

Key challenges of future market places: Identification, interoperability and licensing of software modules



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NANOMATCH GMBH
Eggenstein-Leopoldshafen

www.nanomatch.com

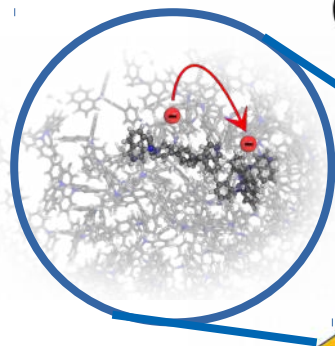
info@nanomatch.com

+49 721 608 26884

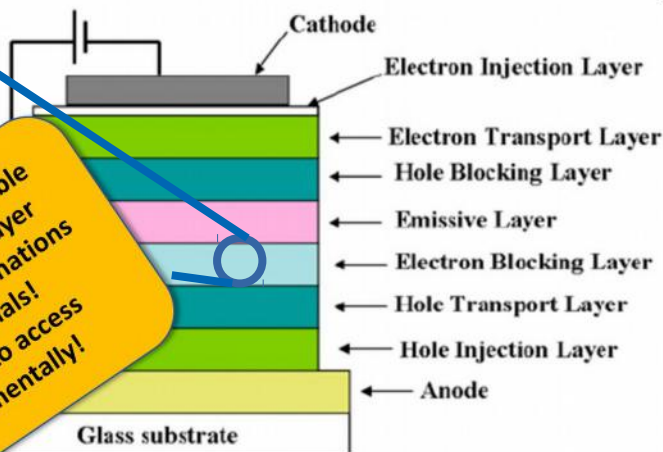


Challenges in Organic Electronics

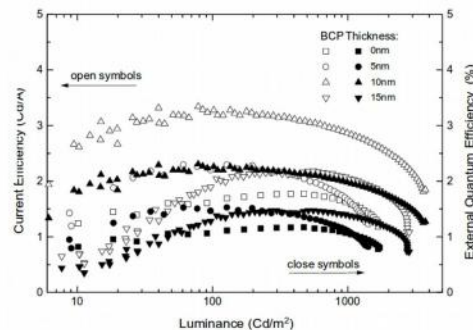
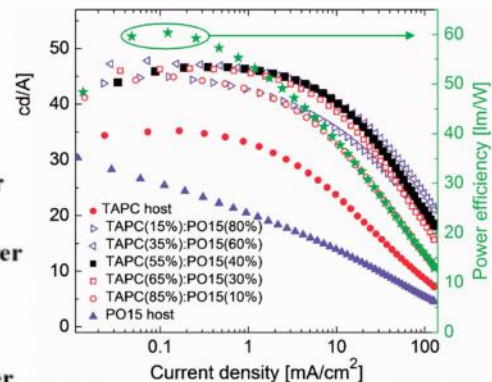
OLED challenges



Vast number of possible combinations of layer parametrs, combinations and materials!
Very hard to access experimentally!

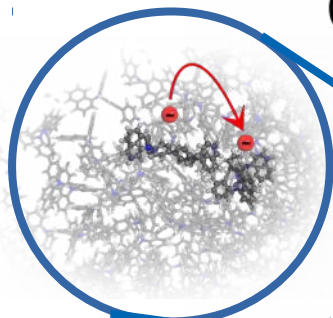


M. Ben Khalifa *et al.*, Organic Electronics 5 (2004) 187–198
 N. Chopra *et al.*, Appl. Phys. Lett. 97, 033304 (2010)
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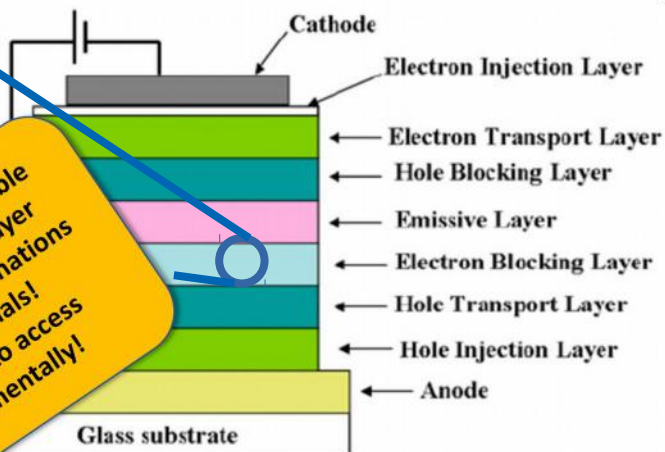


Challenges in Organic Electronics

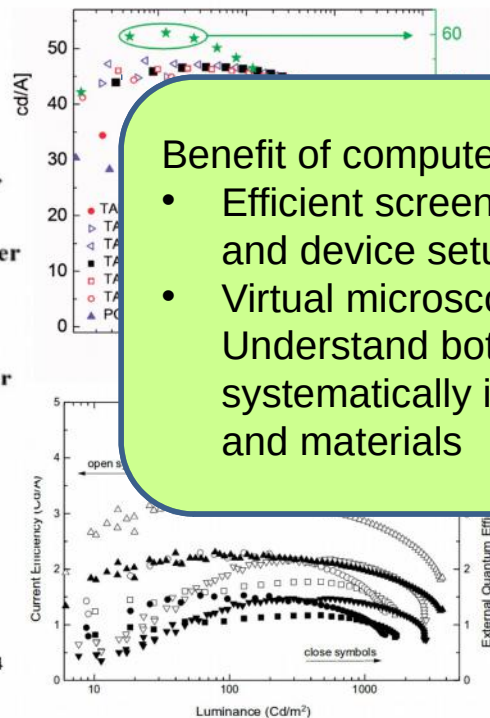
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Benefit of computer simulations:

- Efficient screening of materials and device setups
- Virtual microscope: Understand bottlenecks and systematically improve devices and materials



The multiscale simulation workflow for Organic Electronics

1. Single molecule parametrization (QM)

- Geometry optimization
- Customized force-fields

2. Generation of atomistic morphologies

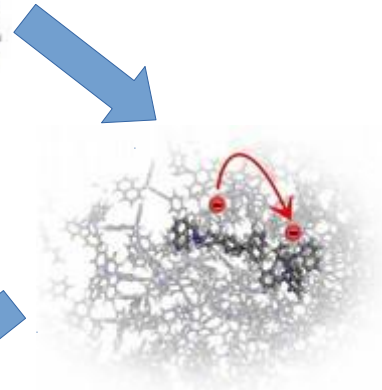
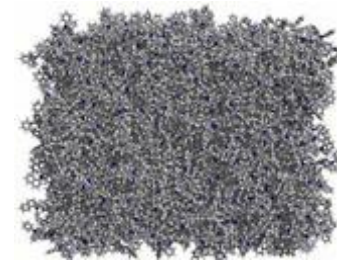
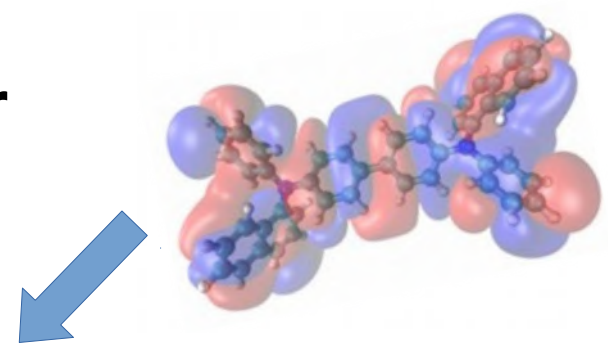
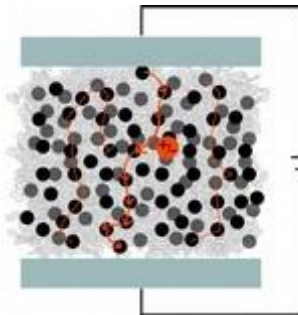
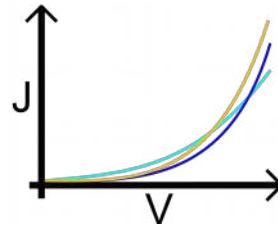
- Molecules parametrized on quantum mechanical level
- Simulation of physical vapor deposition

3. Calculation of charge hopping rates

- Full quantum mechanical electronic structure analysis
- Electronic couplings, reorganization and orbital energies

4. Charge transport simulations

- Time resolved charge carrier/exciton dynamics
- IVs, IQEs, carrier balance, quenching, ...



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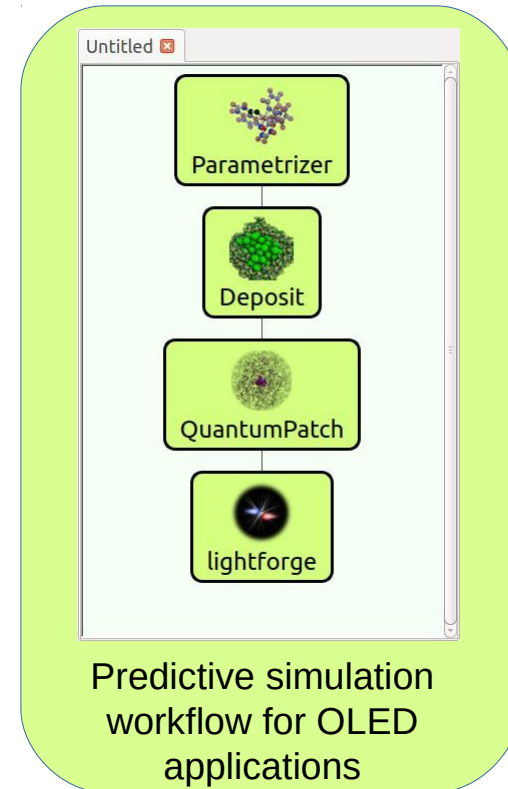
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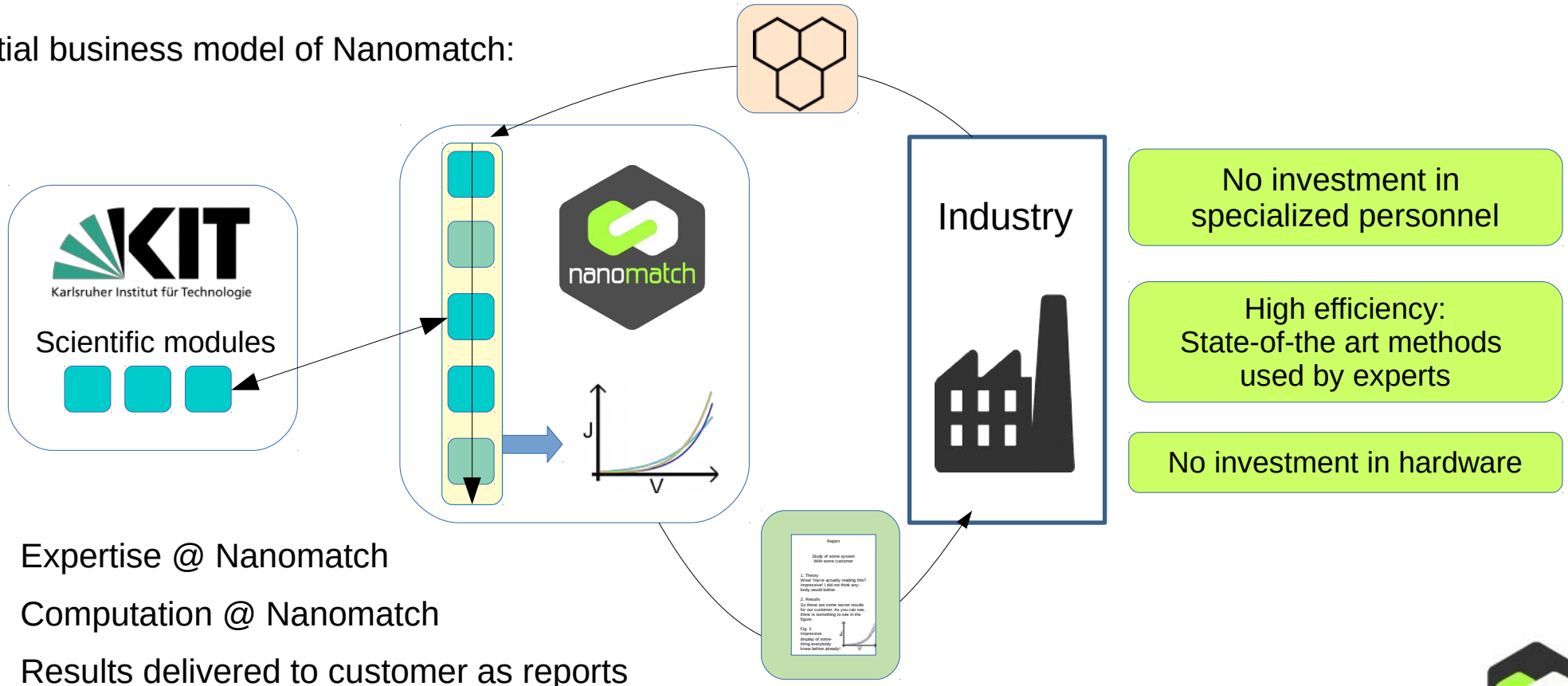
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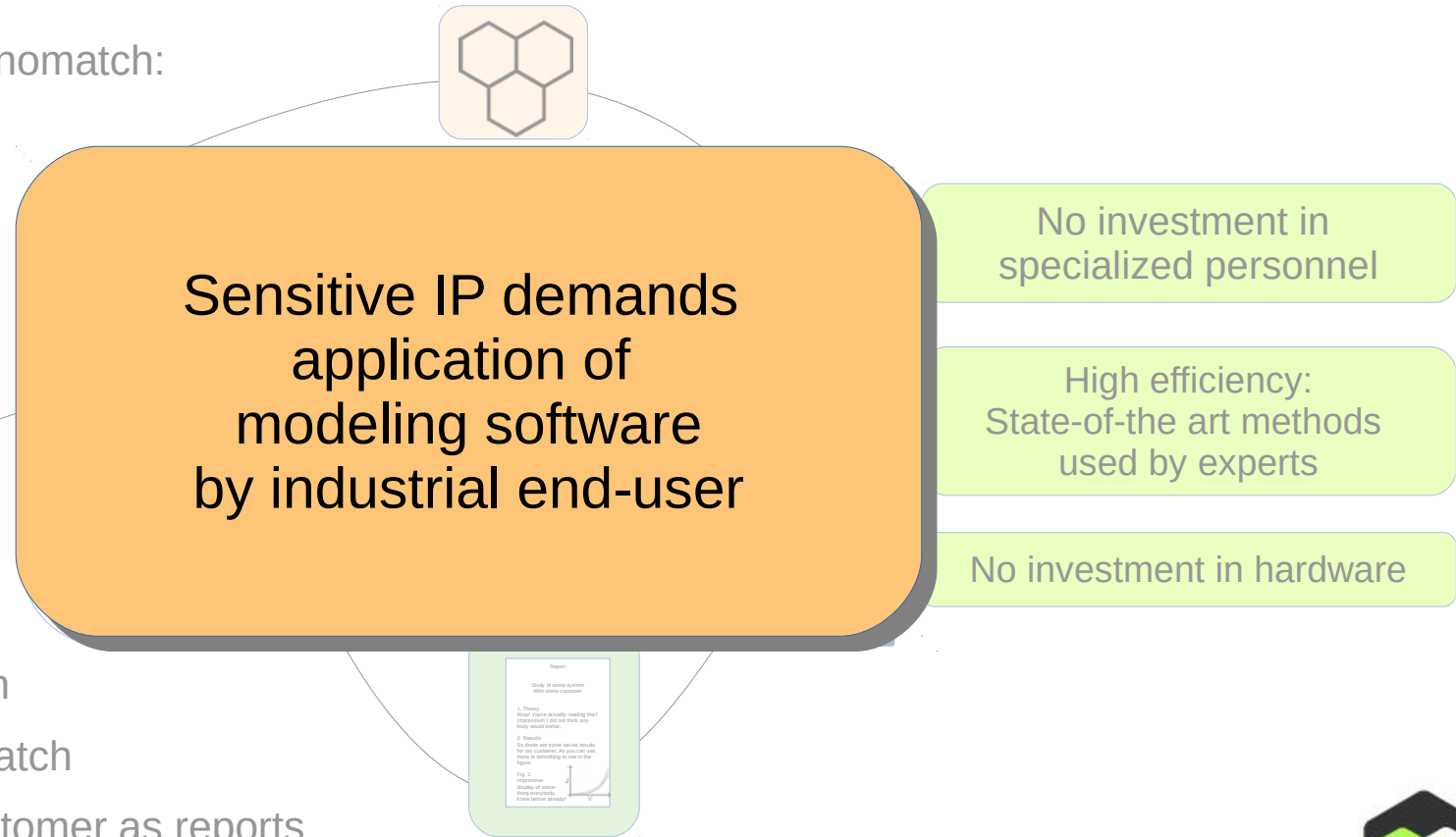
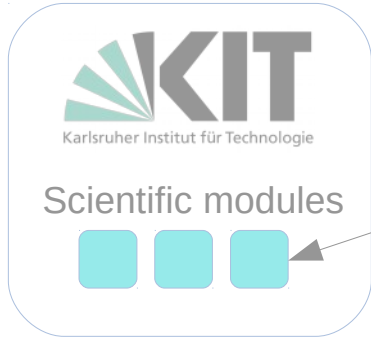
Evolution of a business model

Initial business model of Nanomatch:



Evolution of a business model

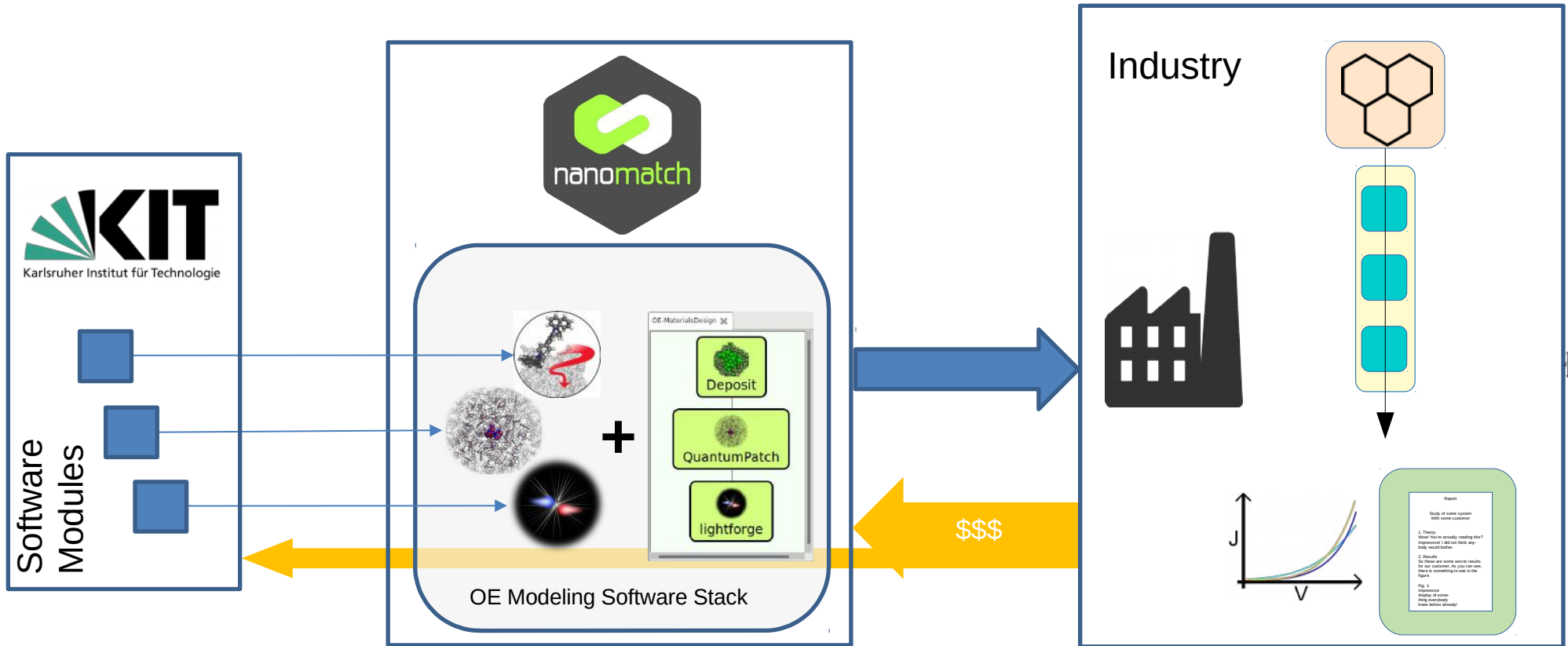
Initial business model of Nanomatch:



- Expertise @ Nanomatch
- Computation @ Nanomatch
- Results delivered to customer as reports



New business model: easy-to-use software solutions



Successful translation of modeling methods

What we learned:

- 1) Application by the industrial researcher is essential due to IP
- 2) Modeling needs to generate obvious added value within the company
 - Faster or more results than by experimental trial and error
 - Support experimental R&D with screening, understanding, etc.

Modeling software needs to ...

... be easy-to-use

... allow high
scalability and
reproducibility

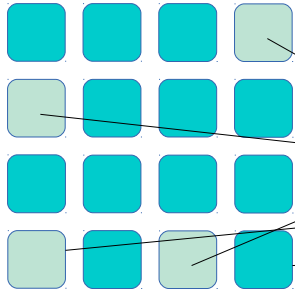
... be adaptable on a
case-to-case basis



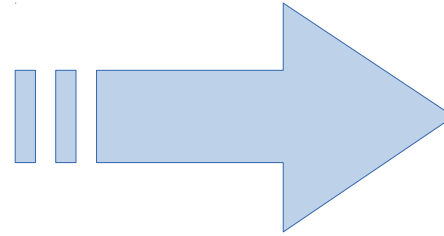
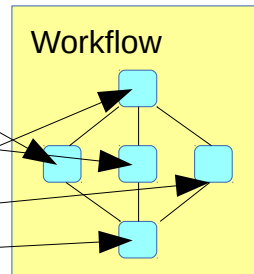
Translation of Materials CAD to Industry via a Market Place

Scientific Modules

EU ROMM



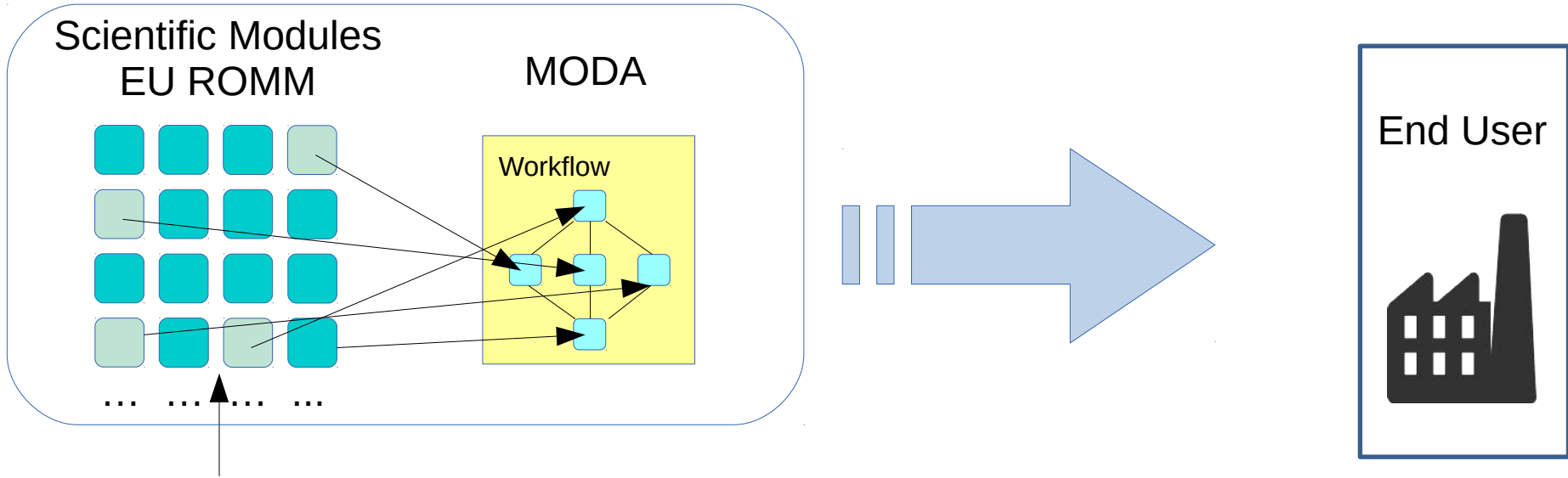
MODA



End User



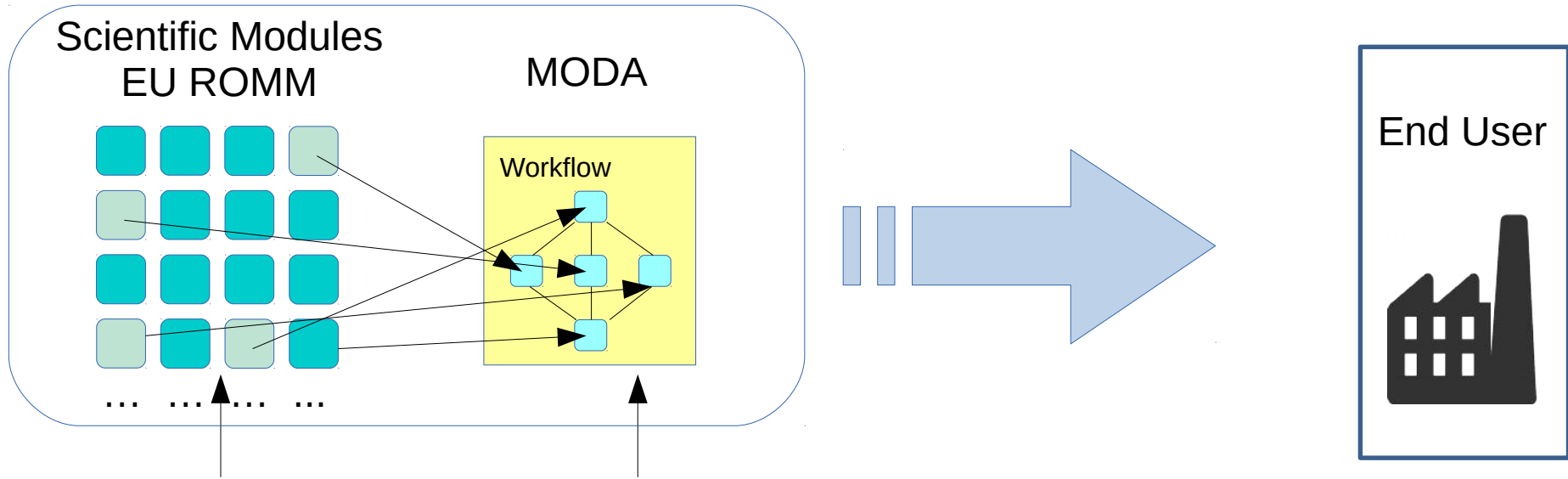
Translation of Materials CAD to Industry via a Market Place



Challenge #1:
Identify suitable software modules in the market place



Translation of Materials CAD to Industry via a Market Place

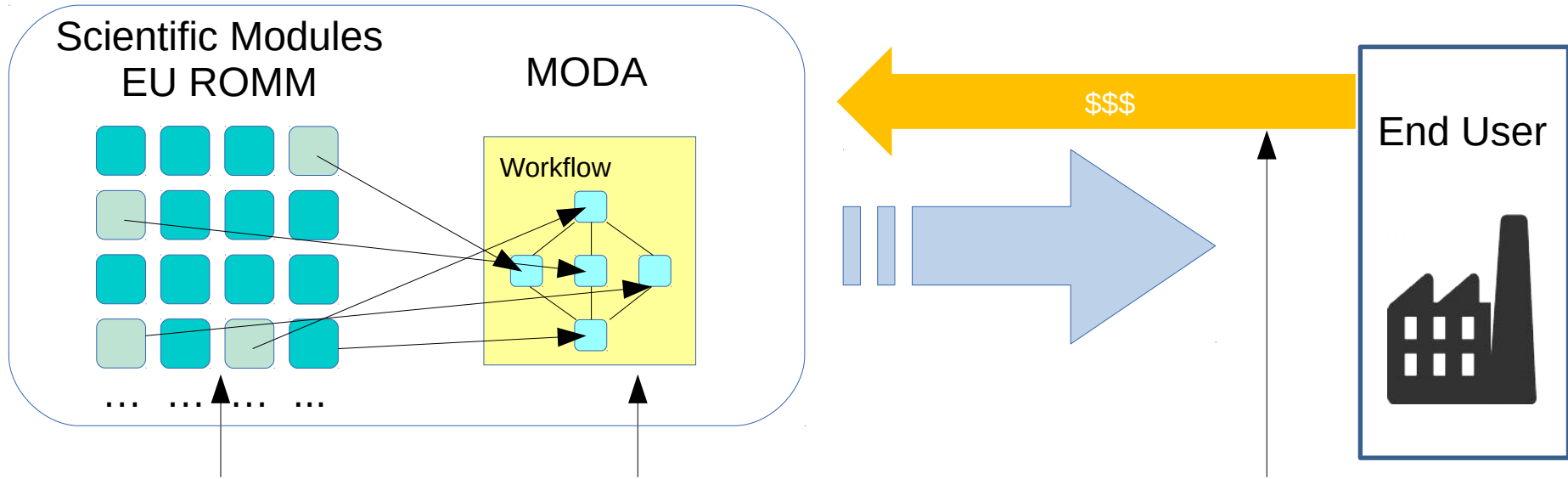


Challenge #1:
Identify suitable software
modules in the market place

Challenge #2:
Interoperability, combination
into workflows, execution on
remote resources
→ Rapid prototyping



Translation of Materials CAD to Industry via a Market Place



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Challenge #3:
Flexible licensing models
and billing processes



Challenge #1: Identification of suitable modules

Example: State-of-the-art “Translation“ in large enterprises:

- Technology scouts
 - Scientific background
 - Knowledge of company’s pains
- Identification of potential solutions via conferences, trade fairs, web
- Gathering details of modules from individual web pages or via personal discussion

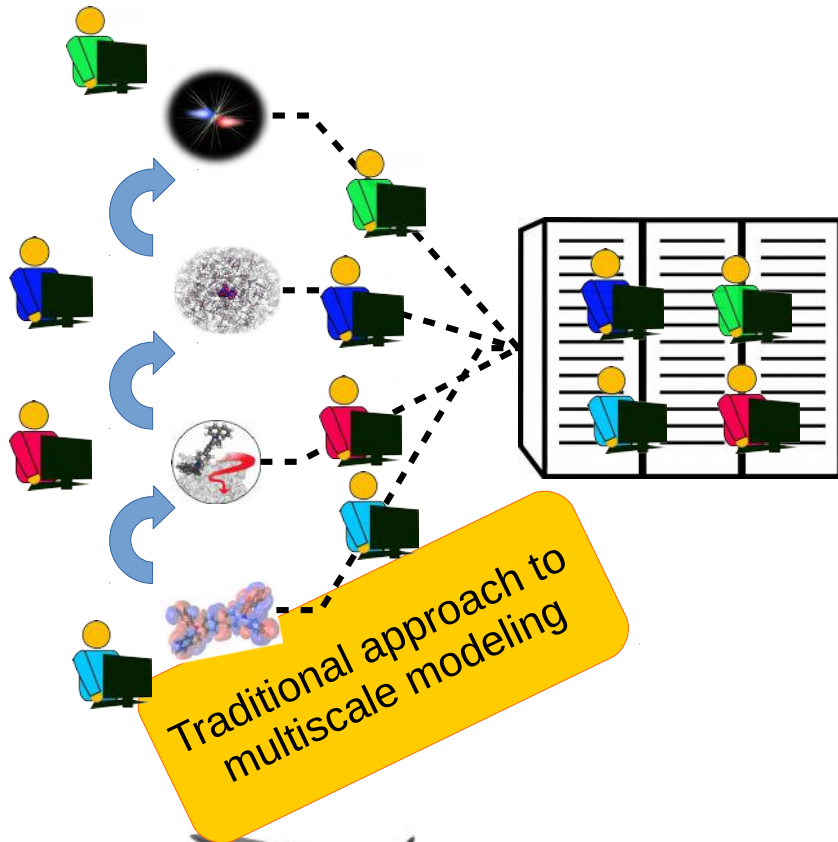
→ Slow, badly scaling process

Requirements for a market place

- 1) Clear definition of application domain
- 2) Clear definition of required input and resulting output **in a common language** (e. g. based on an ontology)
- 3) Modules should enable rapid prototyping
 - Quick identification of modules



Challenge #2: Module interoperability and rapid prototyping in a market place



Challenges in setting up multiscale workflows:

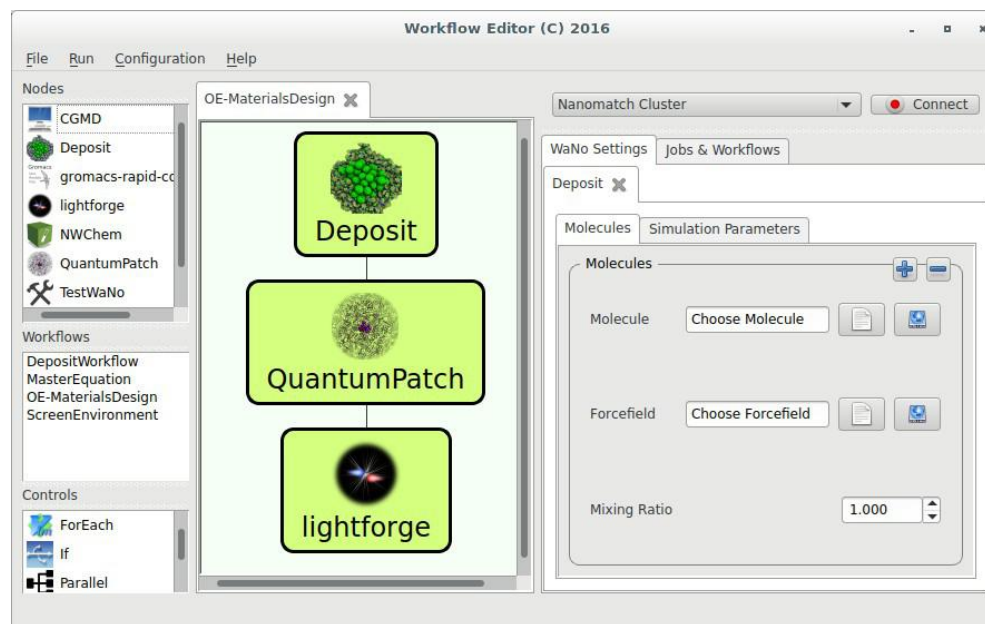
- **High level of complexity** of multiscale modeling: input preparation, data transfer to computing resources, job submission and monitoring, ...
- Data conversion between modules: No standardized language for module I/O limits **module interoperability**
 - Low level of scalability and reproducibility
 - **Technical realization** for interoperability and rapid prototyping required



Translation enabled by SimStack

... a generic workflow platform conquering complexity

- open to arbitrary software modules
- rapid prototyping: 30min to include new modules, 1 h to construct functional workflows
- maximal reusability and scalability
- module interoperability:
 - **Fully automated, file based data transfer between modules**
 - Schema based data transfer in development
 - Compatible with owl ontologies (e.g. EMMO, once developed)

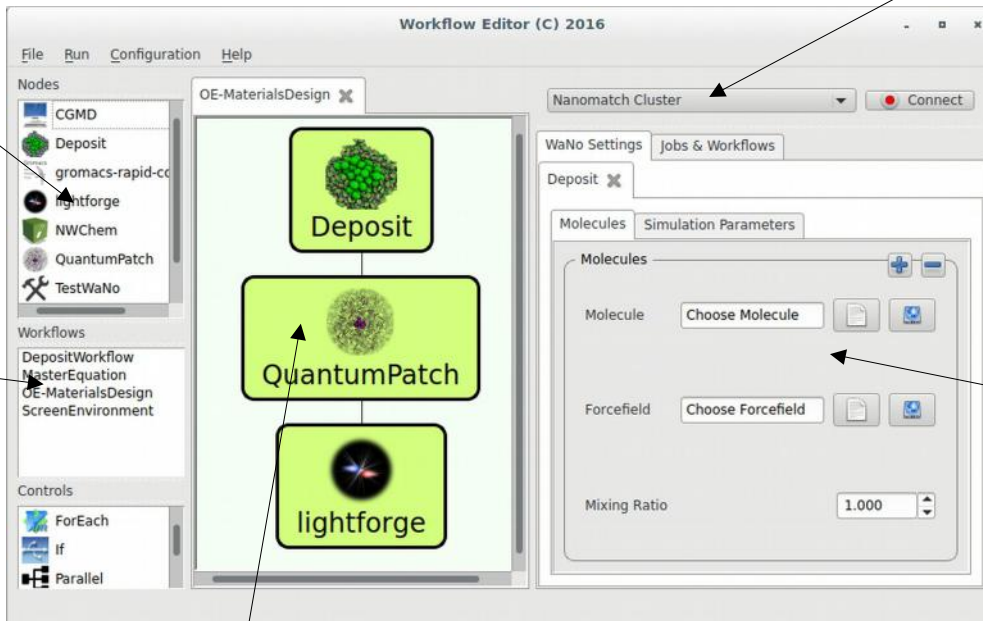


Translation enabled by SimStack

Embedded Scientific modules = „WaNos“

Connect to remote computational resources

Saved workflows for reproducible multiscale simulations



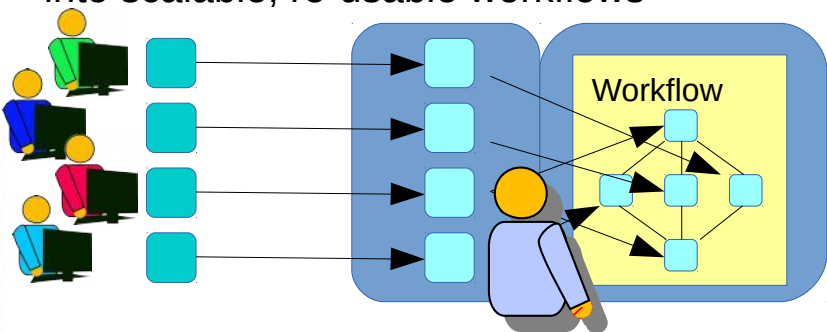
Define input files and parameters for each module

Construct a workflow by drag & drop

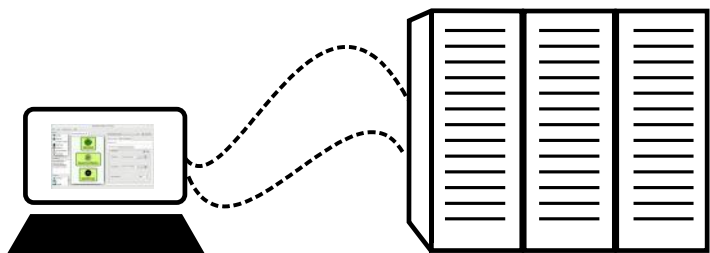


Challenge #2: Module interoperability and rapid prototyping with SimStack

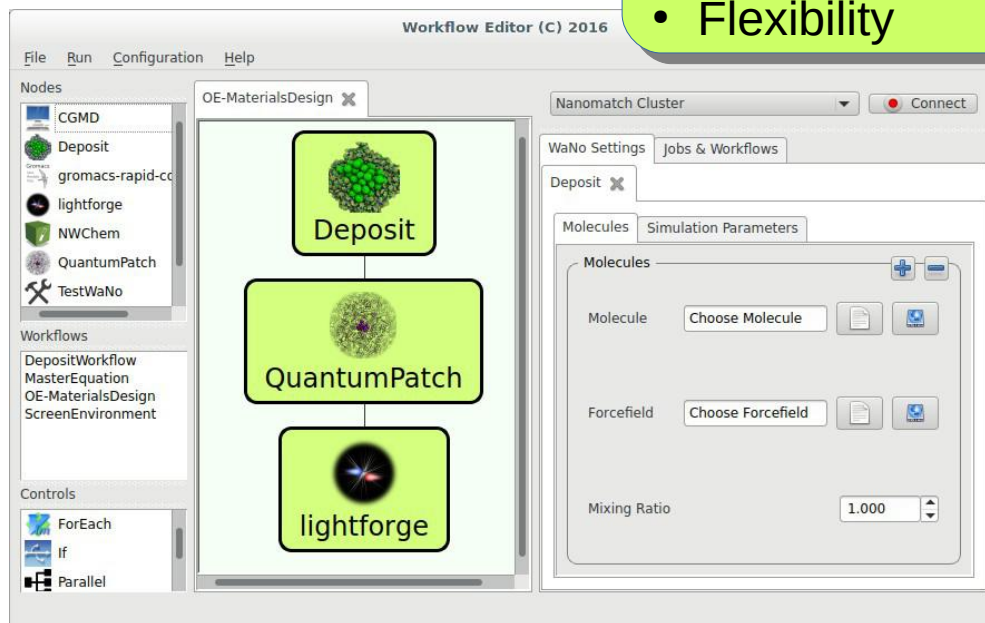
Efficient translation of modules from various sources into scalable, re-usable workflows



One-click execution of workflows on HPC facilities



- Scalability
- Throughput
- Reproducibility
- Flexibility



Challenge #3: Licensing of software modules

Case 1:

- Large enterprise
- Secluded research network
→ in-house HPC resources
- **Annual licensing & local license servers**

Case 2:

- SME
- Limited in-house resources
→ Cloud computing
- **Pay-per-use & license server**

Requirements for a market place

- 1) License models for both cloud-based and in-house computation
- 2) Unified license terms for modules (# cores, # users, annual vs. perpetual license, ...)
- 3) Unified billing via the market place:
Separate billing by each provider limits scalability



Towards successful translation

Challenge #1: Identification of suitable modules

- Unified definitions of application domain and I/O in a common language

Challenge #2: Module interoperability and rapid prototyping

- Technical realization of interoperability, e.g. with SimStack
- Enable rapid prototyping by conquering the complexity of multiscale modeling on HPC resources

Challenge #3: Licensing of software modules

- Flexible licensing and billing concepts for cloud and in-house simulations

