



ENTHOUGHT

Building a materials modelling marketplace:
challenges for SME's and research organisations

Cambridge, Nov 8 2017

Quick intro

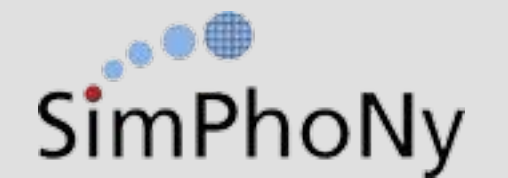
- Enthought is a leader in Scientific Computing, Scientific Digital Transformation, AI, Simulation, & Modeling
- Industries: IIoT, Oil & Gas, Bio-science, Semiconductor, and Polymers
- Enthought is engineering and science focused. They build solutions that accelerate research and engineering analysis.



Quick intro



- Involved in European projects:
 - A. Symphony (FP7) - 2012: **Sim**ulation framework for multi-scale **phenomena** in micro- and **nanosystems**
 - B. FORCE (Horizon 2020) - 2017: Formulations and Computational Engineering
 - C. MarketPlace (Horizon 2020) - 2018: Materials Modeling Marketplace for Increased Industrial Innovation



Building a material modelling marketplace!

*“Materials Modelling Marketplaces are digitalised systems which integrate a range of tangible and intangible components to support innovation based on materials modelling. Marketplaces utilise **web-based platforms** in order to link various materials modeling activities including repositories, modelling workflows, simulation tools, expertise, training, translators, etc.*

*Existing and emerging repositories and materials modeling marketplaces call for additional actions ensuring **coherency and efficiency of information management and exchange**. In particular linking various marketplaces and data repositories requires interoperability to facilitate **common unified access and retrieval of data and information**.*

*There is also a need for efficient and lean **management and curation of data and knowledge** across different platforms. These in turn pose additional requirements for **deep interoperability that go beyond models, reaching out into data and information management in general**.”*

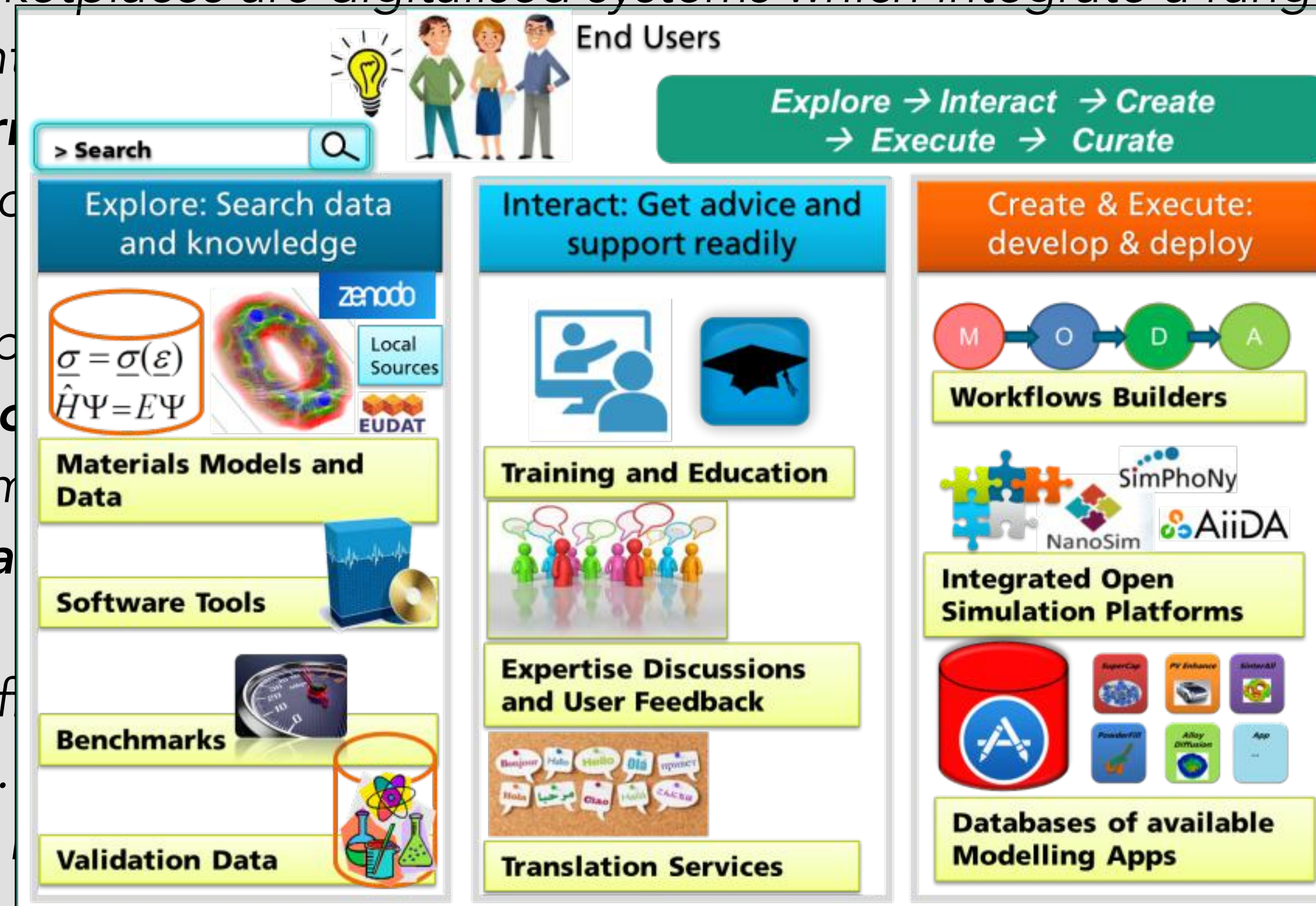
Discussion notes from EMMC IntOP Workshop, Nov 7-8, 201

Building a material modelling marketplace!

“Materials Modelling Marketplaces are digitalised systems which integrate a range of tangible and intangible components and utilise **web-based platforms**, data repositories, modelling workflows

Existing and emerging repositories and actions ensuring **coherence** and **interoperability**, in particular linking various materials data to **common unified access** and

There is also a need for effective communication across different platforms. **Tools and services that go beyond models,**



Marketplaces including etc.

Additional change. In order to facilitate

knowledge interoperability in general.”

Disciplines **17 partners** IntOP Workshop, Nov 7-8, 201

Challenge 1: interoperability

- Code interoperability
- Data interoperability
- Model/workflow interoperability
- Marketplaces interoperability

Challenge 2: people and skills

- Domains/skills required to build a marketplace: **(avoiding any scientific skills)** ontologies, meta-programming, distributed computing and storage, security, numerical methods, web frameworks, online payment processing, scalability and deployment, data integrity, big data processing, API design, CS best practice, ...
- Profiles: PhD students and employees in SME's focused on materials modelling

Challenge 3: legal frameworks

- Managing intellectual property
- Ownership of data
- Compliance: European GDPR, US export restrictions, ...
- Impacts on the technical details of running a secure marketplace: encryption, configuration management, managing security of customer models and workflows

Challenge 4: delivering

- Focus on delivering value (not features or technology)!
 - Importance of the original business use case
- Release process: documentation and training for integrators , backward compatibility, cost of integration, maintenance cost and versioning
- Technology choice: web frameworks, provisioning, cloud infrastructure, etc.
 - Use of industry standards! - Don't reinvent the wheel
 - Dependency on other (open projects) —> Governance requirements

Conclusion

- I've deliberately ignored the scientific aspects. They are probably as challenging as the 4 challenges mentioned in this presentation!
- Business plans for marketplace projects will be a key!
- Technical decisions and quality of deliveries made by project members will have major impact on the success too!
- Position of the EMMC as an umbrella organisation for the open libraries/components/standards/initiatives? + a mechanism of funding for those components?

Q&A