Multiscale simulations of complex materials basing on UNICORE workflows

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Outline

- The Challenges
- Project MMM@HPC overview
- Approach based on UNICORE middleware
  - GridBeans
  - Workflows
  - Data flow management and Licensing Issues
- OpenMOLGrid as Application Wrapper
- Proof of Principle: Simulation of Organic Light Emitting Diodes (OLEDs)
- Live Demo
- Conclusions and outlook
The challenges

- Integration on different size and time scales to address real-life problems in nanomaterials science
- Develop an easy to use solution for non-experts: industrial and experimental groups
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
Can we meet these challenges?

- **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

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


The GUI of DEPOSIT GridBean developed in MMM@HPC
UNICORE Rich Client and Workflows

UNICORE Client layer

Portal client, e.g. GridSphere

command-line client

Eclipse-based client

DEPOSIT GridBean GUI

UNICORE Rich Client

Workflow

Embedded visualisation with Jmol
Control flow: Example
OLED: Simulation protocol

<table>
<thead>
<tr>
<th>continuum model (FEA)</th>
<th>coarse-grained model (CG)</th>
<th>Atomistic model (MM)</th>
<th>QM model (QM)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Elmer</td>
<td>ToFeT (KMC)</td>
<td>DEPOSIT</td>
<td>MOPAC</td>
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<tr>
<td>FEAP</td>
<td>End-bridging MC</td>
<td>LAMMPS</td>
<td>TURBOMOLE</td>
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<td>Transporter</td>
<td>DL_POLY</td>
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<td>BigDFT</td>
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- **macroscopic scale**: \( \sim 10^{-6} \text{ m} \)
- **molecular scale**: \( \sim 10^{-8} \text{ m} \)
- **electronic scale**: \( \sim 10^{-10} \text{ m} \)

Diagram: OLED device structure with layers labeled and scales indicated.
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

Realization: GridBeans and Workflow

Reused GridBeans:
- MOPAC
- Gaussian
- Amber

Newly developed GridBeans:
- DEPOSIT
- TURBOMOLE
- OpenBabel
- PairFinder


Data exchange and licensing issues

- Chemical Markup Language (CML)
- Data flow management with the OpenMolGRID library
  
  
  - Read, write and convert chemical file format
  - Provides a data model
  - Application Wrapper

- Further data models are being evaluated
  

- License management
  
  - OpenSource and Commercial applications in simulations
  - VOMS with UNICORE (UVOS and SAML) is being evaluated
Application Wrapper Lifecycle

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

Simulation protocol

QM: Geometry Optimization
MM: Film deposition
MM: Determination of Site pairs
QM: Pairwise QM calculations J (eV), DE (eV)
CG: Compute Charge mobility
FEA: Calculate Current Density

UNICORE Workflow

1 Molecule
MOPAC GridBean
DEPOSIT GridBean
BABEL GridBean
Pairfinder GridBean
PairwiseQM GridBean
Reduction GridBean

n Molecules
PDB
CML
CML
Pair
CML
Edge
CML
Edge
Demo
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 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
- MMM@HPC Development Kit (Virtual Box)
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