MMM@HPC

Project coordination

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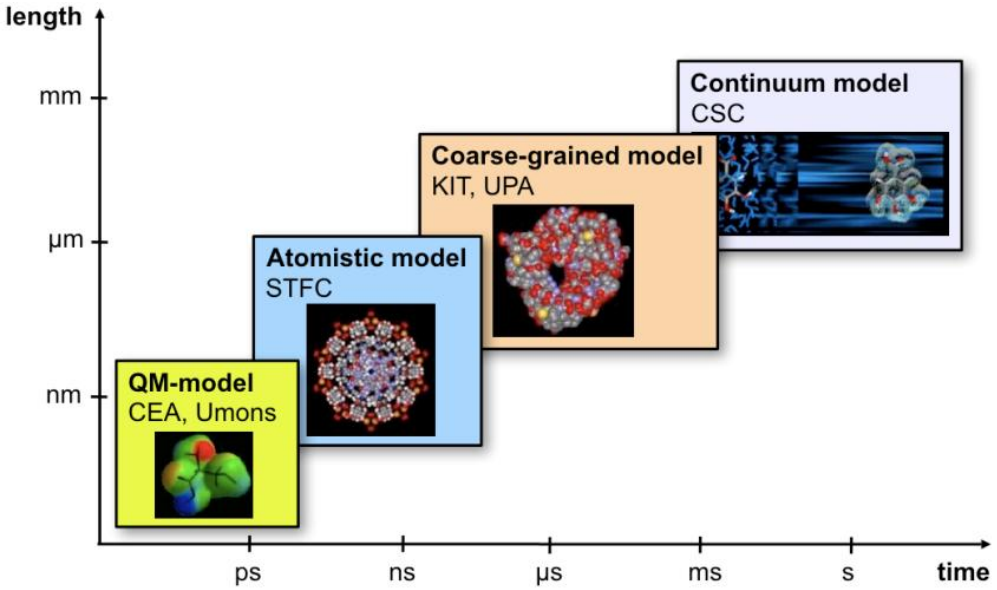
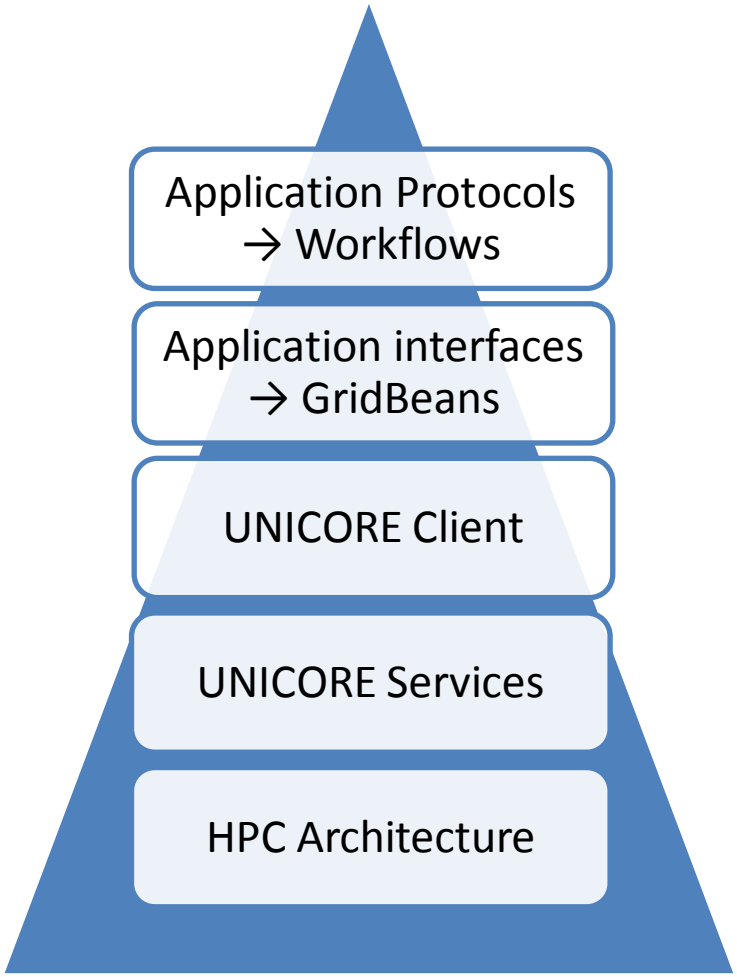
Motivation, objectives and main concept



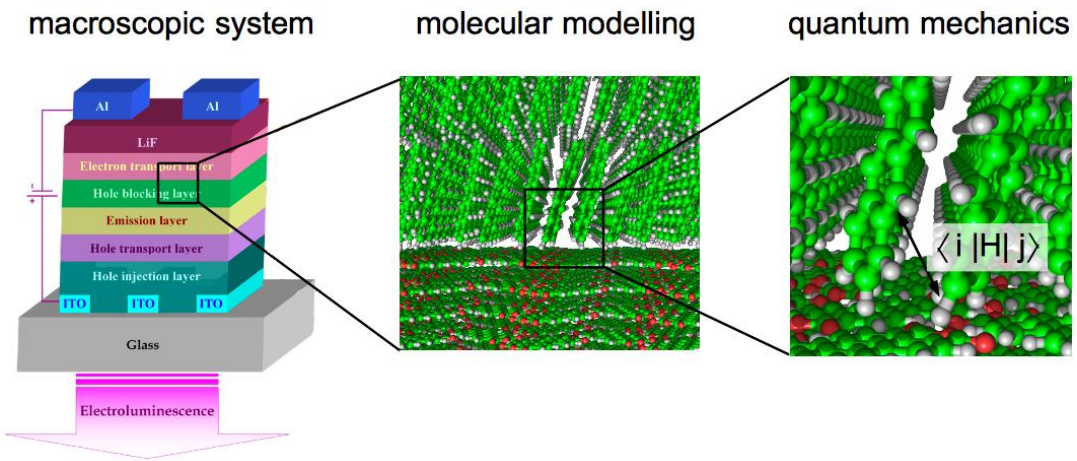


- Great progress in computational materials science (methods & HPC)
- However it still lacks:
  - Integration on different size and time scales to address real-life problems
  - Community and e-infrastructures with both industry and academia involvement

Application example

OLED Simulations (WP9 JRA2)

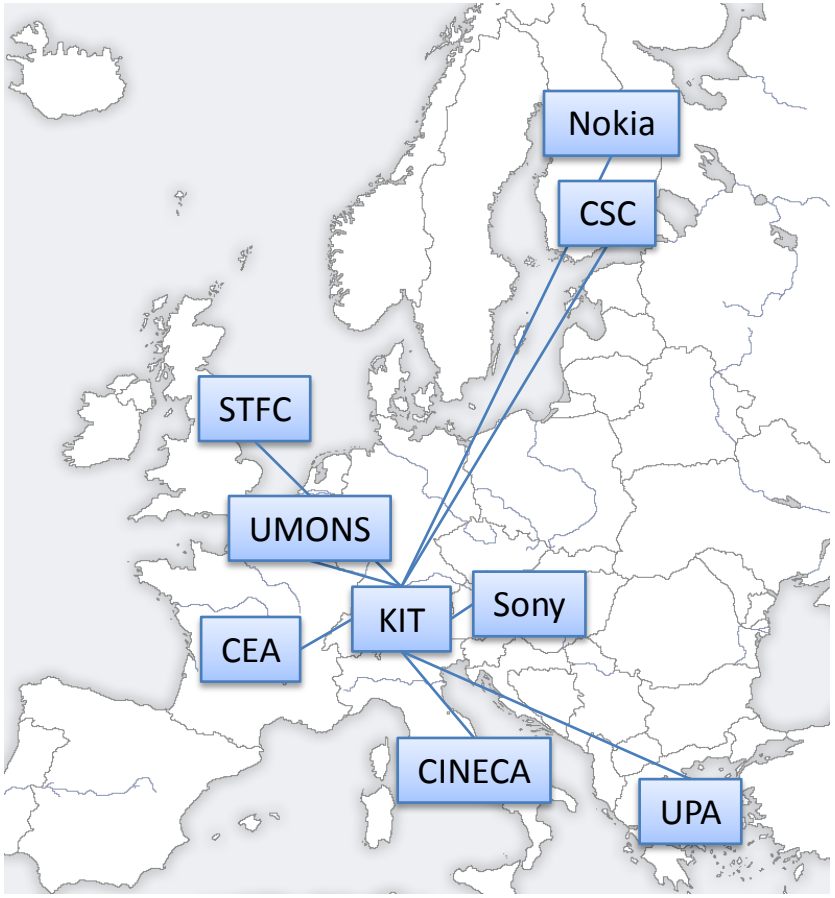
- QM/MM interface simple: no covalent bond breaking
- MM/KMC interface complex, but conceptually simple
- KMC/FEA interface necessary to simulate whole device



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		

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