Ontokin: Building a chemistry knowledge base and services for bespoke chemical models in the process industry

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CMCL Innovations

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CMCL Innovations

CMCL: Computational Modelling Cambridge Ltd.

Mission

Delivering digital engineering software and solutions to industry and academia

Business model

Software | Consulting | Training

Market segments

Powertrains & fuels | Energy & chemicals

Simulation and design software supplier to industry and academia

Over a decade in innovative R&D and advanced engineering services

SME with an organically growing experienced team

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Context:

- We specialise in digital engineering workflows that combine physico-chemical simulation with advanced statistical algorithms
- Ontology engineering forms the basic foundation (“the zeroth step”) in order to harness the data semantics, model interoperability, knowledge base and decision making
- **Use case:** Leveraging Ontokin, a chemical kinetics ontology developed and represented in OWL to offer on-demand chemical models and simulation services

Why Ontokin?

- Problems with the current approach
  - Fragmentation/heterogeneity of data sources and tools in industry
  - Inconsistencies in data, loss of information and logical errors
  - An example: Inconsistencies in chemical models
    - Discrepancies (up to 100 kJ/mol) in enthalpies of formation of same species in different models
    - Many orders of magnitude discrepancy in the rates of the same chemical reactions in different models

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- Ontokin: Formal, explicit specification of a shared conceptualisation
- Ontology representation: Ontokin, formal reasoner-ready using one of the following syntax: OWL/XML, RDF/XML, TTL
- Ontokin→ Chemical knowledge base → Effective decision making

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CAM.CREATE C4T Cambridge Centre for Carbon Reduction in Chemical Technology

The Power of Ontology

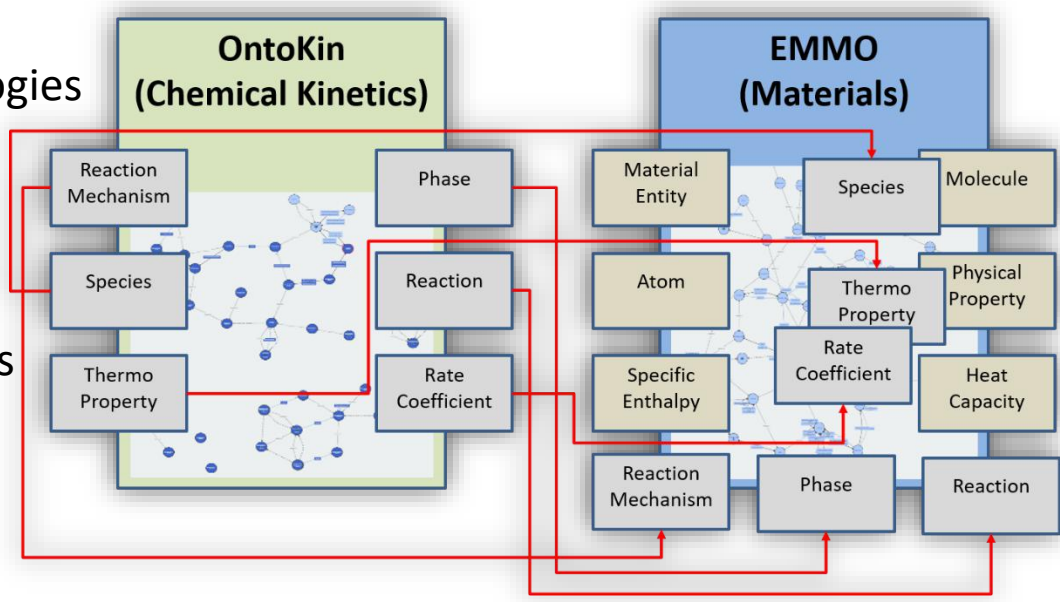
- Ontology sits on top of data to ensure a common meaning
  - Integrate and query heterogeneous resources within and across domains
  - Natural language processing of unstructured literature
  - Data sources enriched with meta-data

- Simplifies software engineering
  - Easy development of services and re-use of exiting resources
  - Advanced query and automation of tasks

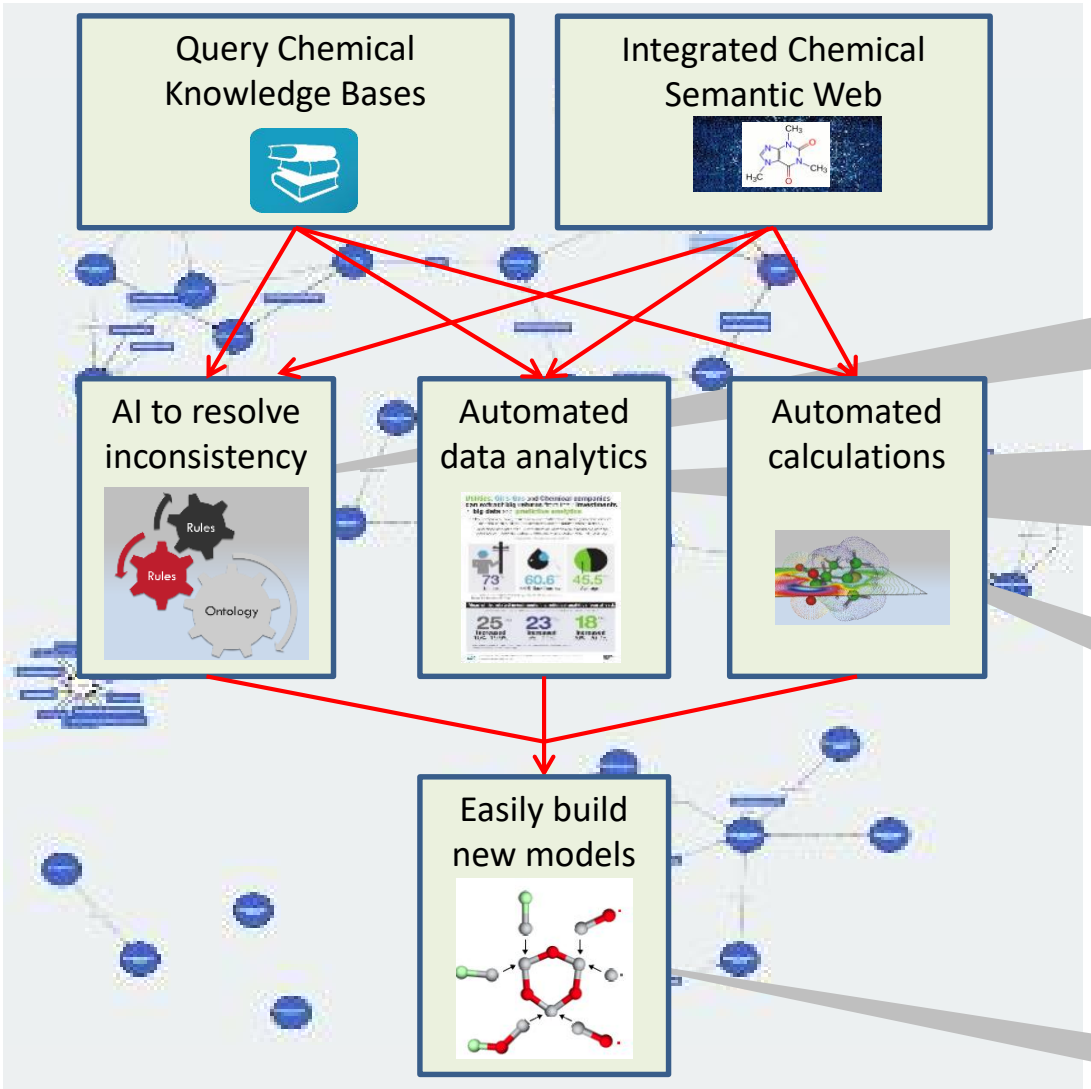
- Extensible
  - Re-use and extend existing ontologies
  - Standardisation via W3C

- Ontokin
  - Data: Computational chemistry calculations, reaction mechanisms

- Utilise machines to automate chemical models – *k*inetics, Cantera, Chemkin, etc.



Purpose & methodology: use-cases for the Process Industry



Ontology to sit on top of data

Services to automate tasks

Curation of knowledge

- Resolve inconsistencies
  - Species data
  - Reaction pathways
- Assessment of new data
  - Millions of compounds published every year
  - New properties added to existing data
- Automated calculation
  - Thermochemical data
  - Reaction rates

Automated bespoke models

- Development and verification of models for industry