Multiscale Materials Modelling on High Performance Computer Architectures



MMM@HPC

Project coordination



Coordinator

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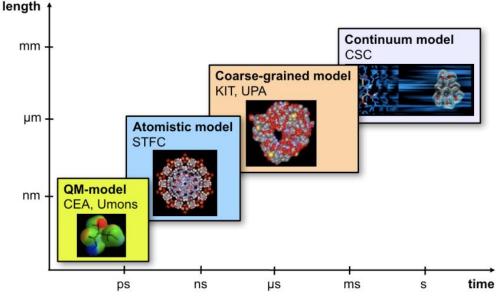




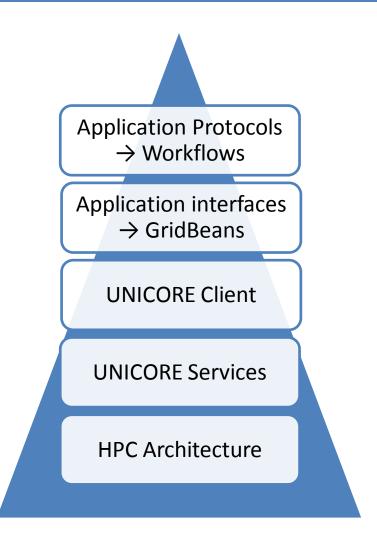
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Motivation, objectives and main concept





- Great progress in computational materials science (methods & HPC)
- However it still lacks:
 - Integration on different size and time scales to address real-life problems
 - Community and e-infrastructures with both industry and academia involvement



Application example

to simulate whole device



OLED Simulations (WP9 JRA2) QM/MM interface simple: no covalent bond breaking MM/KMC interface complex, but conceptually simple KMC/FEA interface necessary

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		

Partners



Participant	Acronym	Country
Karlsruhe Institute of Technology (Coordinator)	KIT	Germany
Commissariat à l'énergie atomique	CEA	France
CINECA Bologna	CINECA	Italy
CSC - IT Center for Science	CSC	Finland
Korea Institute of Science and Technology	KIST	Korea
Nokia Research Center	NOKIA	Finland
Sony	SONY	Germany
Science and Technology Facilities Council	STFC	UK
University of Mons	UMONS	Belgium
University of Patras	UPA	Greece

Overview of infrastructure



	Workflows and other Services UNICORE	 Diverse & modular Open & extendable Secure & stable
	Application Integration GridBeans	 Efficient, adaptable Maintainable & accessible Graphical User Interface
	Key Applications Industry	 OLEDs (MINOTOR/BASF) Li-Ion Batteries (CEA) Carbon Devices (Nokia) Molecular Electronics (Sony)
	Community Building PRACE	 Developers (Academics) Resources (HPC Providers) Users (Industry/SME/Academics)