

Multiscale simulations of complex materials basing on UNICORE workflows



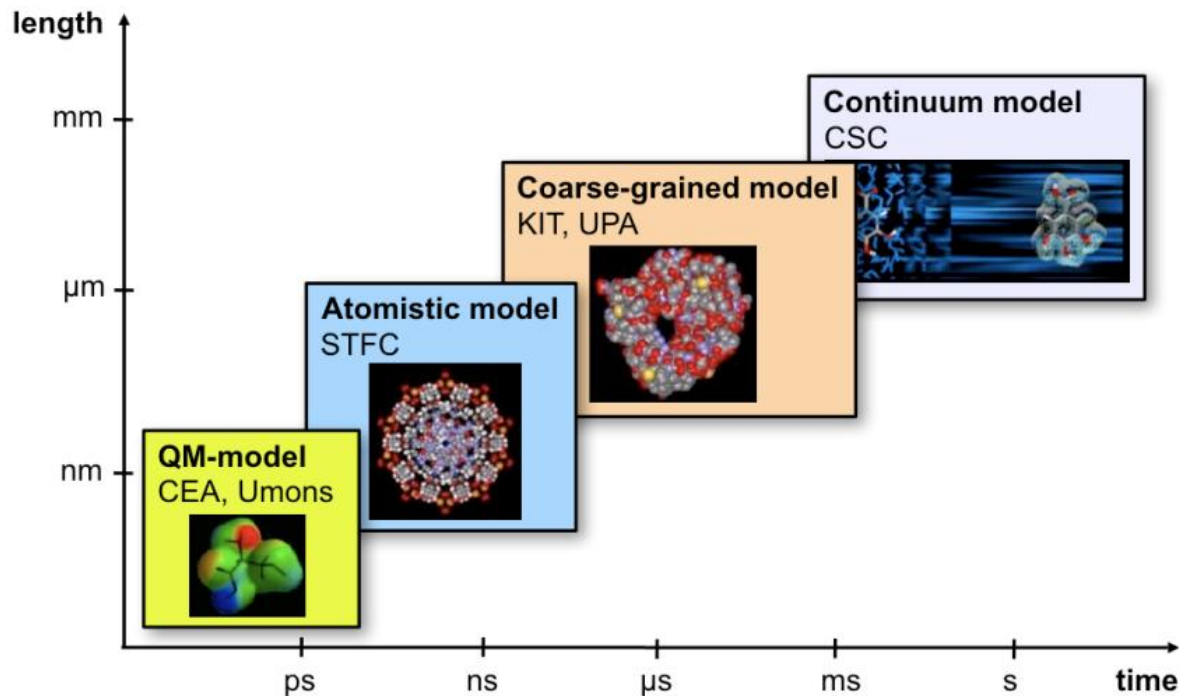
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- The Challenges
- Project MMM@HPC overview
- Approach based on UNICORE middleware
 - GridBeans
 - Workflows
 - Data flow management and Licensing Issues
- OpenMOLGrid as Application Wrapper
- Proof of Principle:
Simulation of Organic Light Emitting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

The challenges



- Integration on different size and time scales to address real-life problems in 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



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)

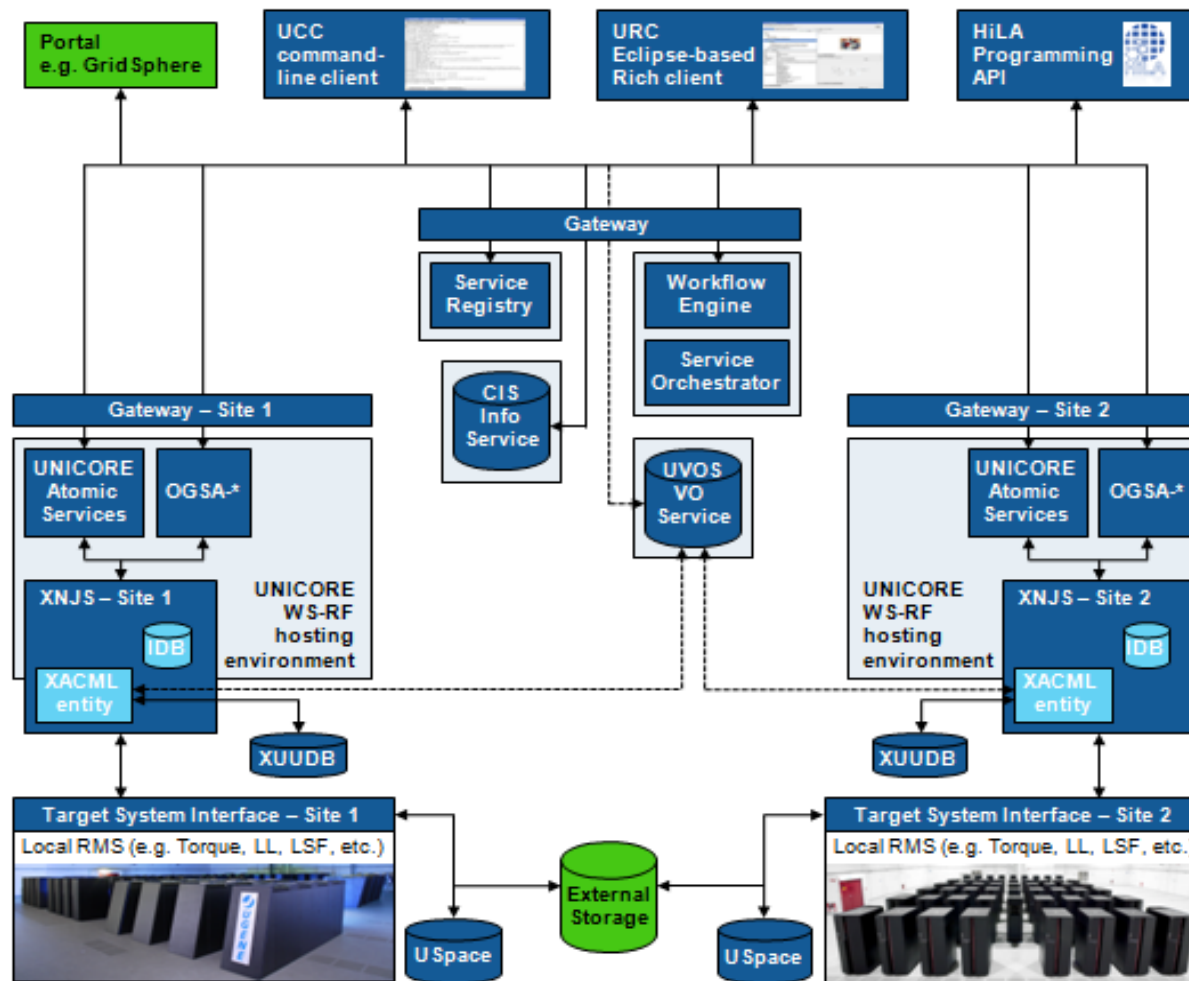
YES!

- 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) .

The logo features the word 'UNICORE' in a bold, blue, sans-serif font. The letter 'O' is replaced by a blue grid pattern.

UNICORE three-layer architecture



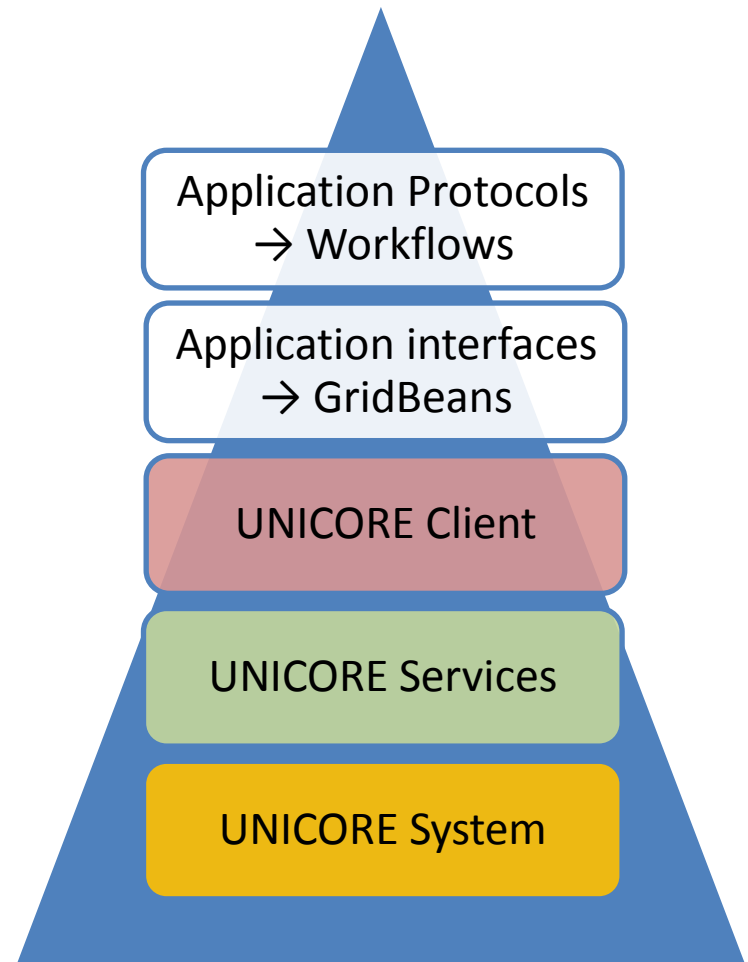
UNICORE Client

UNICORE Services

UNICORE System

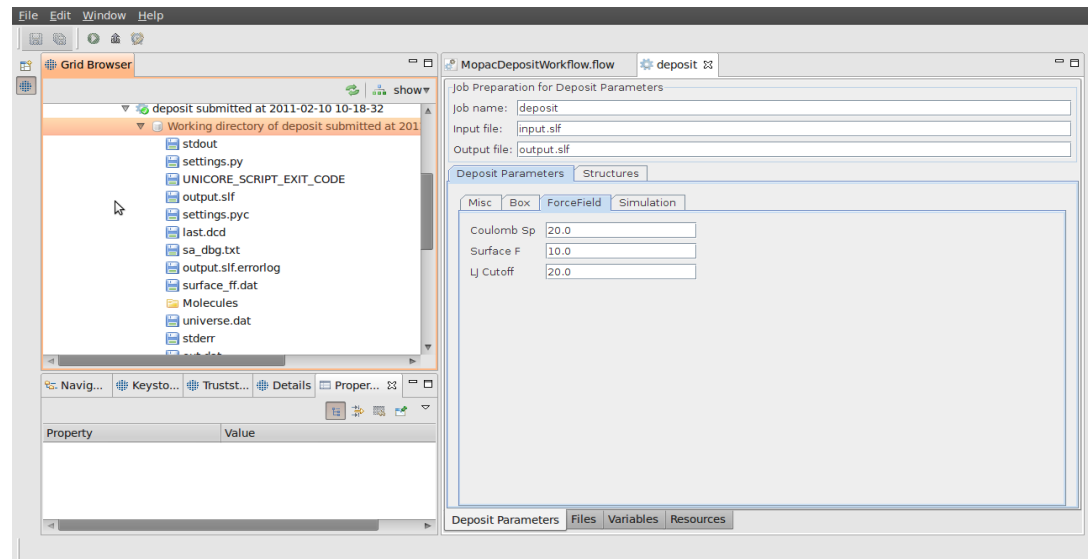
<http://www.unicore.eu/unicore/architecture.php>

- 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



- 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

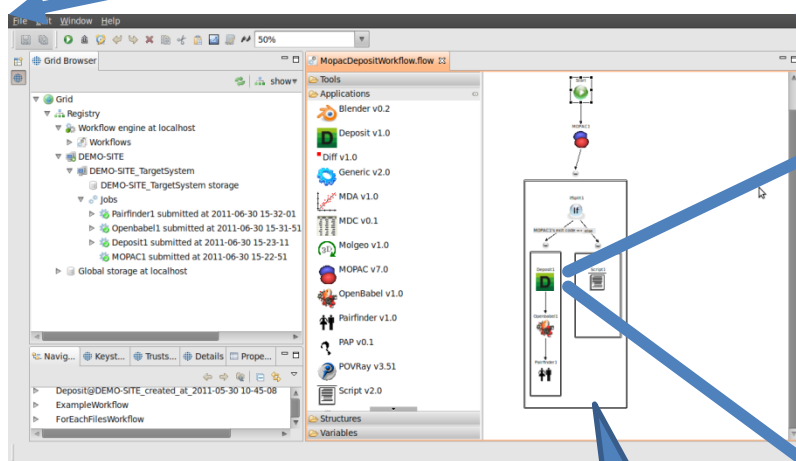


The GUI of DEPOSIT GridBean developed in MMM@HPC

UNICORE Rich Client and Workflows

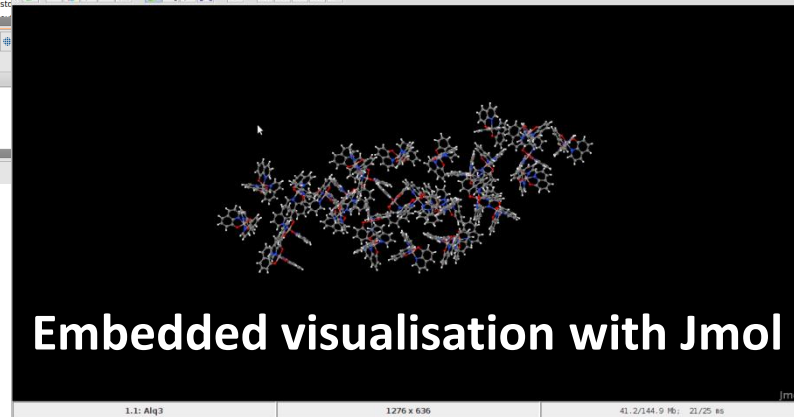
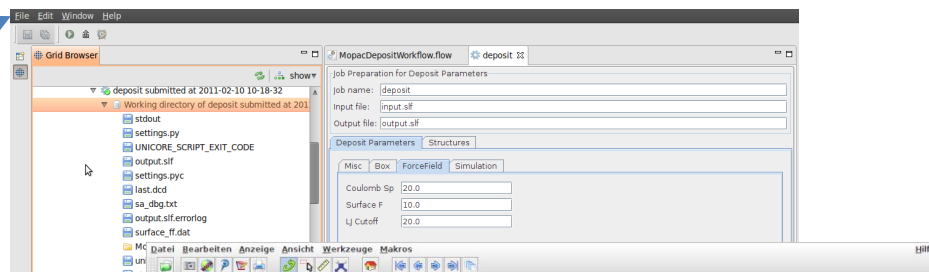


UNICORE Client layer



UNICORE Rich Client

DEPOSIT GridBean GUI



Embedded visualisation with Jmol

Control flow: Example

The screenshot displays the UNICORE Rich Client interface. On the left, the Grid Browser shows a tree view of the grid resources, including 'FZ Jülich', 'Workflow engine Workflow@dgrid-unic.fz-juelich.de', and 'ExampleWorkflow submitted at 2011-12-30 21-15-20'. The main workspace shows a workflow diagram with the following steps:

- Start (Green play button)
- Turbomole geo opt (Blue diamond icon)
- POVChem (Document icon)
- POVRay (Blue sphere icon)

The Tools palette on the right contains the following categories:

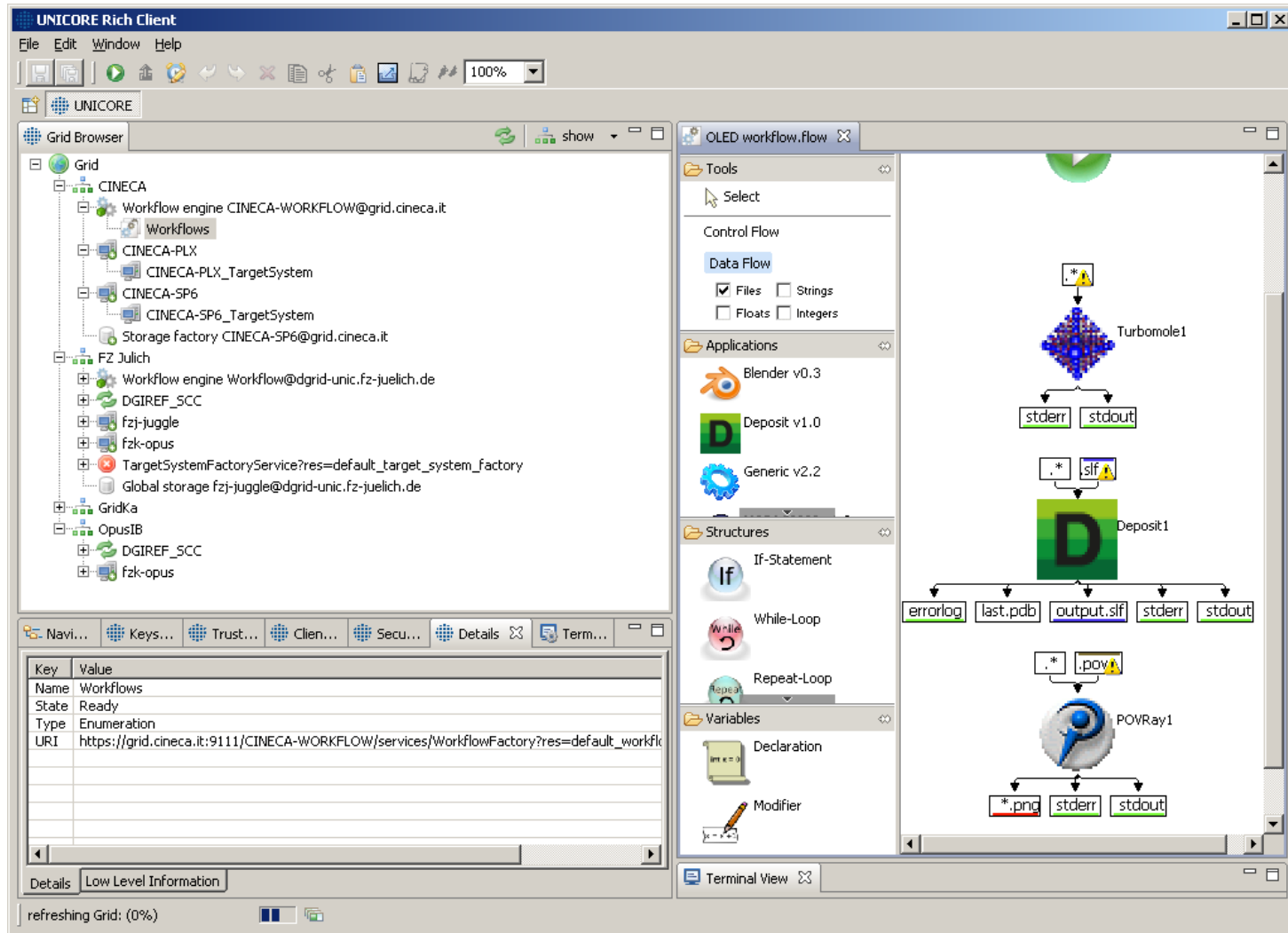
- Tools: Select
- Control Flow: If-Statement, While-Loop, Repeat-Loop
- Data Flow: Files (checked), Strings, Floats, Integers
- Applications: Blender v0.3, Deposit v1.0, Generic v2.2, MOPAC2009 v1.0
- Structures: If-Statement, While-Loop, Repeat-Loop
- Variables: Declaration, Modifier

At the bottom, a status table shows the following information:

Key	Value
Execution Status	RUNNING
Name	ExampleWorkflow submitted at 2011-12-30 21-15-20
Submitted at	2011-12-30 21:15:29
State	Ready
CurrentTime	2011-12-30 22:56:19

Download progress: Downloading remote fil...tent: (0%)

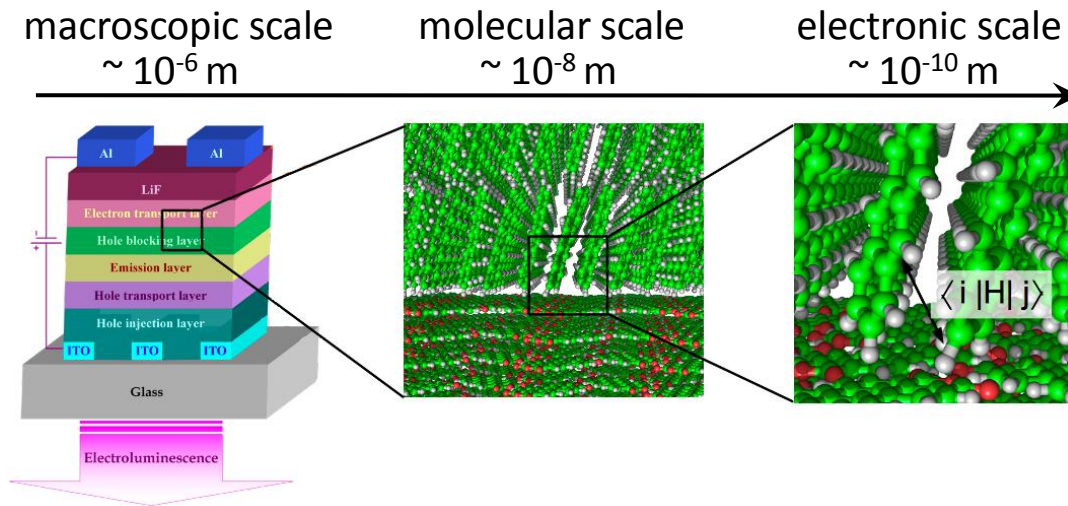
Data Flow: Example



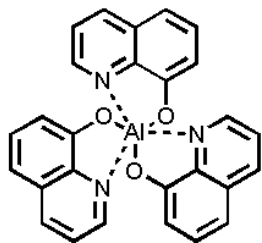
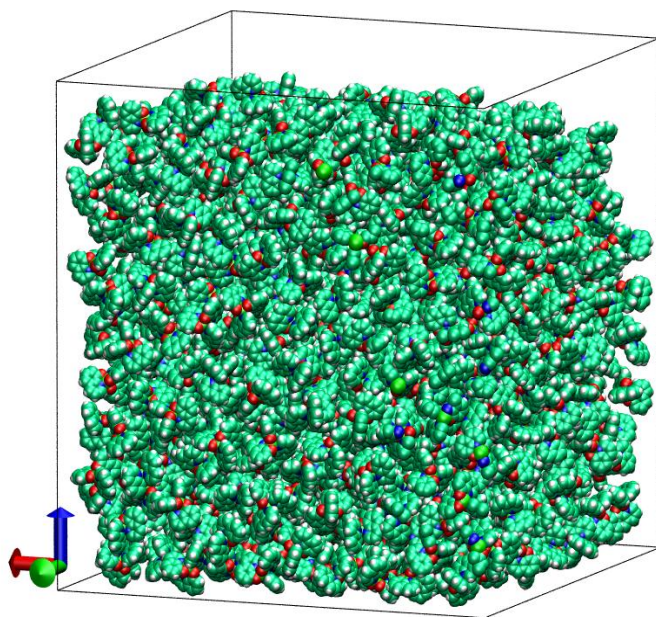
The screenshot displays the UNICORE Rich Client interface. On the left, the Grid Browser shows a tree view of resources including CINECA, FZ Julich, and GridKa. The main workspace shows a workflow editor for 'OLED workflow.flow'. The workflow diagram consists of several nodes: a 'TurboMole1' node (represented by a blue cube) which outputs to 'stderr' and 'stdout'; a 'Deposit1' node (represented by a green 'D') which receives input from a file pattern '*.slf' and outputs to 'errorlog', 'last.pdb', 'output.slf', 'stderr', and 'stdout'; and a 'POVRay1' node (represented by a blue sphere) which receives input from a file pattern '*.pov' and outputs to '*.png', 'stderr', and 'stdout'. The right sidebar contains toolbars for 'Tools', 'Control Flow', 'Applications' (Blender v0.3, Deposit v1.0, Generic v2.2), 'Structures' (If-Statement, While-Loop, Repeat-Loop), and 'Variables' (Declaration, Modifier). A 'Terminal View' tab is visible at the bottom.

Key	Value
Name	Workflows
State	Ready
Type	Enumeration
URI	https://grid.cineca.it:9111/CINECA-WORKFLOW/services/WorkflowFactory?res=default_workfl

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



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

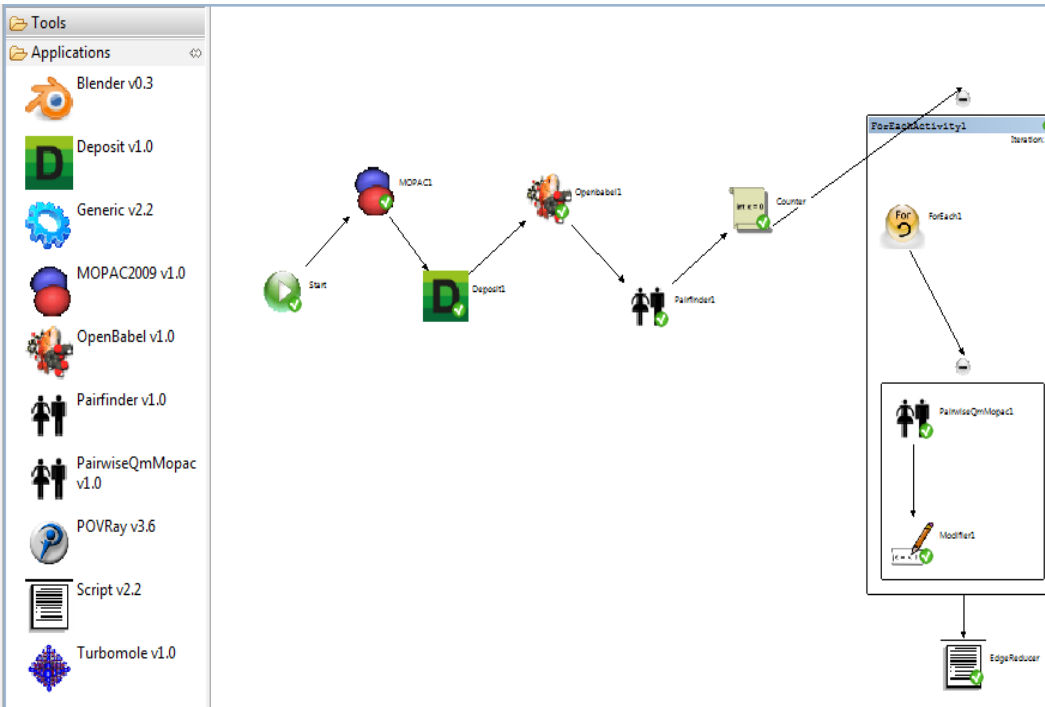
- Film deposition (or MD)
 - Generate disordered film morphologies
- QM calculations of hopping sites
 - Calculate HOMO, LUMO, LUMO+1 etc energies.
 - Electronic couplings reorganization energies
 - Calculate charge hopping rates
- Kinetic Monte Carlo (KMC)
 - Calculate charge (electron-hole) mobility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

Reused GridBeans:

- MOPAC
- Gaussian
- Amber

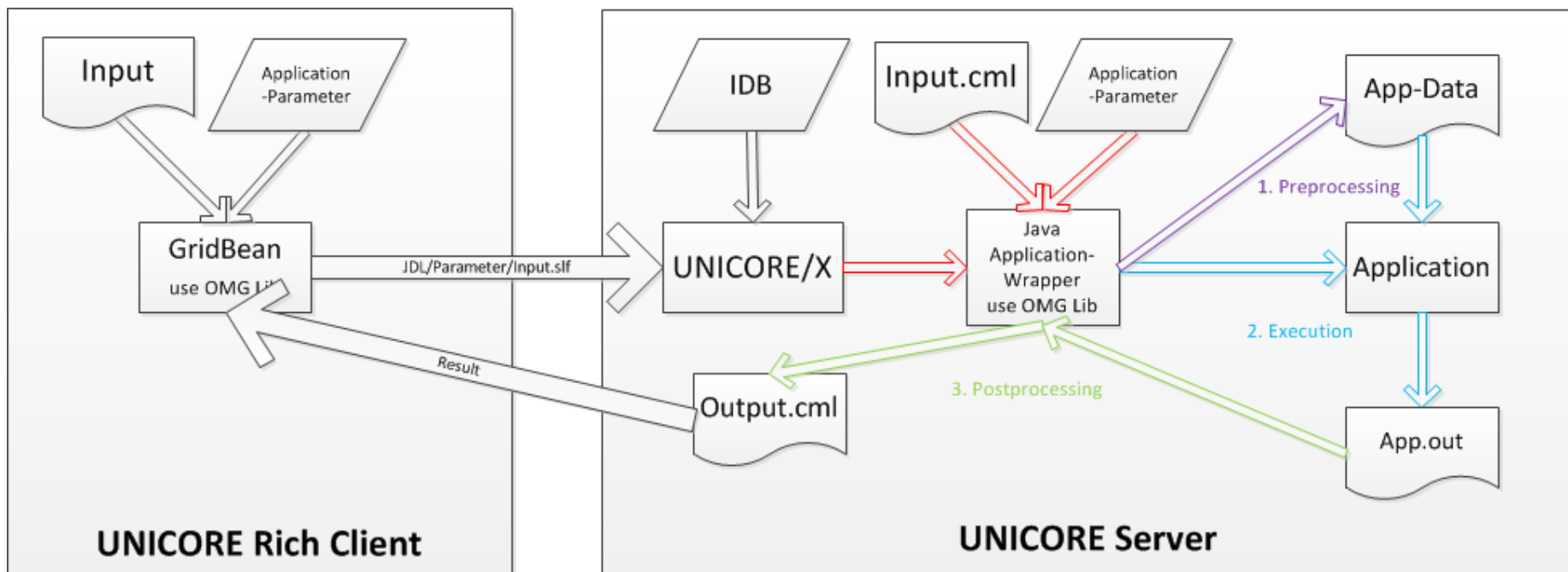
Newly developed GridBeans:

- 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.

- 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
 - Application Wrapper
- Further data models are being evaluated
 - MEMOPS (UML based) R. Fogh et al., J. Integr. Bioinf. 7, 123 (2010).
- License management
 - OpenSource and Commercial applications in simulations
 - VOMS with UNICORE (UVOS and SAML) is being evaluated



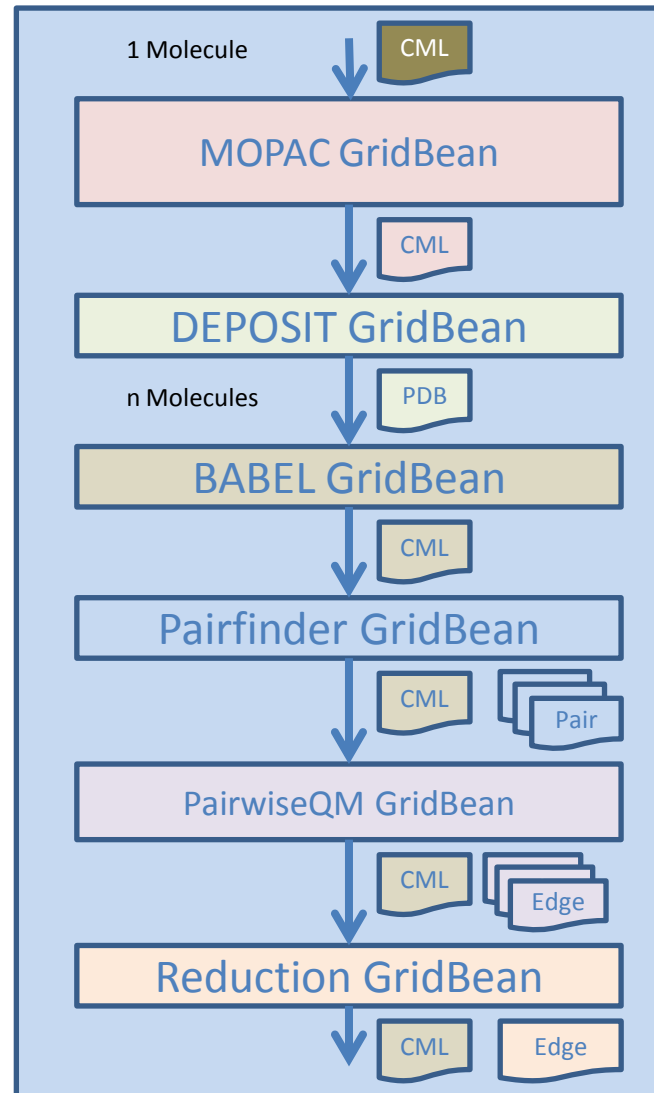
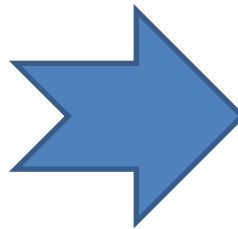
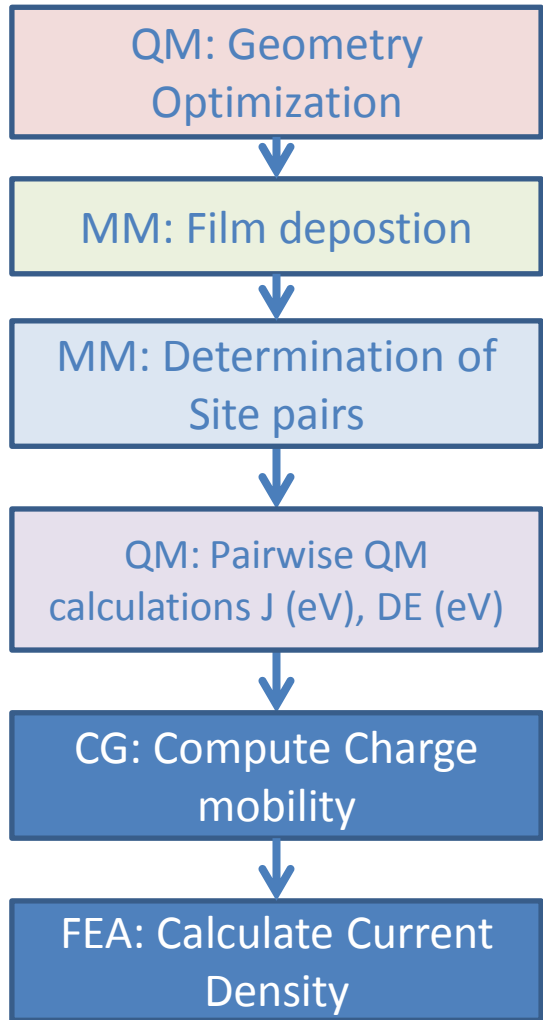
Application Wrapper Lifecycle

- 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



UNICORE Workflow

Demo

- 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)

Acknowledgments



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



- Partner projects, supporting infrastructures and software

