

Silvia Chiacchiera (UKRI/STFC)



VIMMP

VIRTUAL MATERIALS
MARKETPLACE

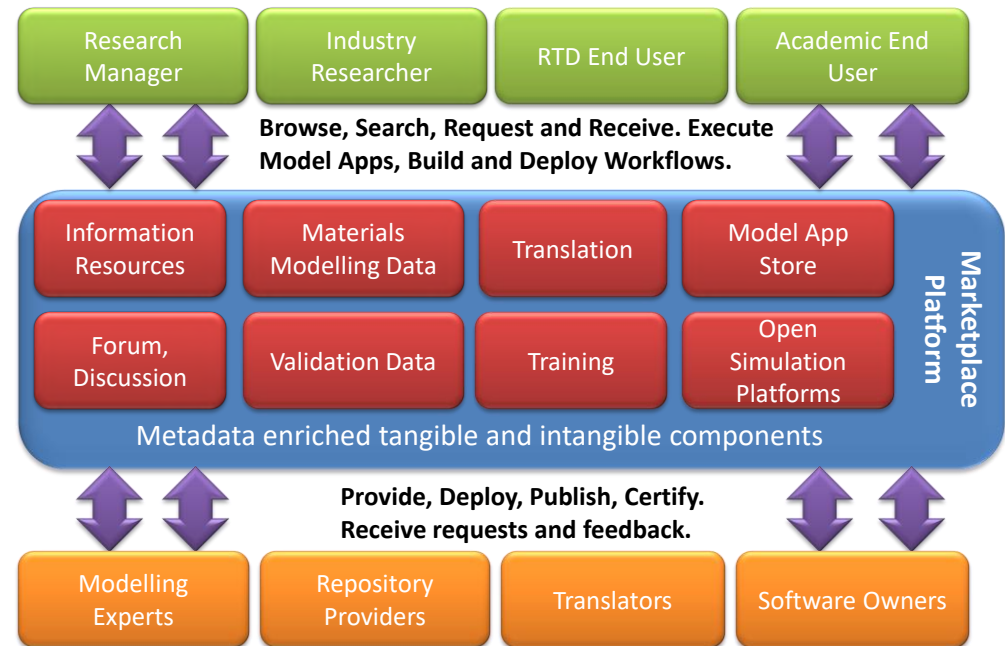
Materials Ontology Workshop

Brussels, 29th June 2018

VIMMP – Virtual Materials Marketplace (GA 760907)

VIMMP Marketplace Concept: serving all stakeholders and **facilitating the exchange between providers and consumers** of products and services.

The VIMMP will provide End User Interfaces to Information, Resources, Discussion Forum, Databases and repositories, Translation and Training services, Validated Models and Modelling Apps, the ability to utilise Open Simulation Platforms to build and deploy workflows and to execute materials modelling Apps via cloud-based computing resources.



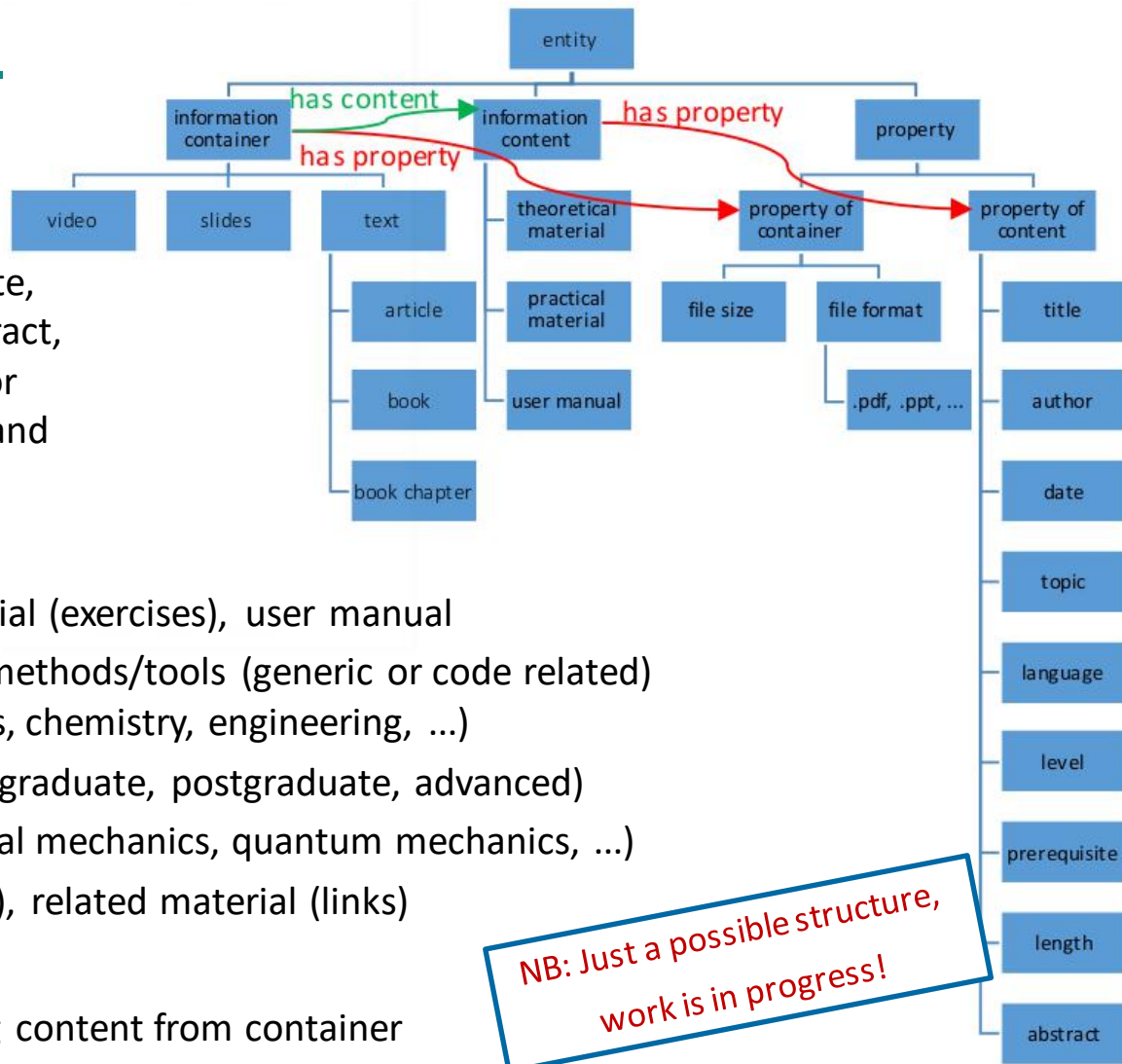
UKRI/STFC (Science and Technology Facilities Council)

Scientific Computing Department, Daresbury Laboratory, UK

- **Software** development / **Research** in collaboration with academia and industry.
- Lead of WP1 (Metadata, Interoperability design and standards) in **VIMMP**.
- **STFC** people in VIMMP: Ilian Todorov, Michael Seaton, Silvia Chiacchiera, Martin Horsch [from July 2018]
- Within VIMMP we will: extend MODA, develop ontologies for the each branch of the VIMMP marketplace components, i.e.:
 - Training ontology, Expert ontology, Translation ontology, Verification, validation and benchmark ontology, etc...
- **Status**: collecting and organizing keywords, reviewing existing relevant ontologies

Training material

- **Basic information:** title, author (name, affiliation, webpage), date, language, length/duration, abstract, type (text, e.g. article, chapter, or book, video, slides), file format and size
- **Specific information**
 - theoretical, practical material (exercises), user manual
 - topic and area: numerical methods/tools (generic or code related) or material science (physics, chemistry, engineering, ...)
 - level (general public, undergraduate, postgraduate, advanced)
 - prerequisites (e.g., statistical mechanics, quantum mechanics, ...)
 - part of a collection (yes/no), related material (links)



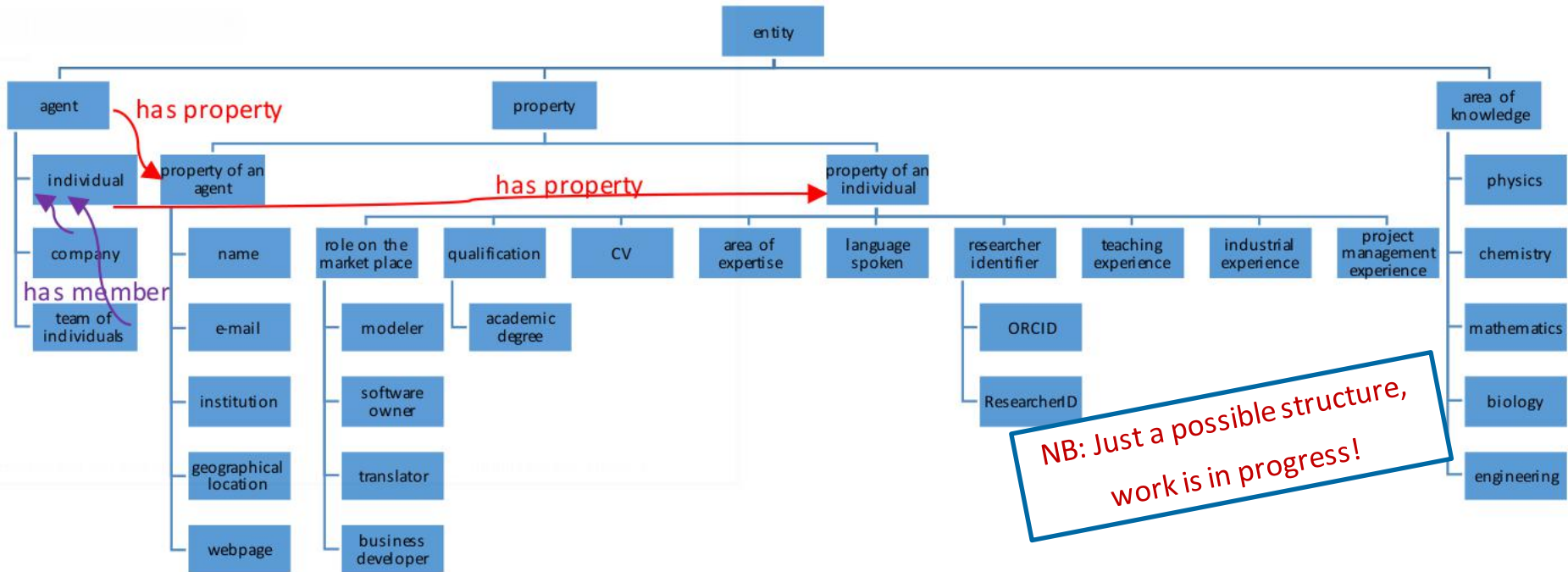
On the right: a taxonomy, separating content from container

Note: A formal characterization of a document is also possible, using the BFO-based ontology IAO (Information Artifact Ontology, <https://github.com/information-artifact-ontology/IAO>) or the UNDO (United Nations System Document Ontology, <https://w3id.org/un/ontology/undo>)

Expert

- **Basic information:** type (individual, team, company), name, institution, geographical location, e-mail, web-page
- **Information on individuals:**
 - role on the market place: modeler, software owner, translator, business developer, ...
 - qualification; highest education degree: level (bachelor, master, PhD), area (Physics, Chemistry, Engineering, Computer Science, Mathematics), institution
 - area of expertise (could be different), sub-area
 - link to a CV
 - industrial/teaching/project management experience (yes/no)
 - indicators (ORCID, ResearcherID,...)
 - Languages
- **Translation (from industrial problem to modelling)**
 - Material: phase, pure/mixture, key feature (suspension, polymer, ...)
 - Phenomena (rheology, optical properties, electrical properties, ...)
 - Properties (viscosity, refraction index, electrical conductivity, ...)

Expert (2)



Above: a taxonomy, separating the agents acting on the market place from their properties.

We are currently reviewing existing relevant ontologies for branches such as: areas of knowledge, classification of materials and chemical entities, workflows.

We will use Protégé as an ontology editor.

Verification, validation and benchmarking

- Verification of software codes:
 - Fundamental tests: time integration (e.g., is energy conserved?), electrostatics, ...
 - Comparisons with exact results (when possible)
 - Comparisons with independent numerical results (same method or others)
 - Existence of a repository, Continuous Integration (CI) of changes
 - Test suite (number of tests, code coverage)
- Benchmarking of software codes:
 - Performance, scaling (weak and strong)
 - Ranges of usage (max number of particles, ...)
- Validation of model parameters: parameter provider, model, target property, experimental value, reference publication

Note: For some categories we may provide **workflows** in the market place

Caveat: With numerical methods, often difficult to disentangle the aspects tested (method, model and code)



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