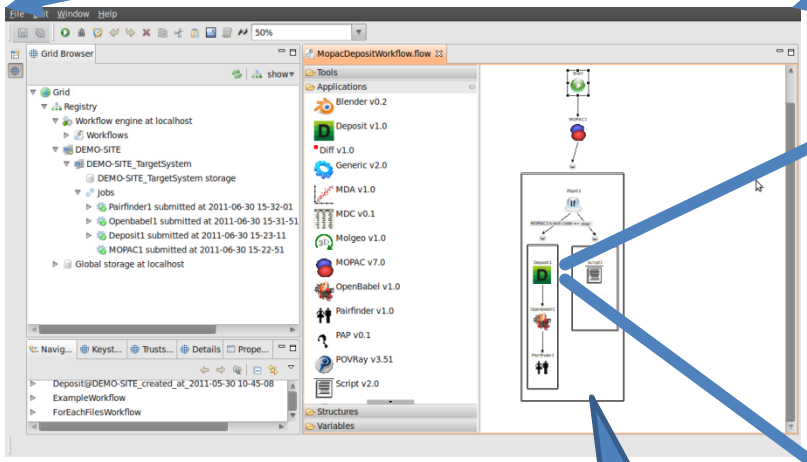
Application protocols: UNICORE workflows

UNICORE Client layer

Portal client, e.g. GridSphere

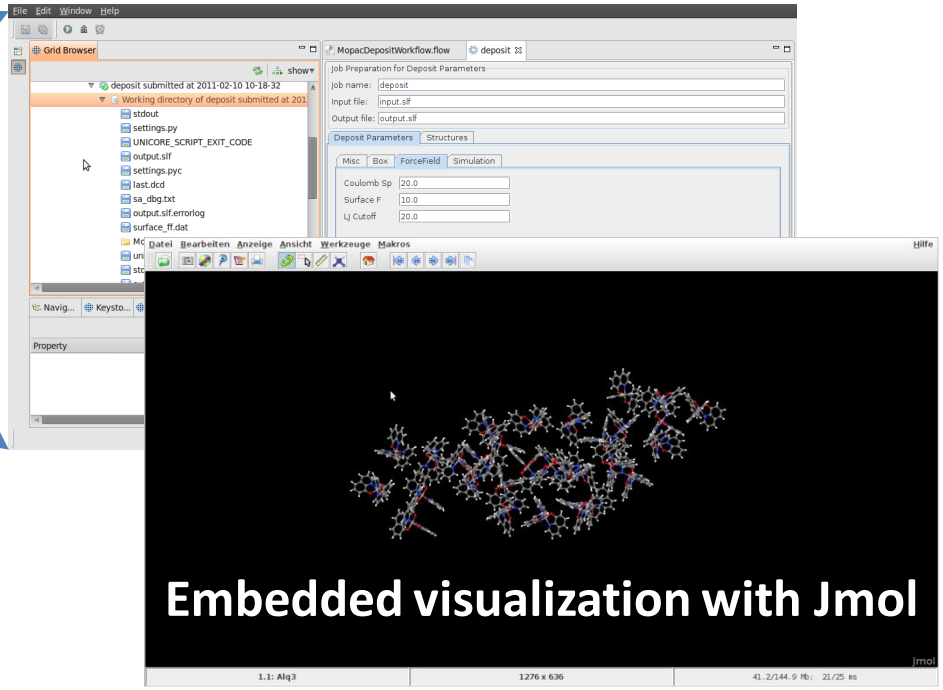
command-line client

Eclipse-based client



UNICORE Rich Client

DEPOSIT GridBean GUI



Workflow

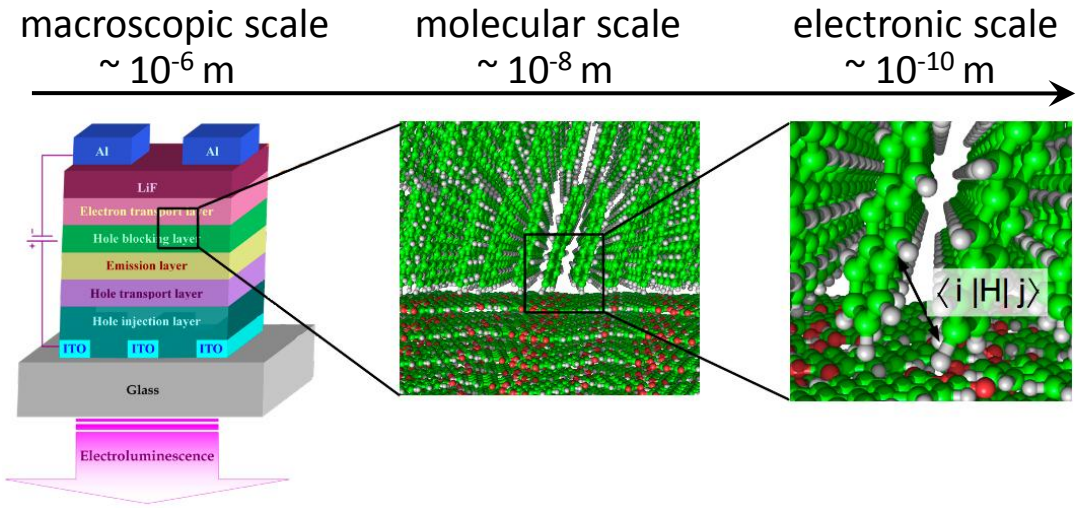
Data exchange and licensing issues

- Data standards
  - Pursue to employ Chemical Markup Language (CML)
- Data flow management with OpenMolGRID
  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

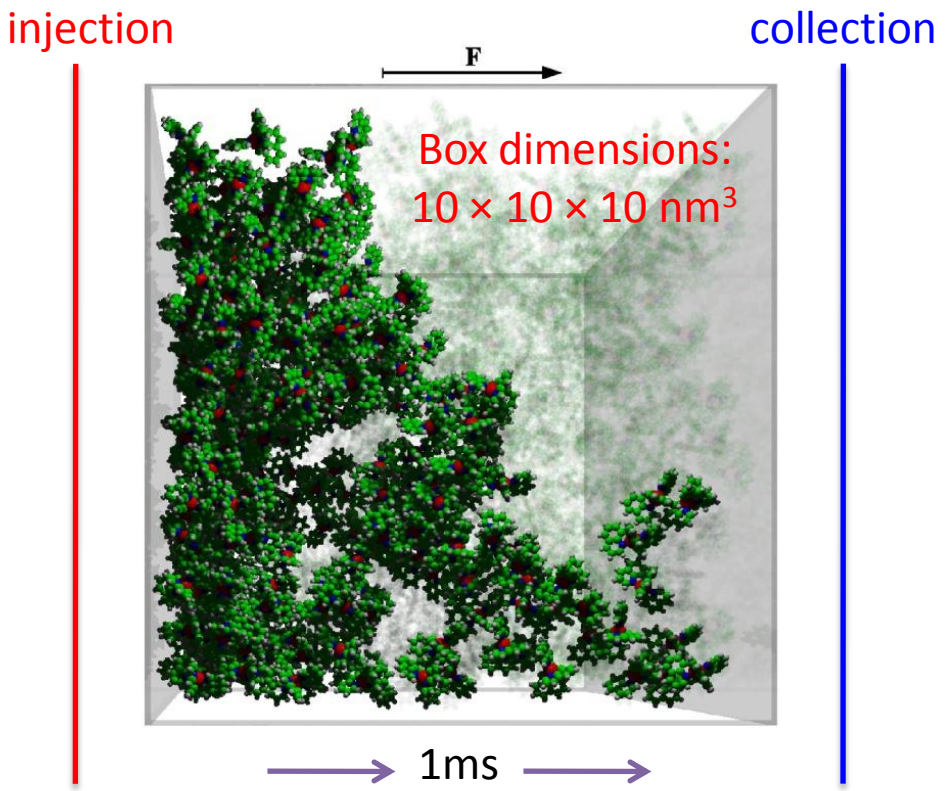
OLED Simulations

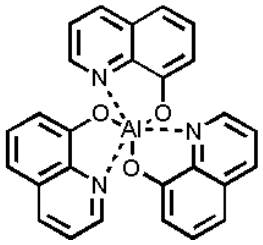
- QM/MM interface simple: no covalent bond breaking
- MM/KMC interface complex, but conceptually simple
- KMC/FEA interface necessary to simulate whole device



QM scale	MM scale	Coarse-grained scale	Continuum scale
TURBOMOLE	Amber	Kinetic Monte Carlo	Elmer
MOPAC	Gromacs	End-bridging MC	FEAP
BigDFT	DEPOSIT	Transporter	
VASP	DL_POLY		
GPAW	LAMMPS		

Charge transport in Alq_3 disordered films

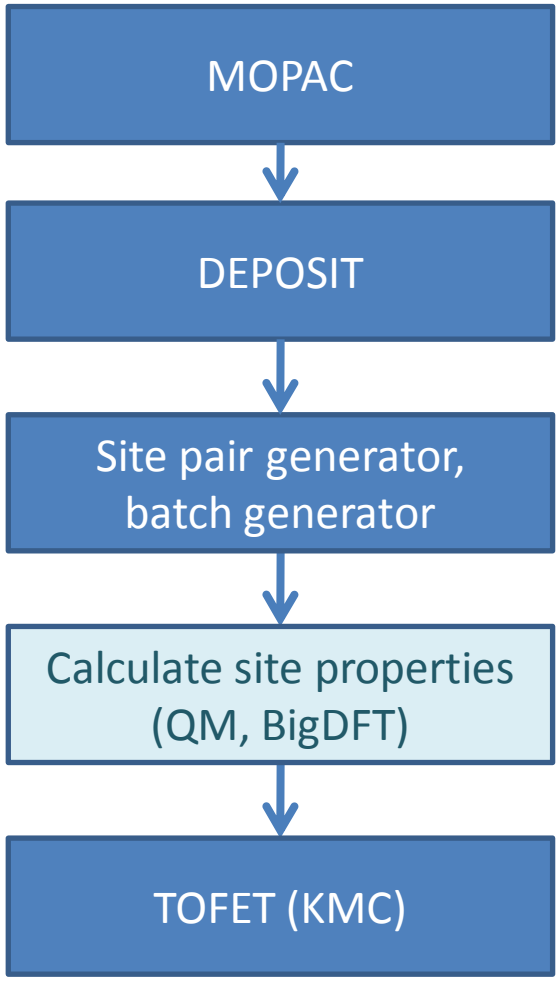


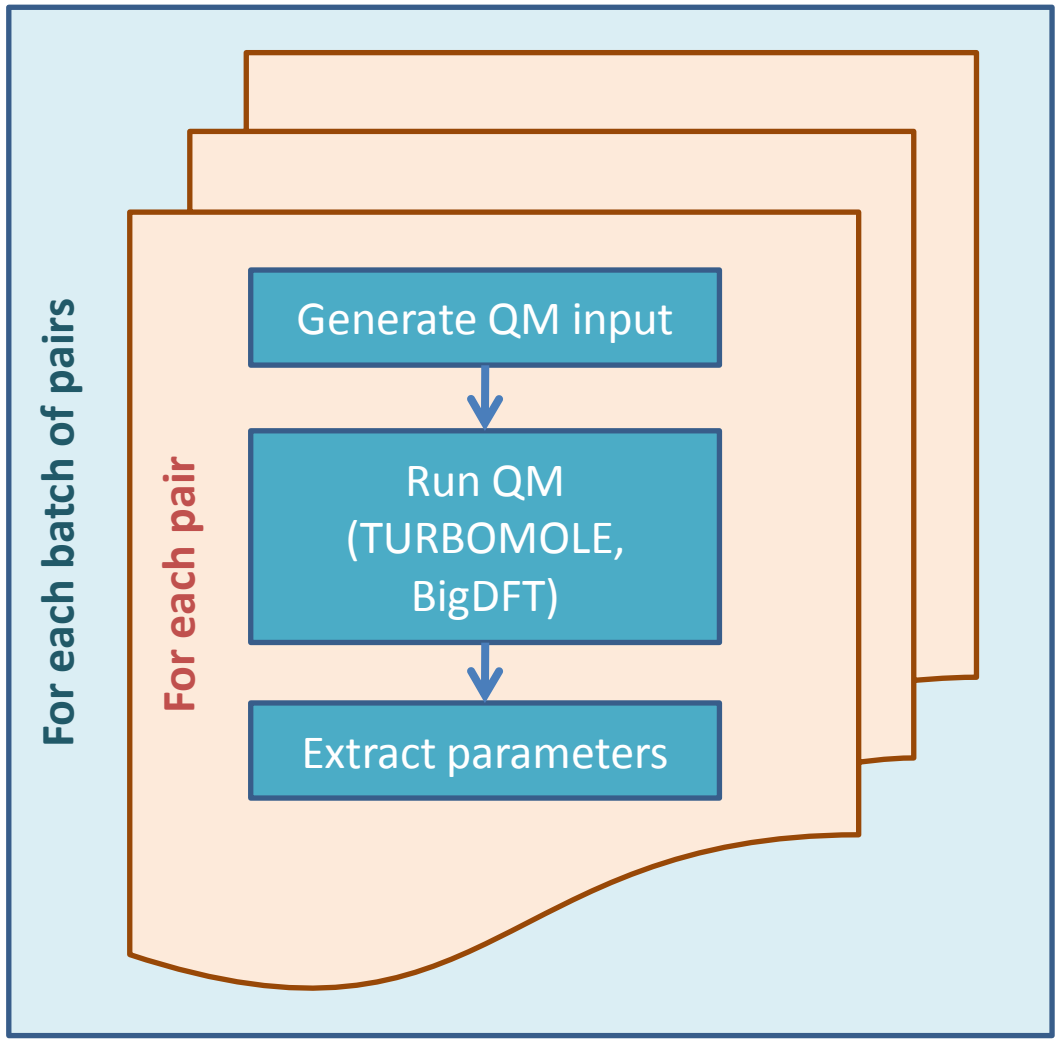


J. J. Kwiatkowski, J. Nelson, H. Li, J. L. Bredas, W. Wenzel, and C. Lennartz, Phys. Chem. Chem. Phys., 2008, 10, 1852–1858.

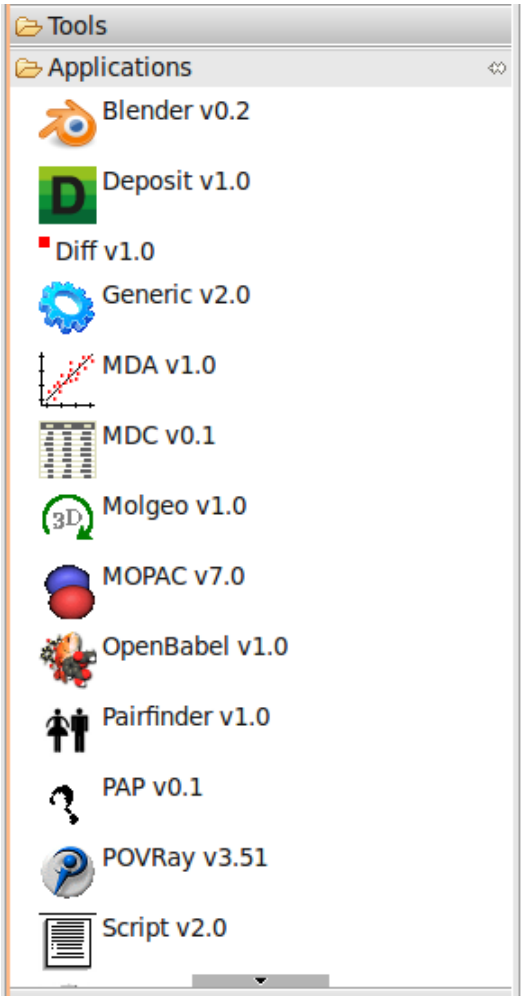
- Film deposition (or MD)
  - Generate disordered film morphologies
  - Optimization via Metropolis & simulated annealing
- QM calculations of hopping sites
  - Calculate HOMO, LUMO, LUMO+1 etc energies.
  - Electronic couplings reorganization energies
  - Calculate charge hopping rates
- Kinetic Monte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

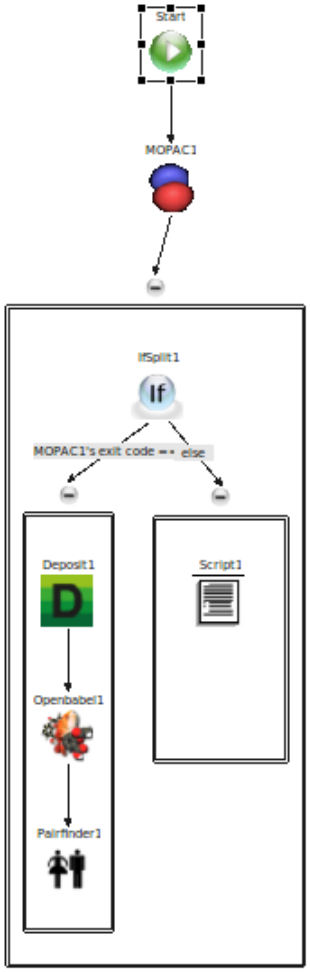
The workflow





Realization: GridBeans and Workflow





Reused GridBeans:

- MOPAC
- Gaussian
- Amber

Newly developed GridBeans:

- DEPOSIT
- OpenBabel
- PairFinder

Conclusions and Outlook

- New GridBeans
- Working workflow for OLED simulations
- Integration of the FEM step into the OLED workflow
- Proof-of-principle simulation of whole OLED devices
- Deployment and test operation of the workflow

Acknowledgments

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