Multiscale Materials Modelling on High Performance Computer Architectures

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on behalf of the MMM@HPC consortium

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Outline

Introduction

- Application area and importance
- Challenges
- Service Oriented Architecture
- Solution strategies

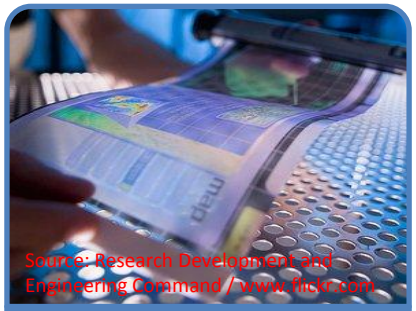
Implementation

- Implementation strategies
- Methodology – technologies used

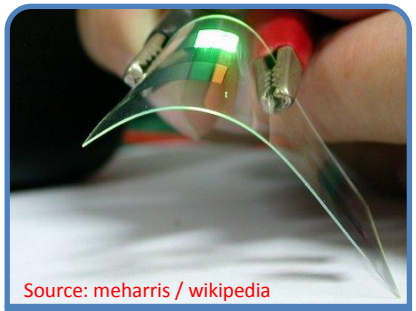
Discussion

- Key results: Proof of principle
- Conclusions and outlook

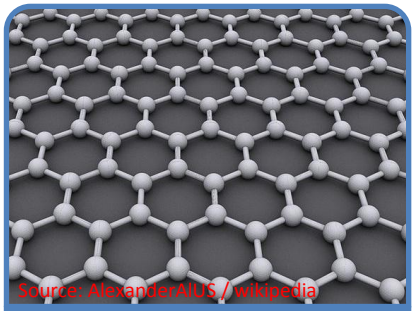
Application area and importance



Organic electronics



OLEDs

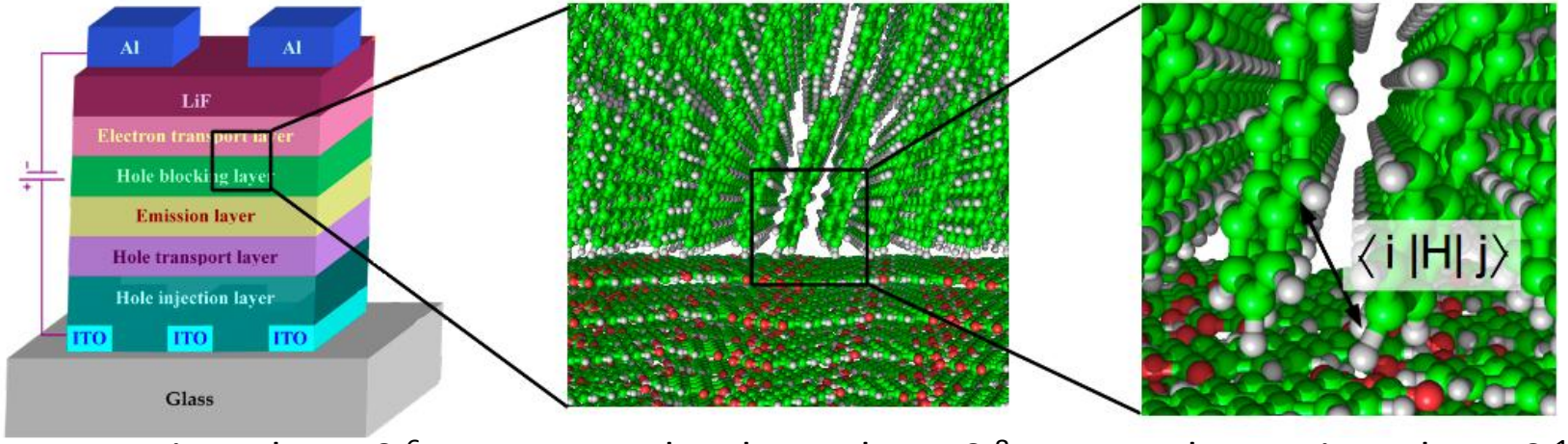


Carbon electronics

Li ion batteries

- Modelling and computer simulation essential
  - Reduce time-to-market
  - Reduce product development costs
  - Increase agility of industrial R&D
- Very complex models and environments for simulation
  - Accessible only for few experts
  - Low effectiveness and general applicability

Example: Multiscale modelling of OLEDs

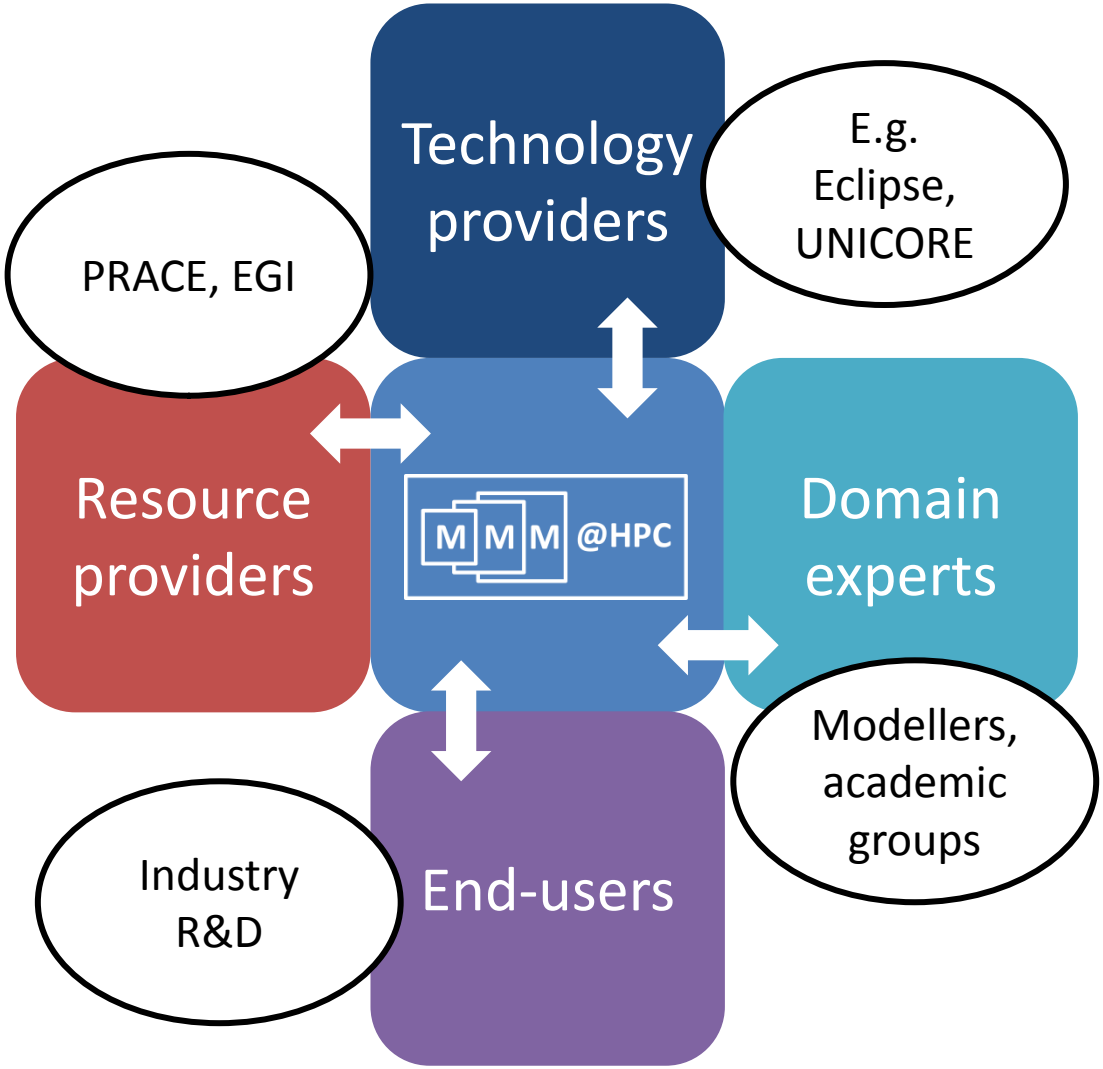


macroscopic scale ~ 10^{-6} m molecular scale ~ 10^{-8} m electronic scale ~ 10^{-10} m

Continuum model (FEA)	Coarse-grained model (CG)	Atomistic model (MM)	Quantum mechanical model (QM)
Elmer	ToFeT (KMC)	DEPOSIT	MOPAC
FEAP	End-bridging MC	DL_POLY	TURBOMOLE
	Transporter	LAMMPS	BigDFT

Structure optimization → Morphology generation → QM dipole calculations → Find donor-acceptor pairs → QM for DA pairs → Charge mobility calculation

Involved communities

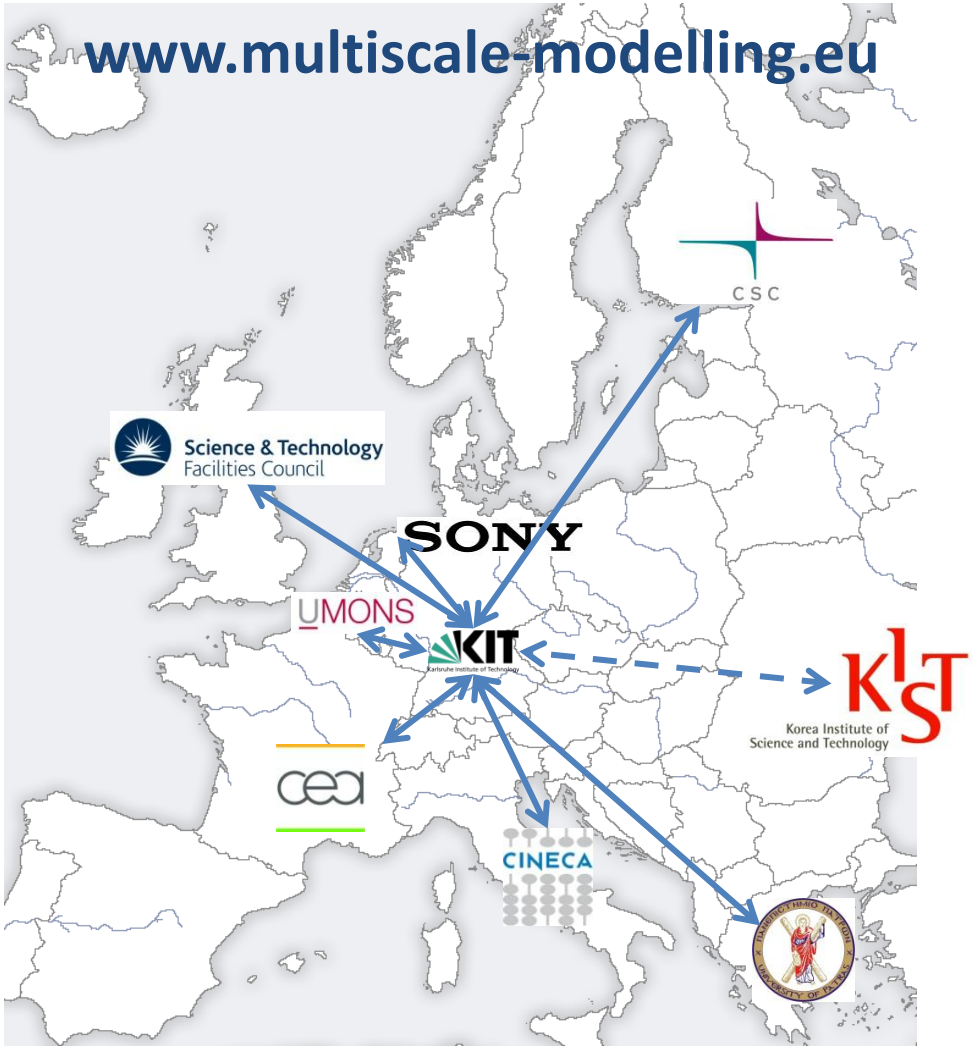


Provide basic services: GridBeans, Data modelling — **R&D**

Domain experts develop workflows and perform PoP simulations — **Early adoption**

End-users employ ready-to-go models as workflows — **Community building**

The MMM@HPC project



- HPC centres:
  CINECA, CSC, KIT and KIST (Korea)
- Domain experts:
  Uni Mons, CEA, CSC, STFC, Uni Patras, KIT
- End-users:
  CEA, SONY, KIT
- LoS from PRACE
- Spin-off Nanomatch

Challenges and proposed solution strategies

Computing capacity and capability

- High Performance Computing on PRACE resources
- High Throughput Computing on EGI resources

Security and reliability

- Grid Security Infrastructure
- UNICORE: x.509, SSL, SAML

License issues

- Open Source Licenses
- UNICORE: UVOS, SAML,VOMS

In this talk

Application integration and reusability

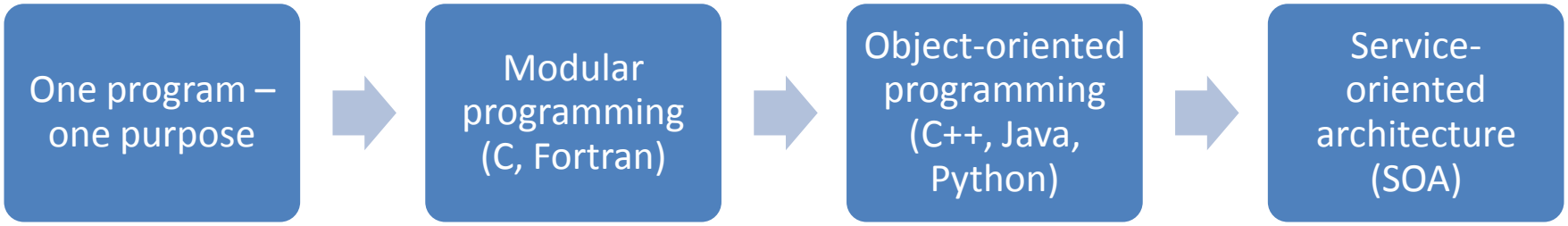
- Service Oriented Architecture (SOA)
- Application interfaces: GridBeans
- Application wrappers: OpenMolGRID
- Sequential modelling with UNICORE Workflows

Data complexity and interoperability

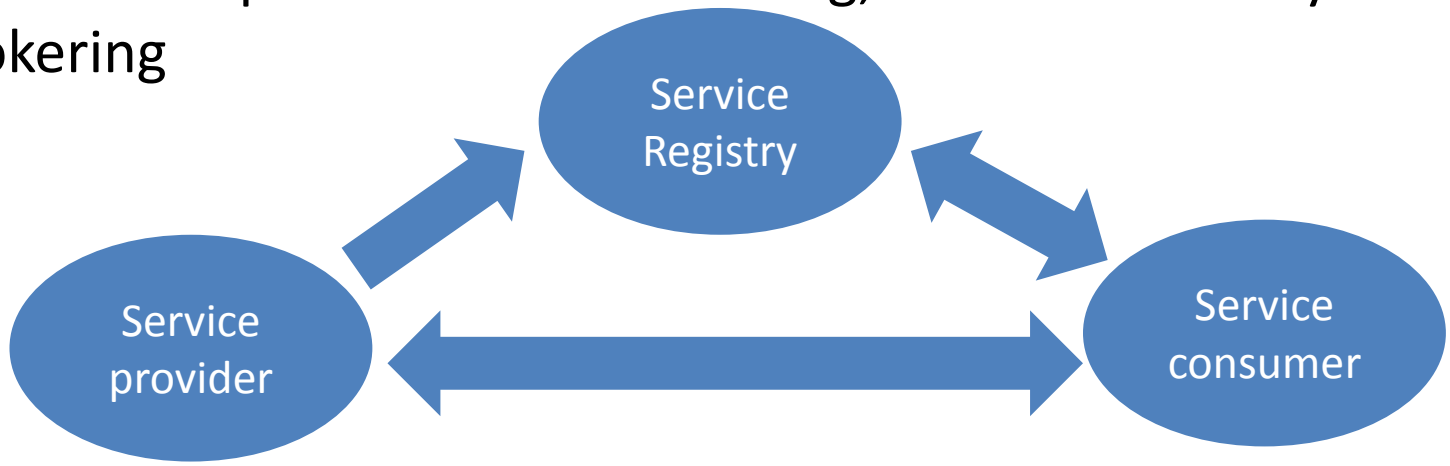
- Pre- post-processing with OpenMolGRID
- Dataflow Management
- Data-model based services

Short history of software …

- Evolution of programming paradigms



- Main SOA component: object-based service that allows distributed processing
- Further components: load balancing, service discovery and brokering



Service Oriented Architecture (SOA)

"A set of components which can be invoked, and whose interface descriptions can be published and discovered" (W3C)

- High reuse with no customization!
- Low effort to create new "ad hoc" composite applications from existing services
- Low effort for changing application

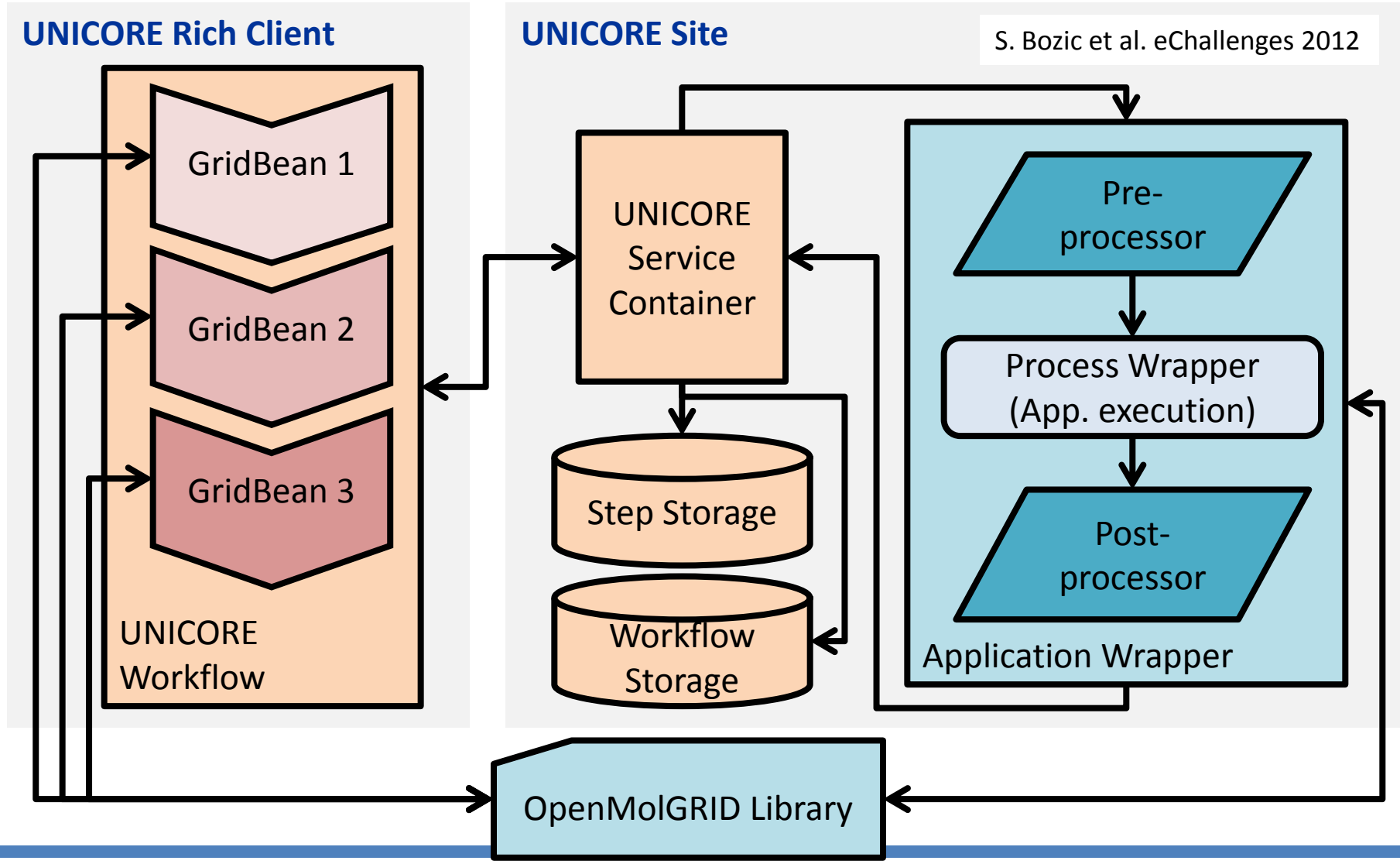
- SOA principles: **standardized service contract, loose coupling, abstraction, reusability, autonomy, statelessness, discoverability and composability**
- Standards for SOA implementation: Web Services
  - WSDL or WADL for describing the service
  - SOAP or REST for messaging

What is UNICORE?

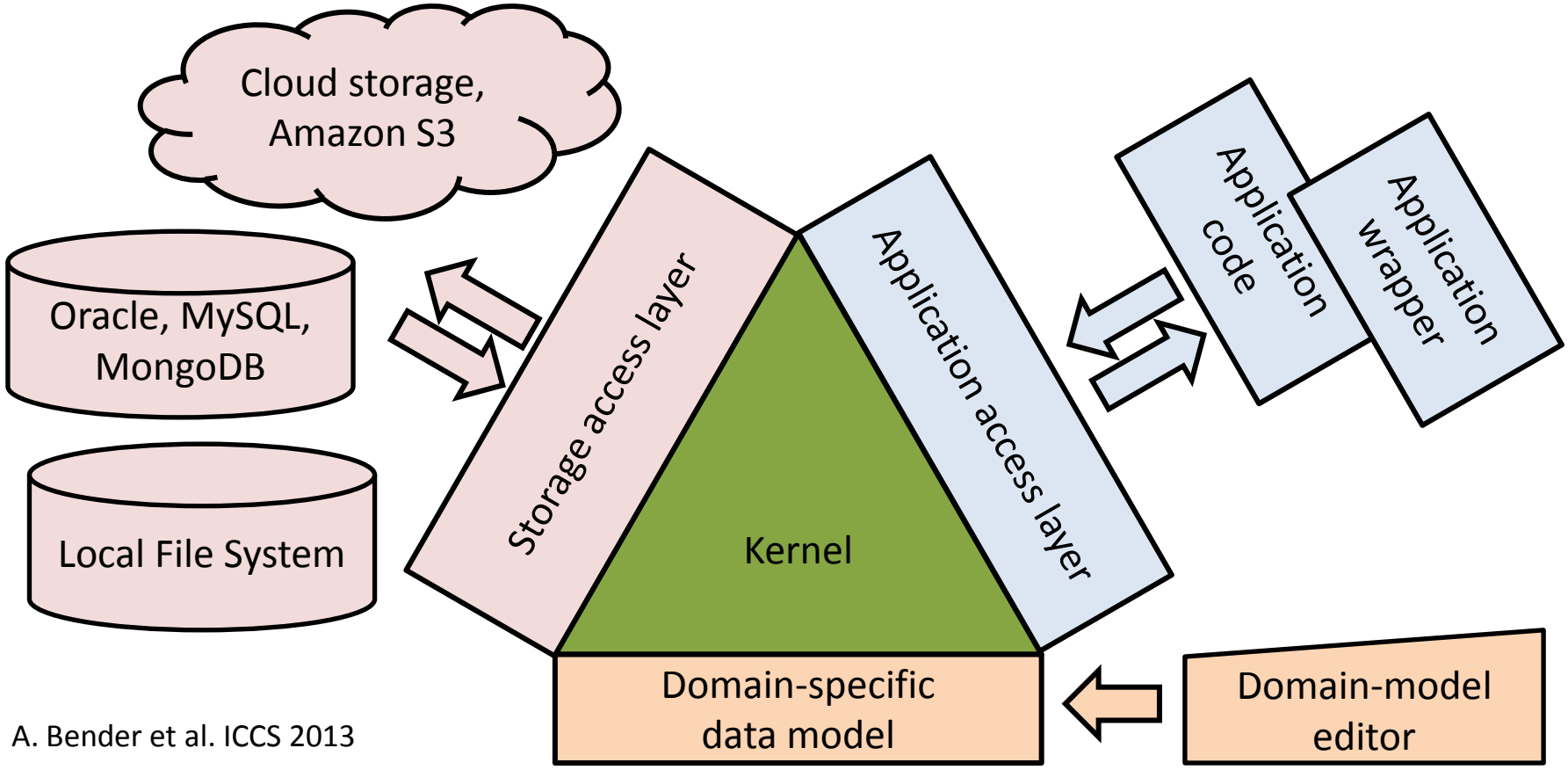
- UNICORE: UNiform Interface to COmputing REsources
- Grid computing technology supported by the European Middleware Initiative (EMI)
- Seamless, secure and intuitive access to distributed grid resources
- Used in daily production at numerous supercomputer centres worldwide - in PRACE (EU), in XSEDE (USA)
- Open source under BSD license
- Implements SOA using standards from the Open Grid Forum (OGF), W3C and OASIS

A. Streit et al., Annals of Telecommunications 65, 757 (2010)

Platform architecture



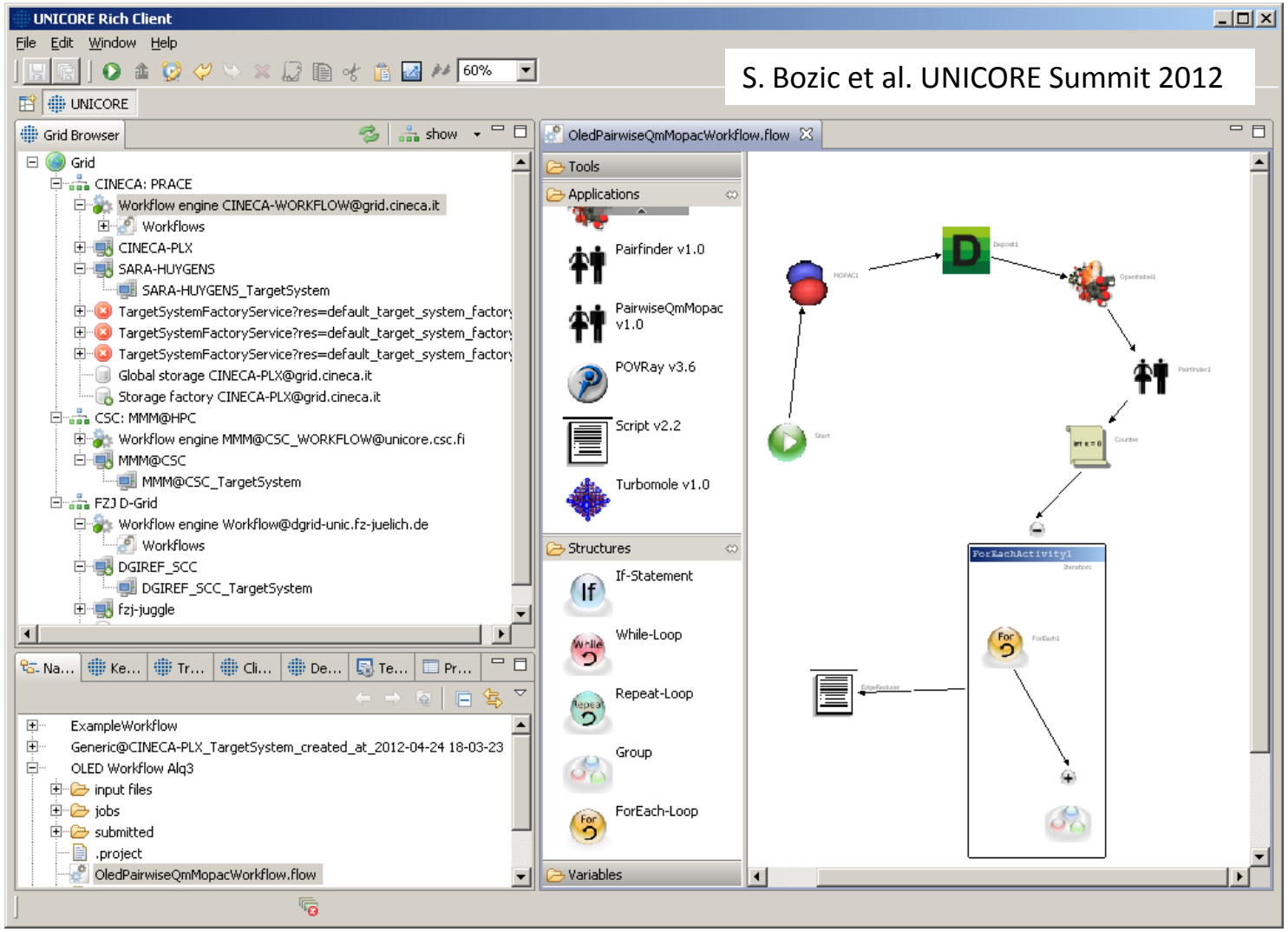
Data model driven approach



A. Bender et al. ICCS 2013

- Better than “yet another standard format”
- Separates storage, access and definition of data

Proof of principle: OLED workflow



S. Bozic et al. UNICORE Summit 2012

Community support

Developers of application interfaces

- Develop GridBeans, Application Wrappers
- Combine technology and single-domain expertise
- Setup and maintenance of tools and services

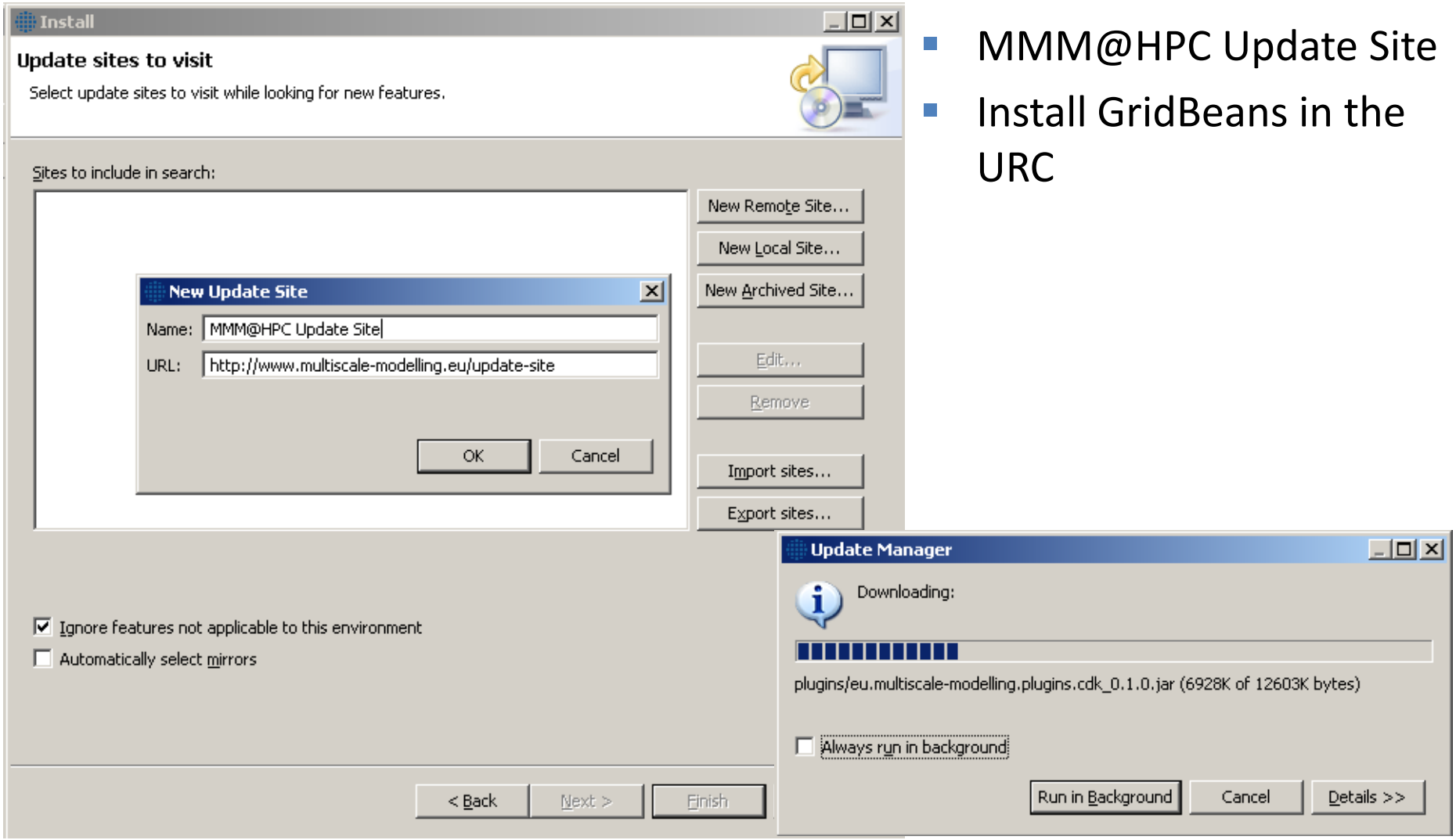
Workflow designers

- Construct workflow models for different applications
- Expertise with modelling in several application domains
- Assistance with integrating GridBeans

End-users

- Employ ready-to-go models as workflow simulations
- No technology or modelling expertise
- Help with using the models

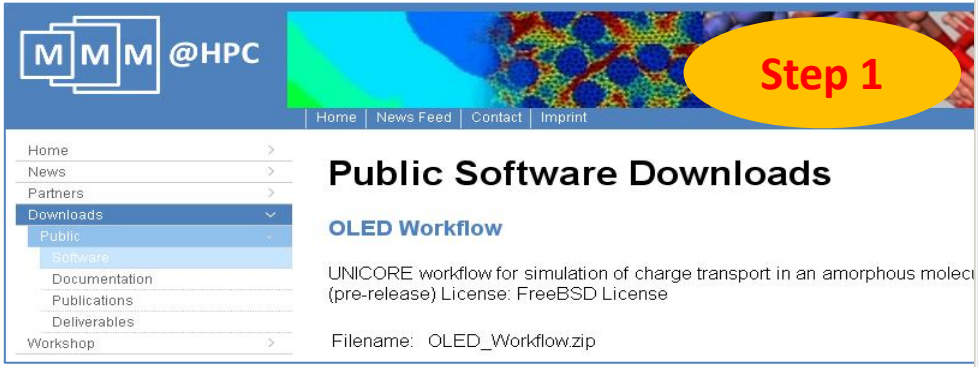
GridBean Deployment Service



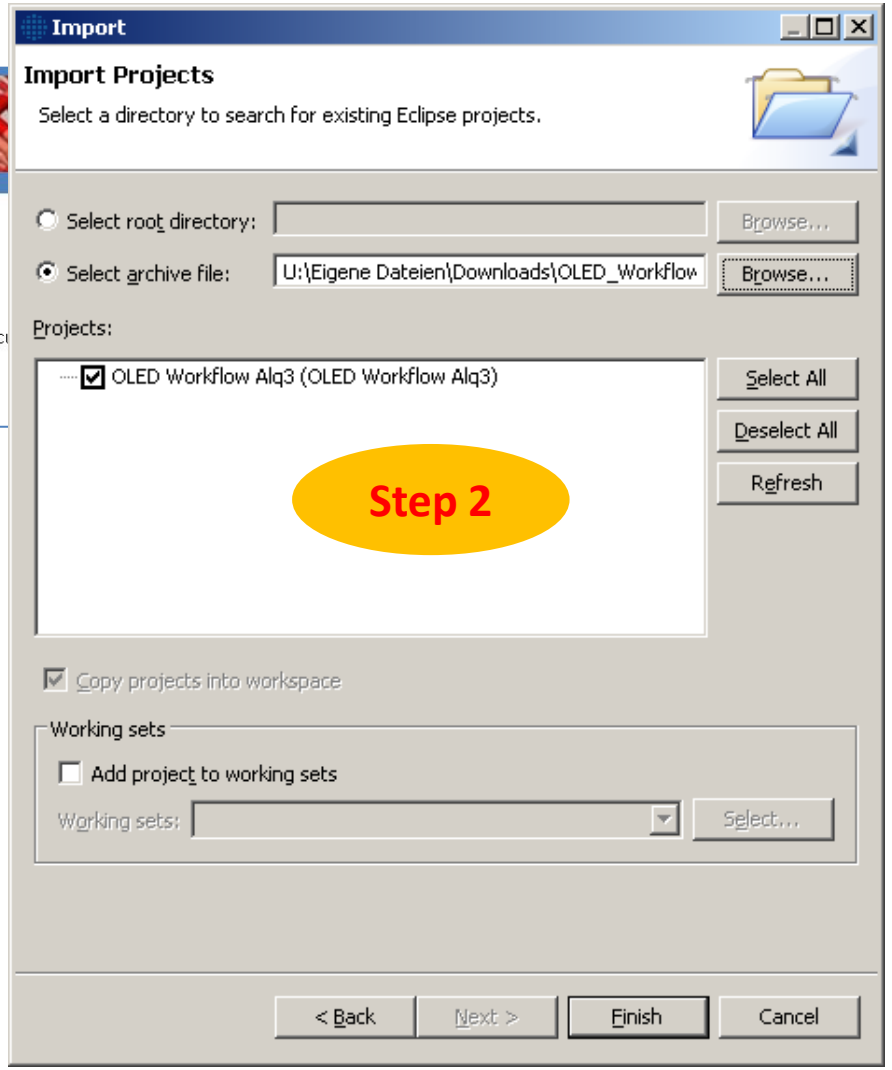
- MMM@HPC Update Site
- Install GridBeans in the URC

Workflow downloads and Live CD

www.multiscale-modelling.eu



Powered by UNICORE OPEN SOURCE



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- Funding from the EC

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- Partner projects, infrastructures, companies, and technology providers

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