Making High-Performance Computing Essential to the Formulation Industry

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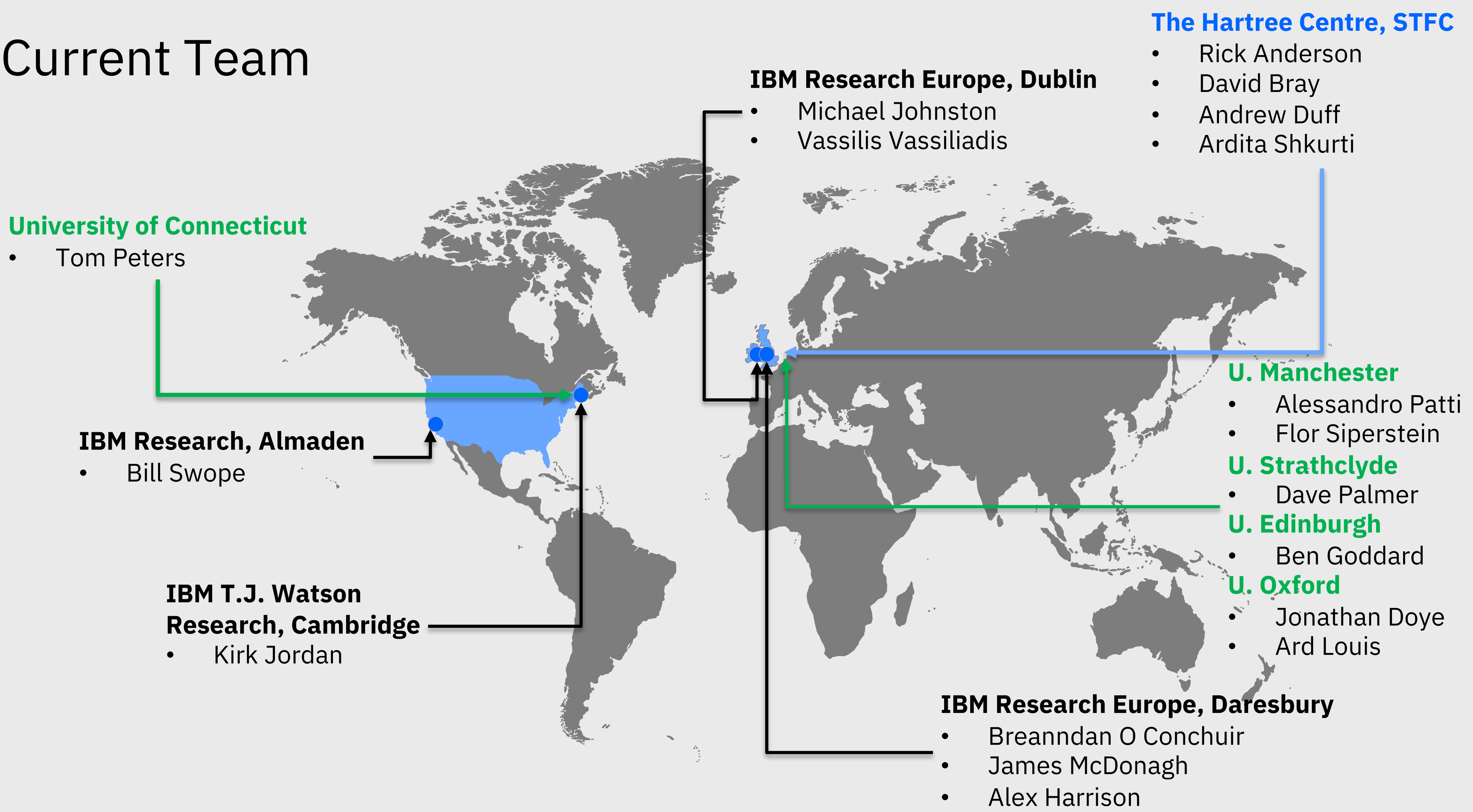
Context

Current Team



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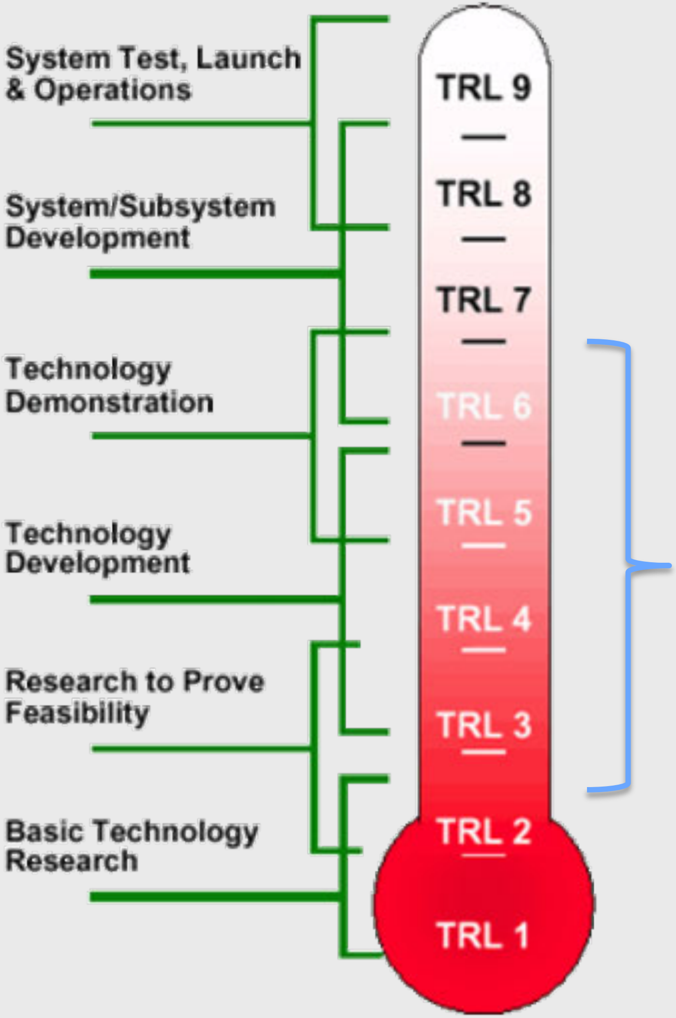
Research Focus



Focusing on TRL 2-6

2. Technology concept formulated
6. Technology demonstrated in relevant environment

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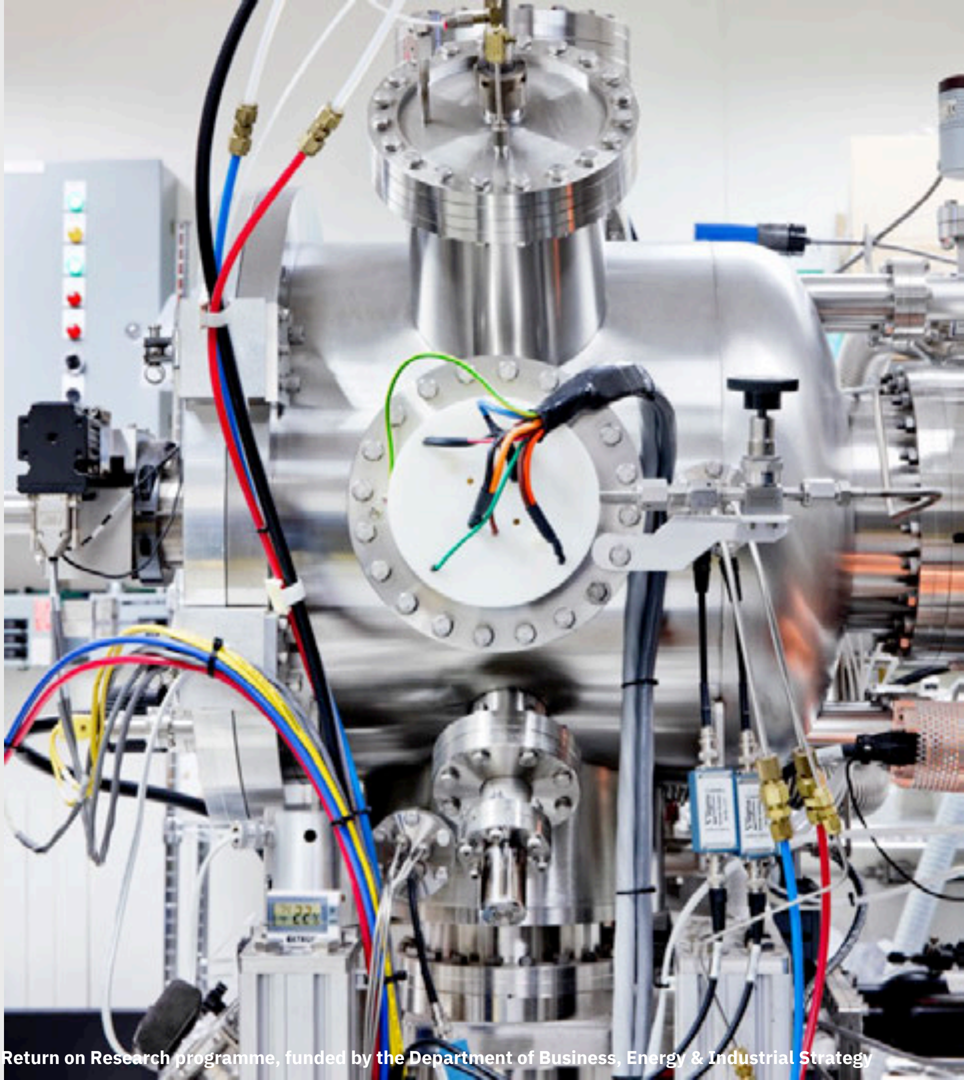
Hartree Chemistry

Research Goal

Computational results representative of experimental measurements



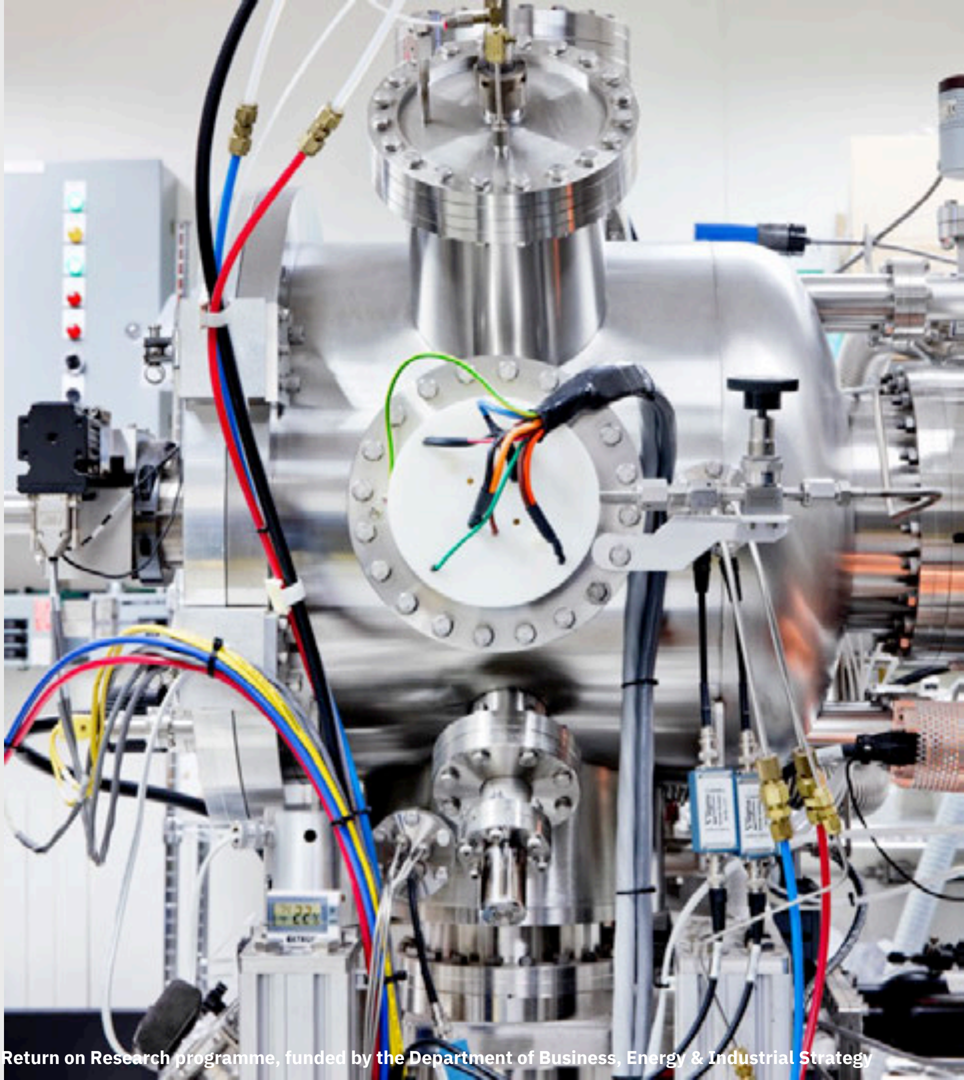
Hartree Chemistry

Research Goal

Computational results representative of experimental measurements

Business Need

- Better faster cheaper product development
- Improved product understanding
- Development for sustainability



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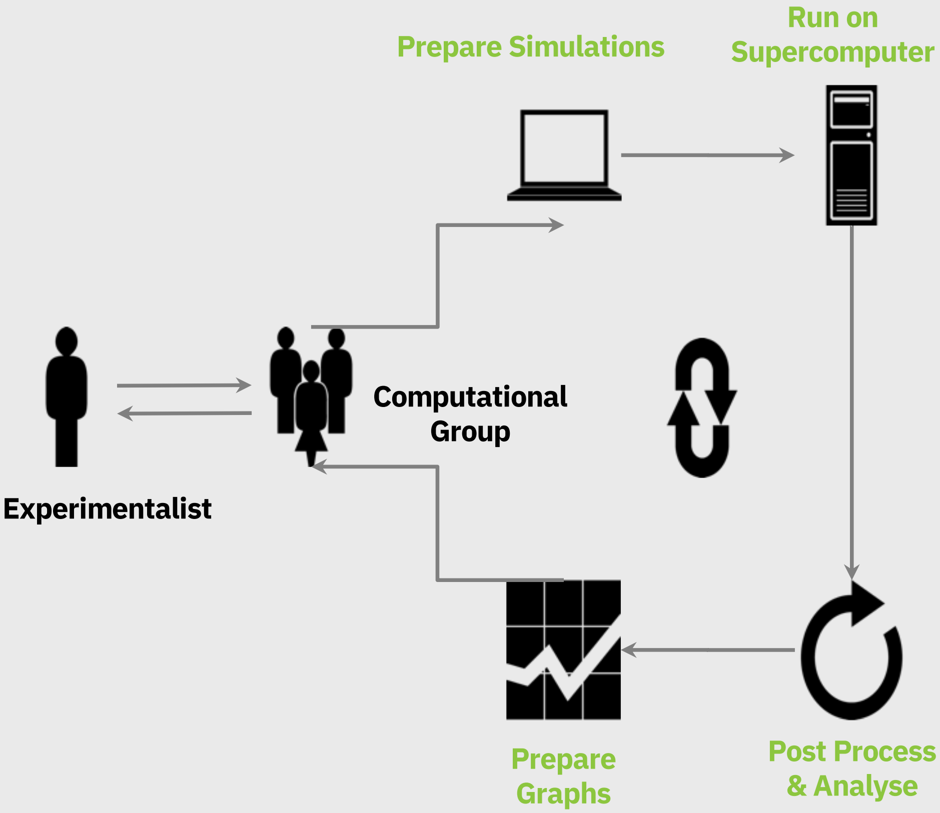
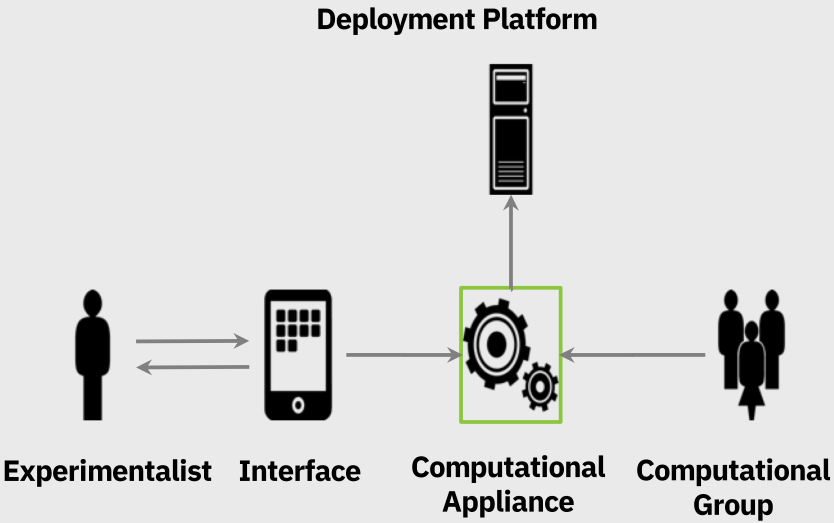
How computational methods are traditionally consumed in industry



An alternate model for consuming computational methods in industry



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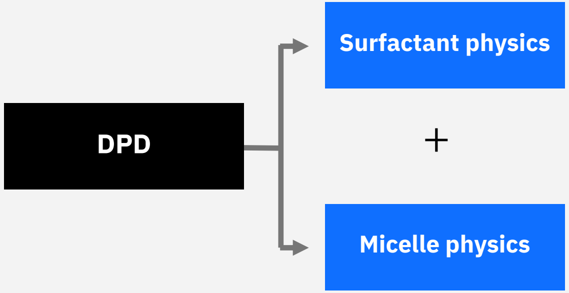
Simulation Methodology

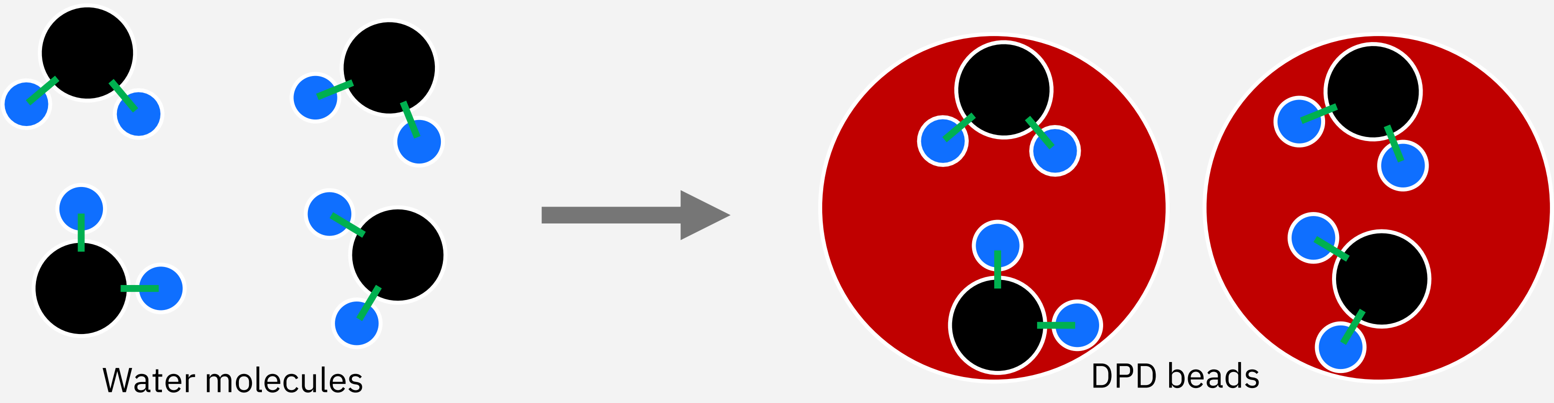
Dissipative Particle Dynamics (DPD)



Interbead DPD Potential

$$\overrightarrow{F_{ij}} = \overrightarrow{F_{ij}^{C}} + \overrightarrow{F_{ij}^{D}} + \overrightarrow{F_{ij}^{R}}$$

$$\overrightarrow{F_{ij}^{C}} = \begin{cases} A_{ij}\left(1 - \frac{r_{ij}}{r_c}\right)\frac{\overrightarrow{r_{ij}}}{r_{ij}} & r_{ij} < r_c \\ 0 & r_{ij} > r_c \end{cases}$$



Parameterisation

Bespoke DPD Force-Field Parameterisation

- Parameterisation is the process by which a force field is fit to reproduce known data
- This is a pre-requisite to an accurate, informative and trustable simulation.
- We are currently building automated methods to parameterise DPD force fields

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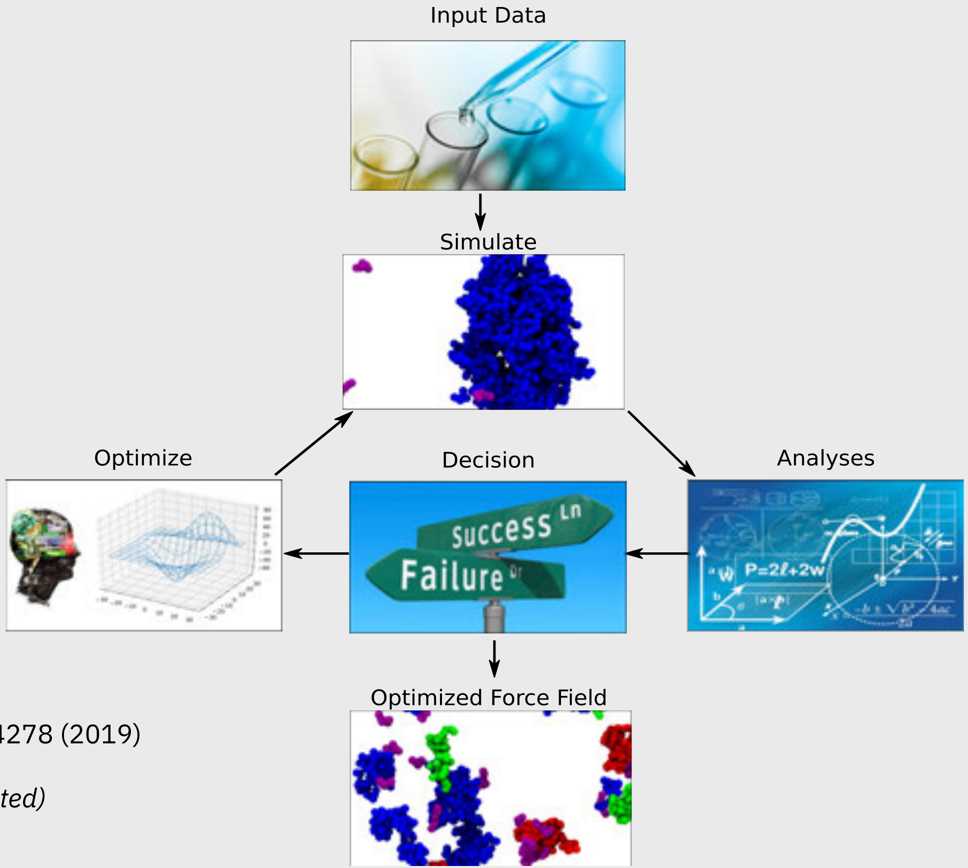
- We are currently building automated methods to parameterise DPD force fields
- Local and global optimisation methods are being explored including gradient descent and AI enhanced methods such as Bayesian optimisation
- Generate tailor-made models for industrial systems using relevant or easily attainable experimental data – top-down or on-the-fly



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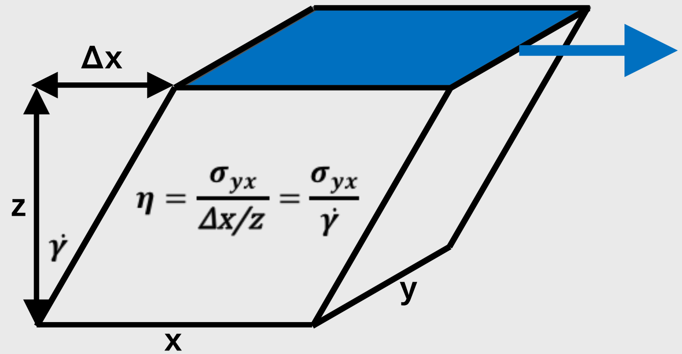
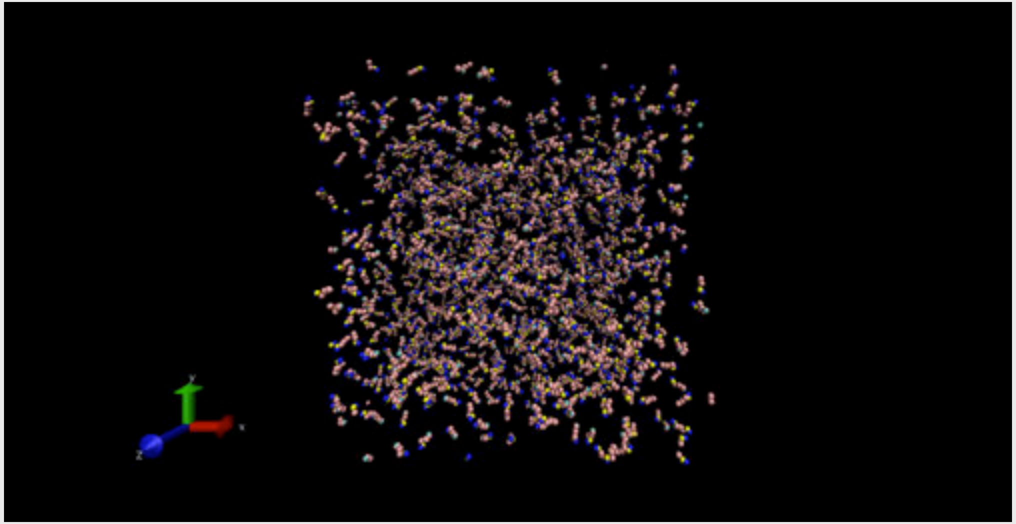
Johnston et al. *Journal of Physical Chemistry B, (2020) (Accepted)*

Virtual Experiments

High Shear Rheology Simulations

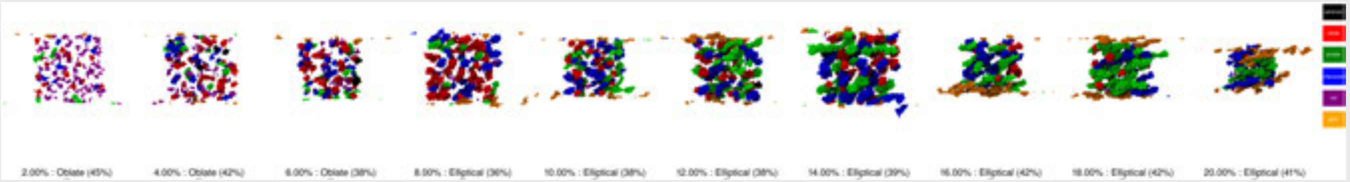




- Lee-Edwards shearing boundary wall conditions
- Clustering algorithm
- Timeseries equilibration metrics

<u>Simulation Output</u>

- Micelle statistics, size and shape distributions
- Viscosity, stress, shear & micelle orientation measurements



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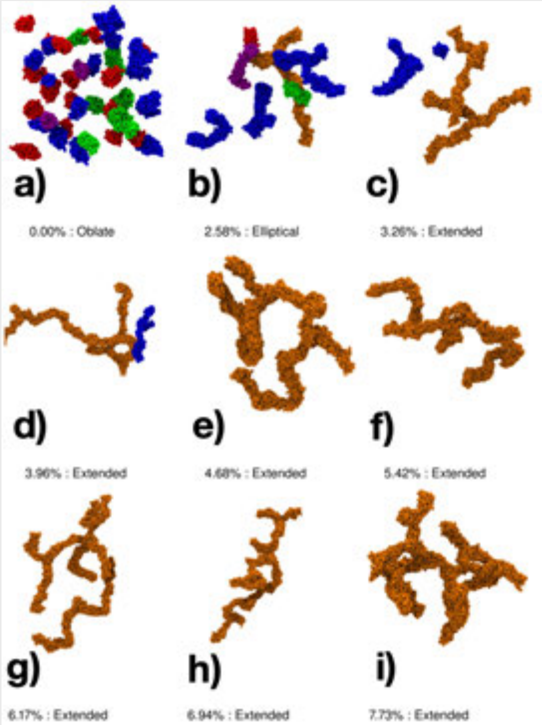
Concentration Scans



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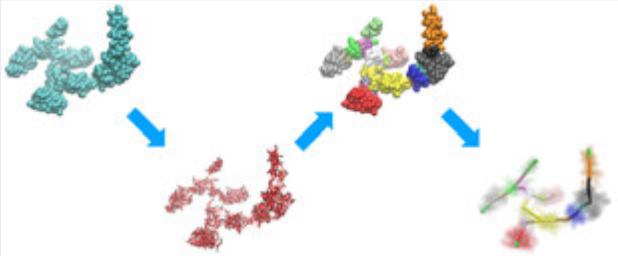

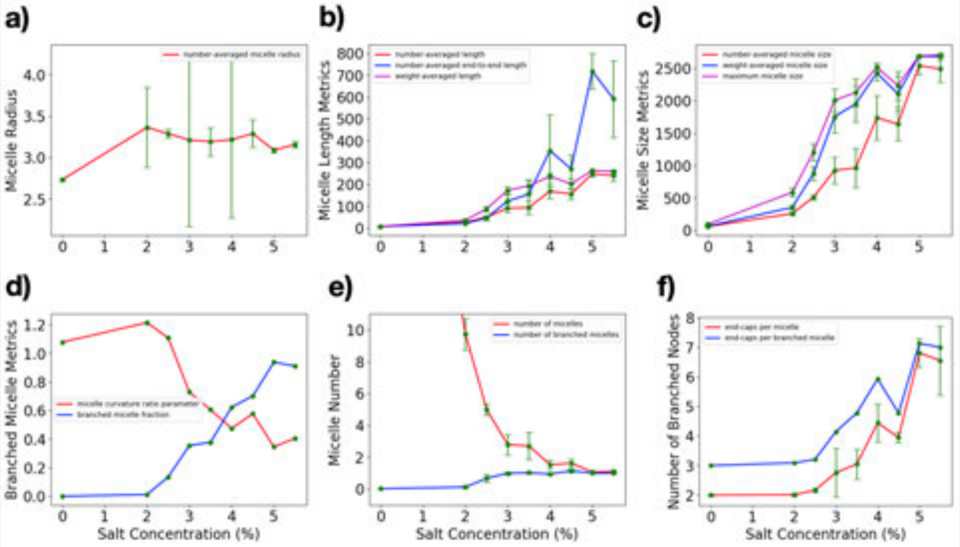

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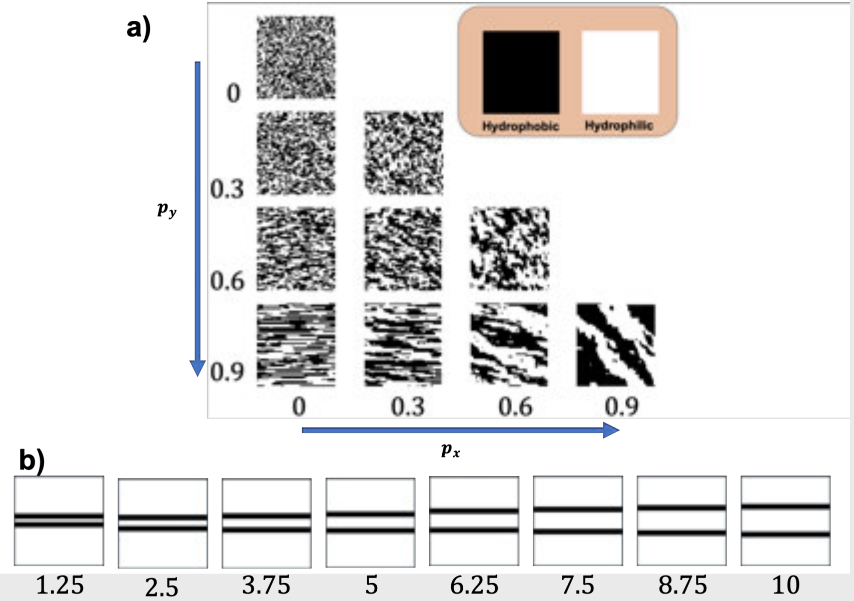
Patterned Surface Adsorption



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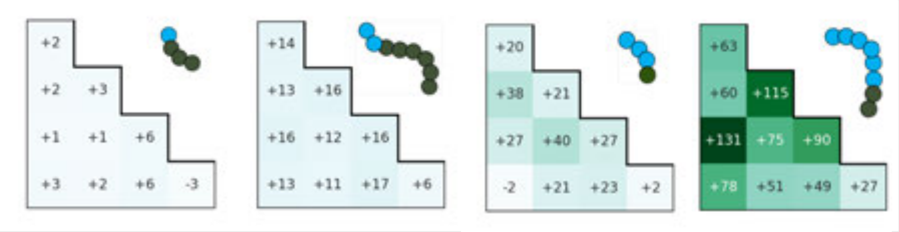

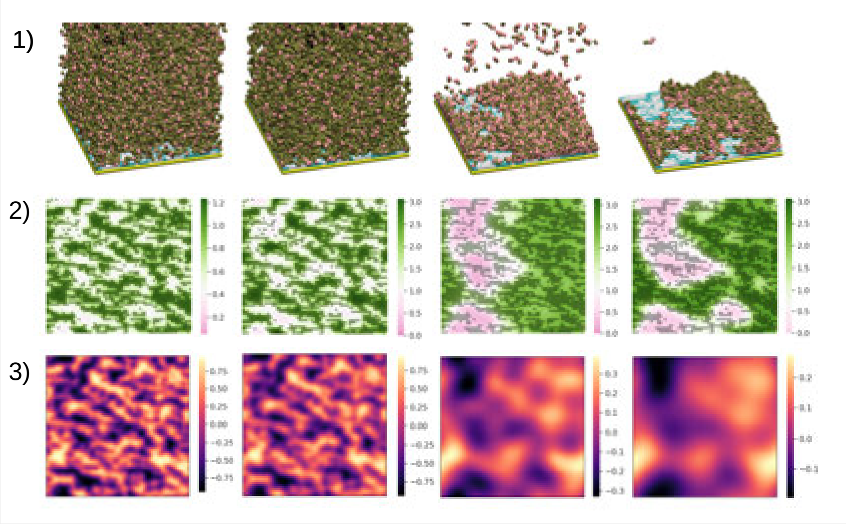

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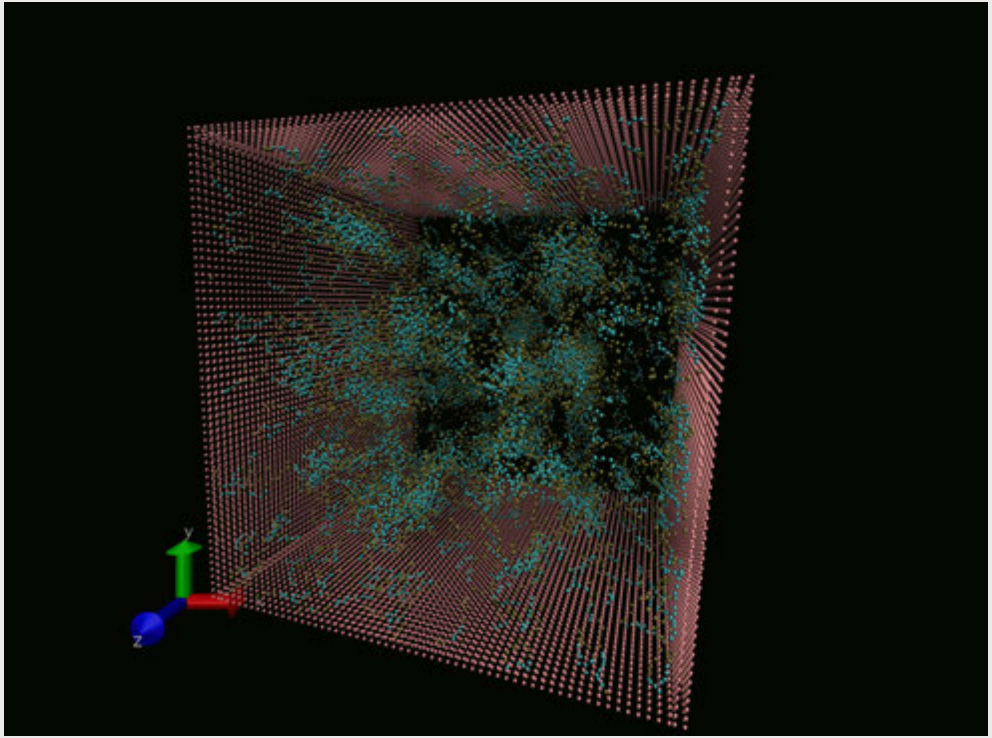
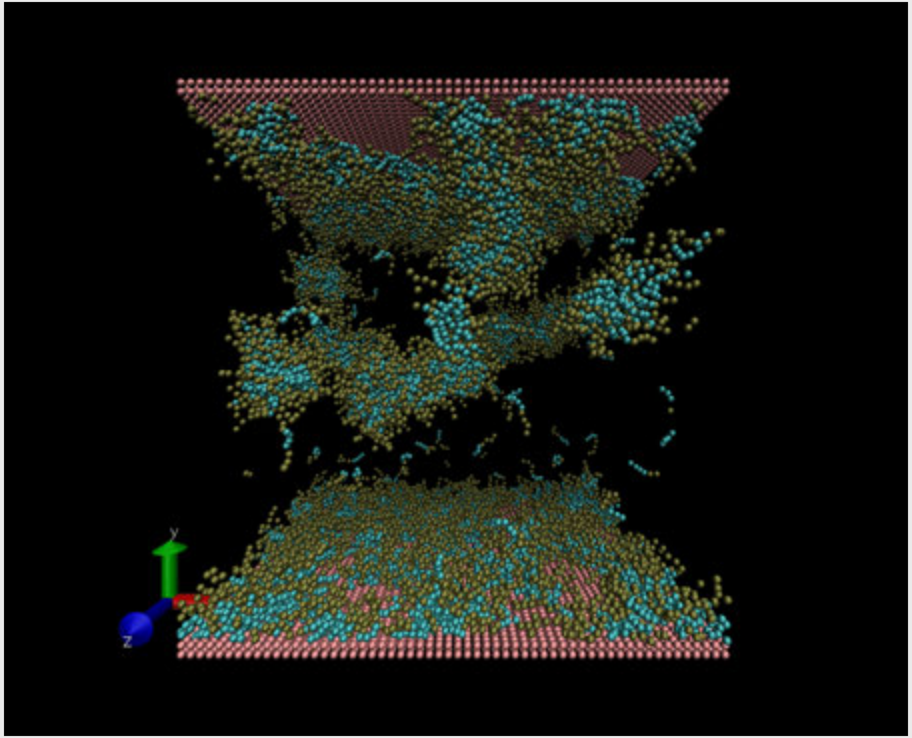
Rheology in Confined Environments

Nanochannel fluid flow with slip/no—slip wall conditions



Parallel plate shear flow with slip wall conditions



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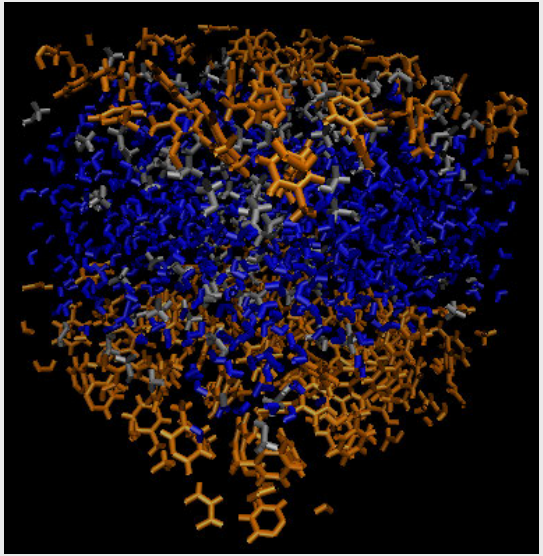
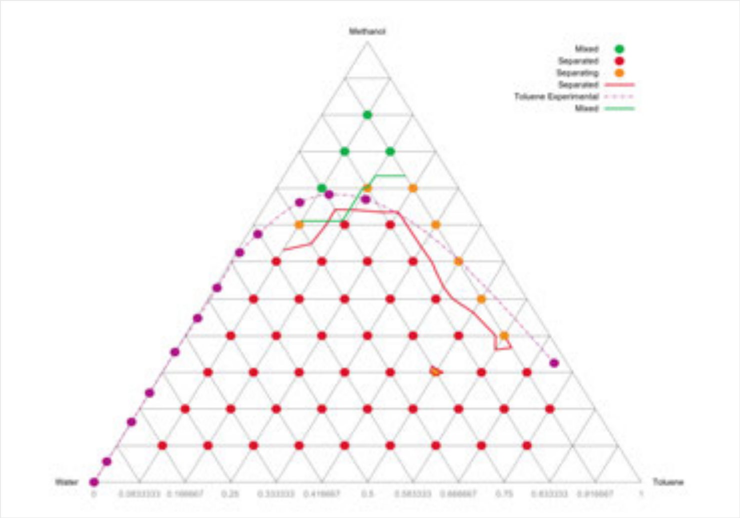
Ternary Phase Diagrams

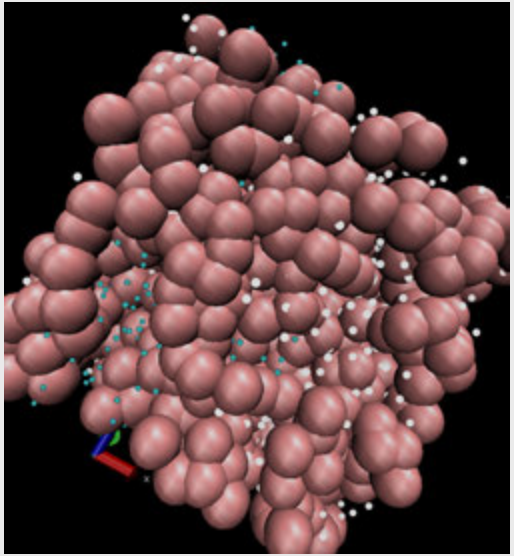
Predicting ternary phase diagram from molecular simulations

We use DPD as a fast efficient simulation methodology to predict the diagram

We also apply MD to elucidate the molecular scale phenomena







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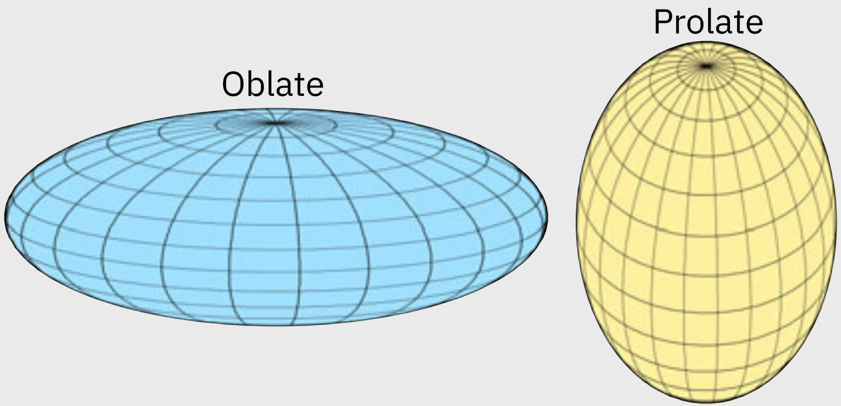
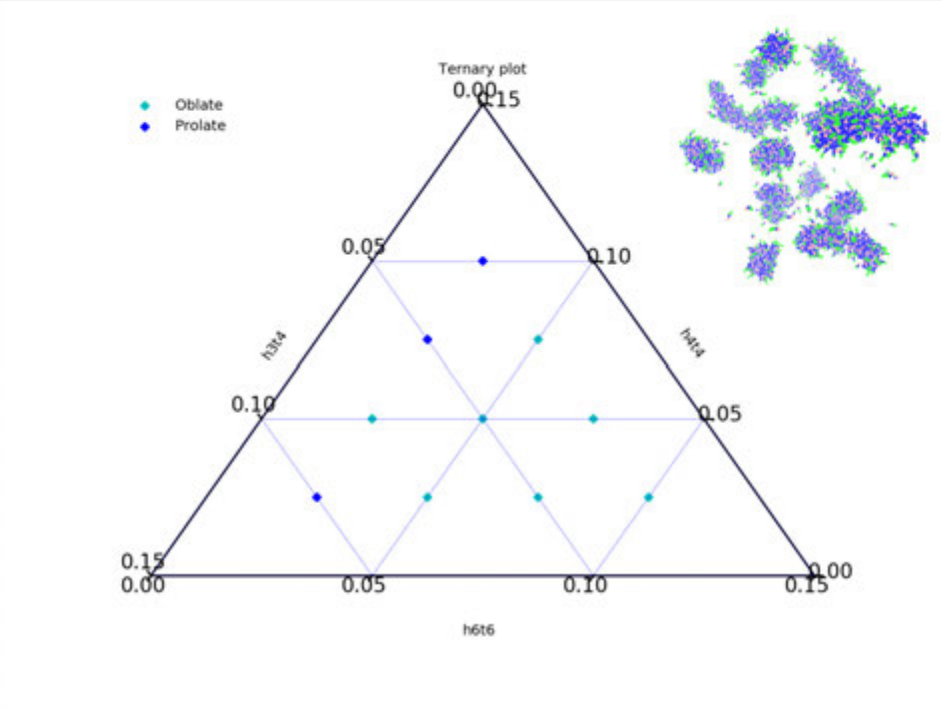
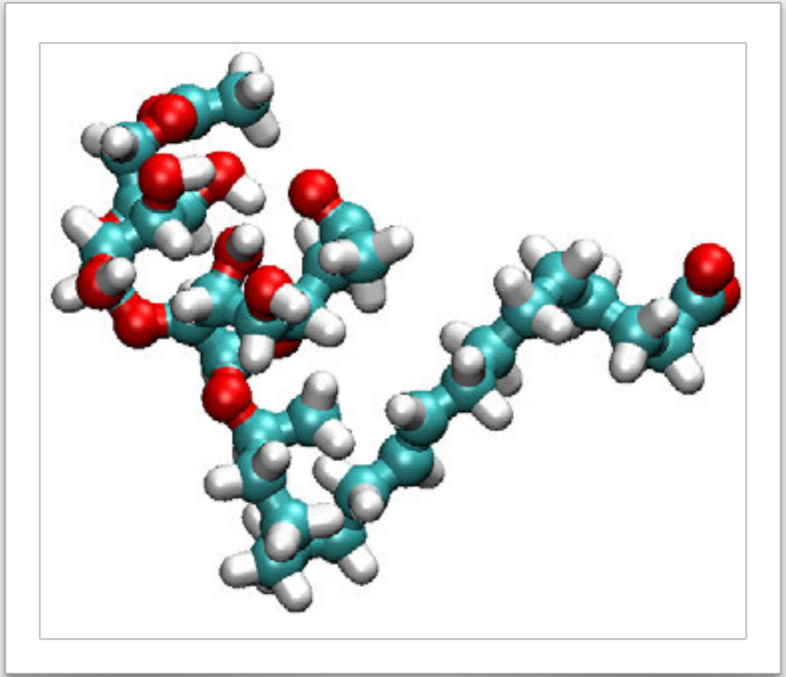
Mesoscopic Phase Detection

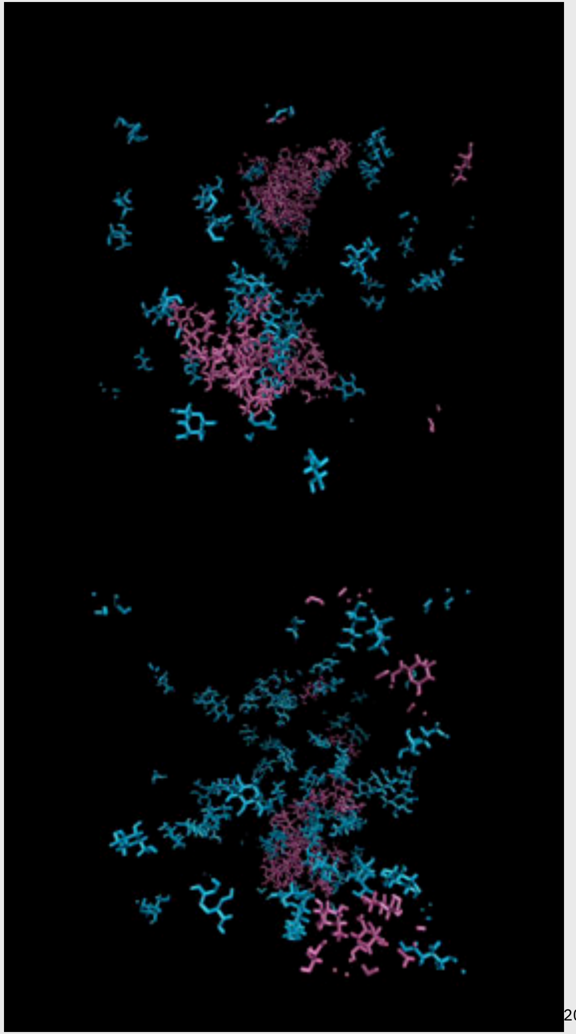
- Developing methods for detecting different mesoscopic liquid phases and aggregate shapes.
- Using DPD to access the scales of mesoscopic structures
- A phase is identified by applying shape metrics to aggregates.





Biosurfactants





- Industry needs biosurfactants: Eco-friendly & sustainable
- Currently ranking a variety of MD force fields for simulating sugars

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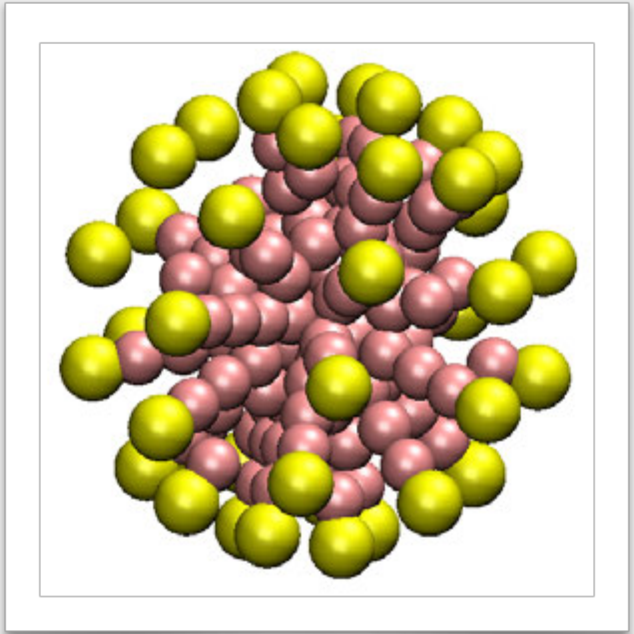
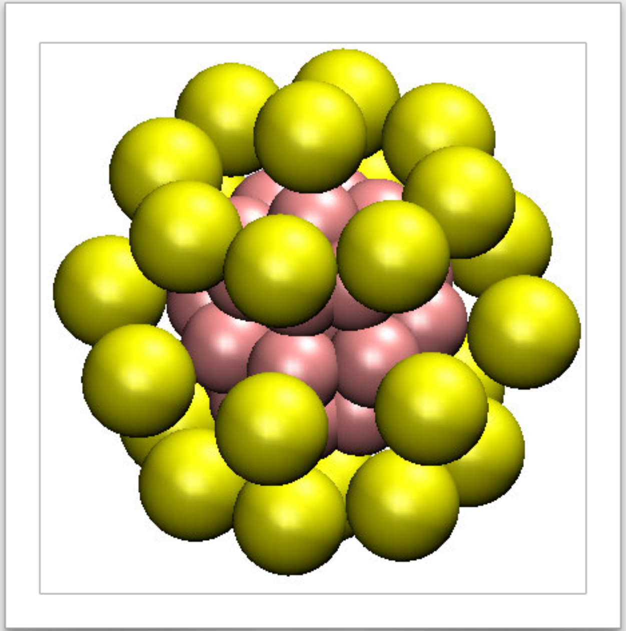
Nanoparticle Design





- Design functionalised nanoparticles for controlled delivery mechanisms
- Generate a variety of nano particles and investigate their transport properties

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Consumable Software

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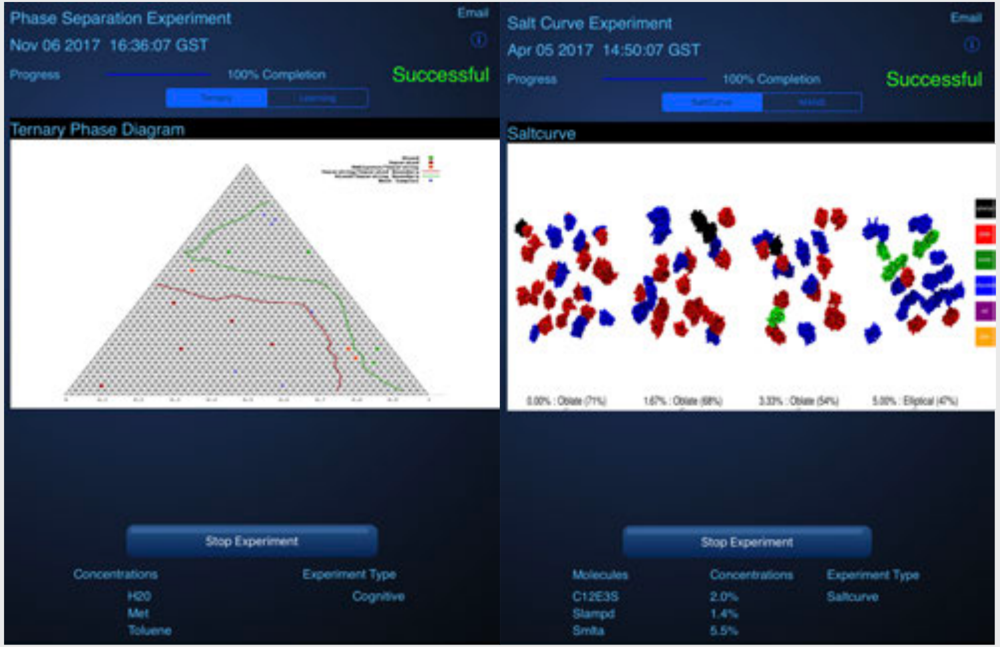
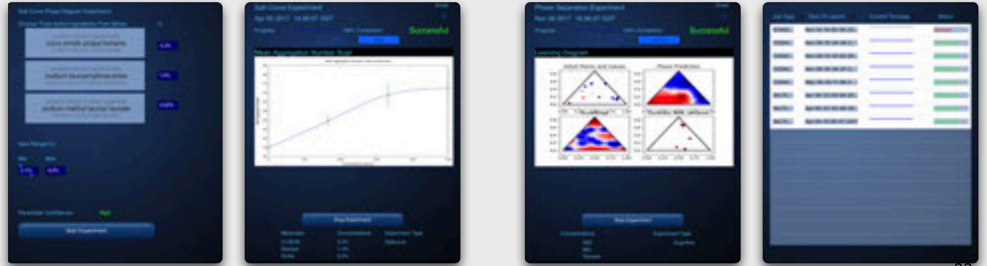
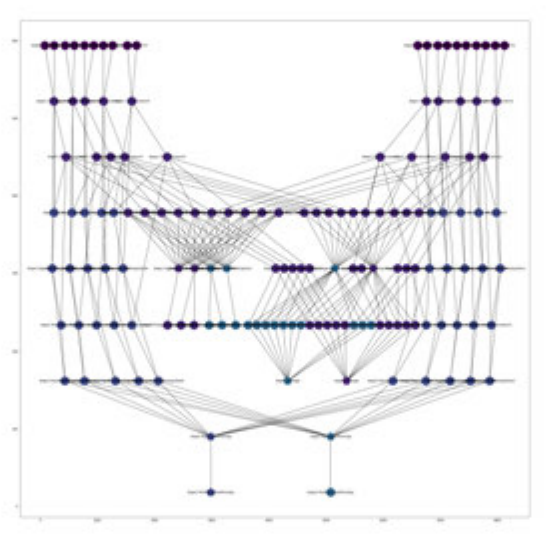
Formulation Applications



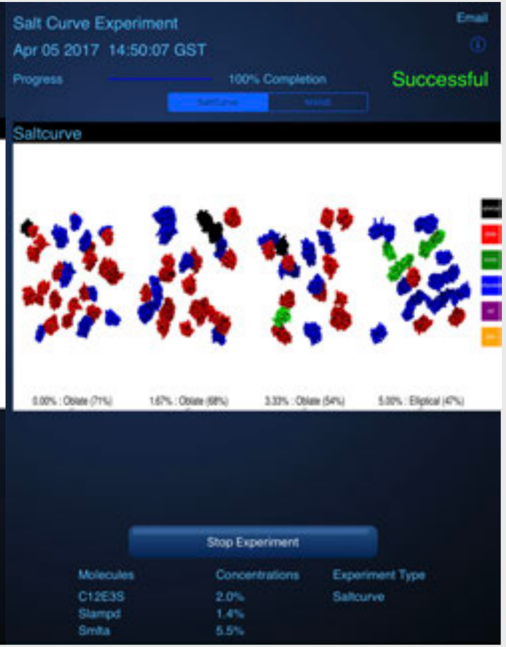
Real-time data visualisation



Formulation Applications



- Inclusive
- Robust
- Platform agnostic
- Scalable
- Data-flows
- Cloud native



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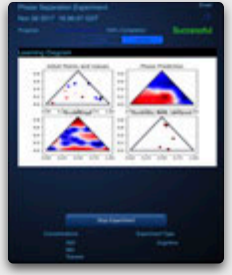

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Industrial Collaborations

July 1, 2020 | Written by: Breanndan Conchuir, James McDonagh , and Michael Johnston

Categorized: Chemistry | IBM Research - UK | STFC-Hartree Center

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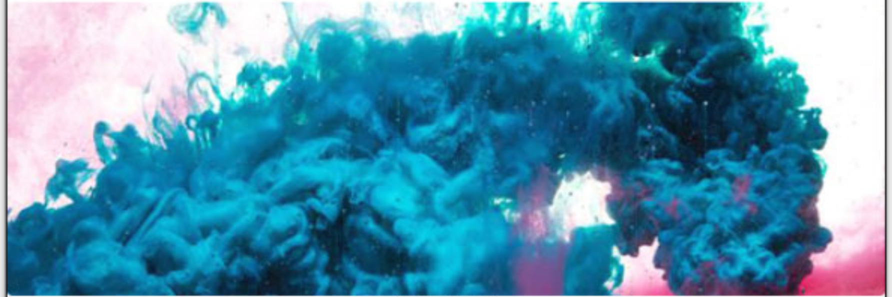
Think back to your chemistry 101 class where you were fumbling around with test-tubes and pipettes attempting to unlock the secrets of Nature. Such experiments were quick to construct and straightforward to complete.

However, real industrial chemical research is not so simple. Scientists need to perform a lot of complicated and laborious formulation chemistry experiments in order to design many of the ubiquitous products which we use daily.

Computational Formulation for Polymers



(Credit: Dreamstime)

15 June 2020

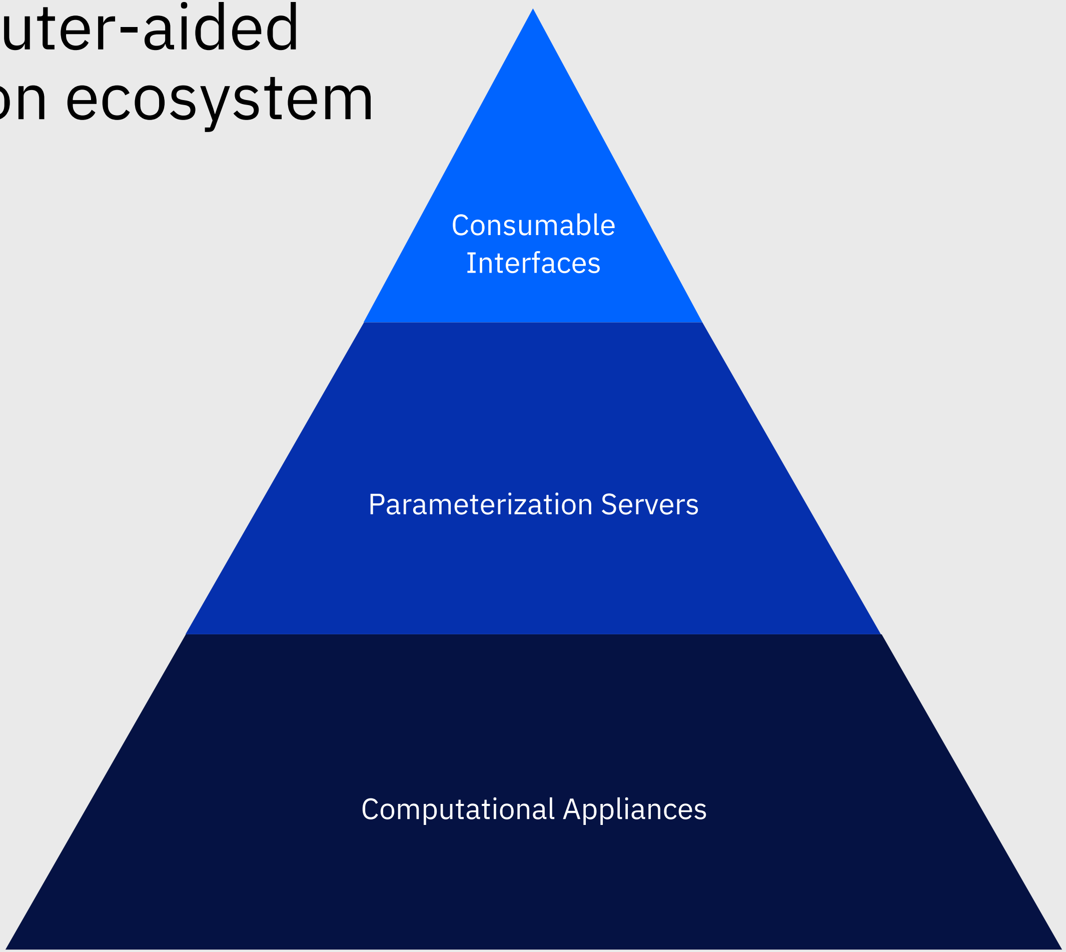
Researchers based at the STFC Hartree® Centre worked with Johnson Matthey, using computational techniques to automate and accelerate the process of identifying properties of novel chemical formulations.

Challenge

Chemical formulation is at the heart of many manufacturing processes. It is critical in areas as diverse as medication, personal care products and engine oils. Typically, formulation research is carried out experimentally in a laboratory. Johnson Matthey were looking for a way to automatically predict the properties of novel formulations, generating strong reproducible insights in to product development. These computational tools would enable digital pre-screening of novel formulations, guiding the decision making behind which new formulations should be prioritised for expensive laboratory testing.

Summary

The computer-aided formulation ecosystem



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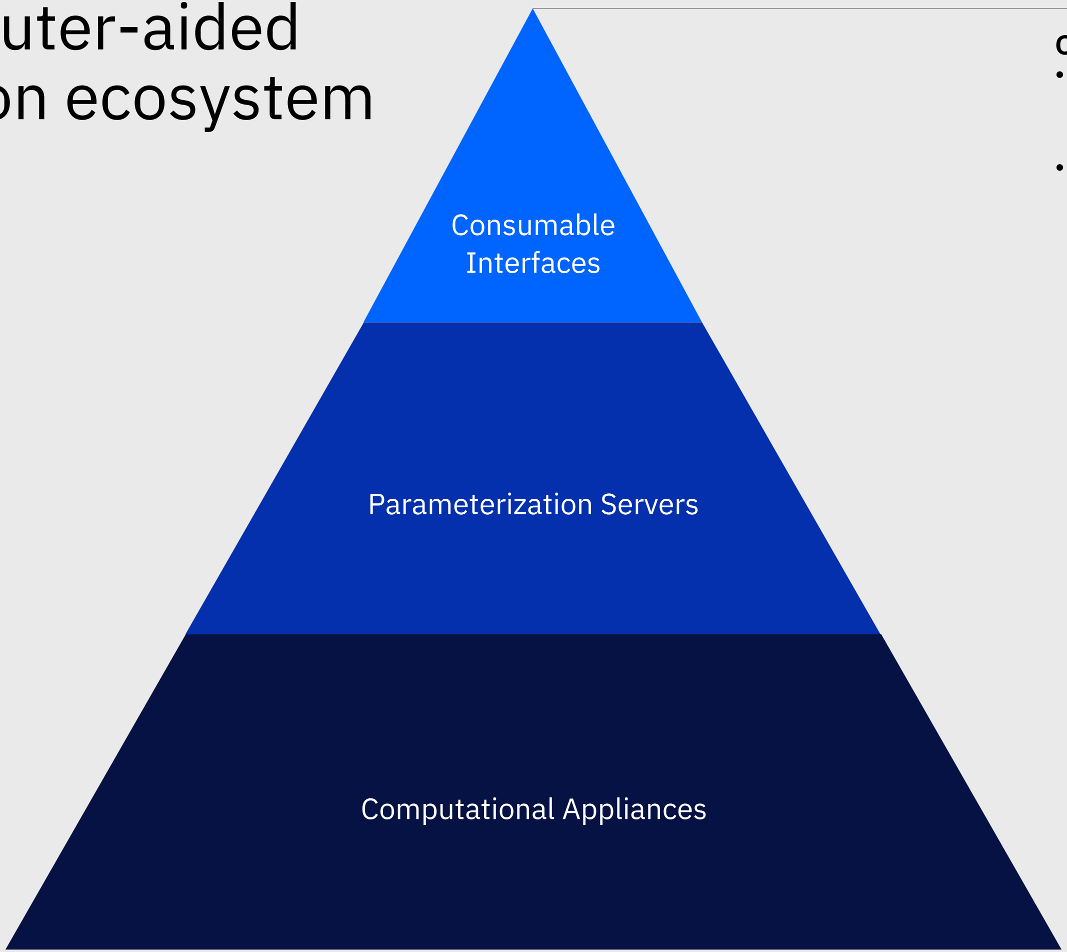
The computer-aided formulation ecosystem



Consumable Interfaces

- *Capability*: Allow non-experts to easily run complex experiments on HPC systems
- *Exploitation*: Appliances created by researchers can be vended via mobile or web interfaces.

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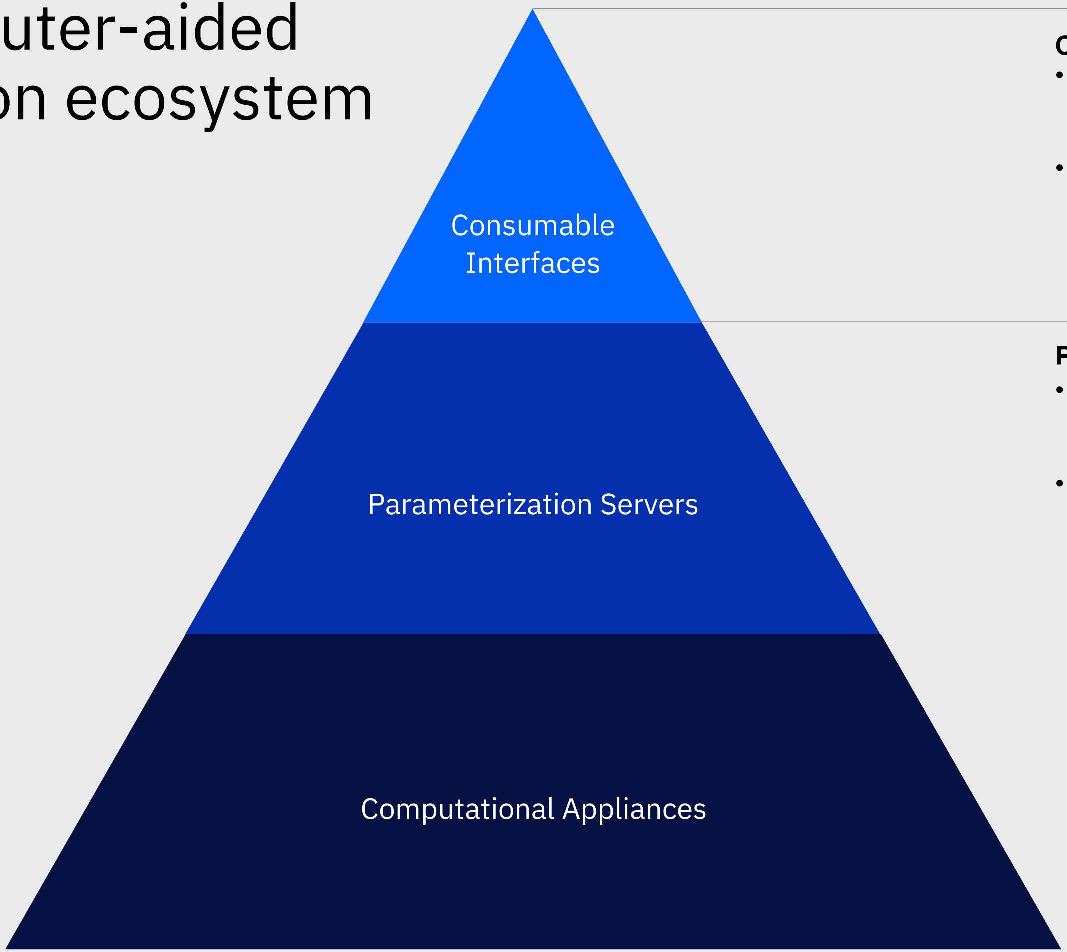
The computer-aided formulation ecosystem



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Parameterization Servers

- *Capability*: Develop technology to automatically train particle/MM models for in-silico design problems
- *Exploitation*: Parameterization servers for training models. Deploy to computational appliances.

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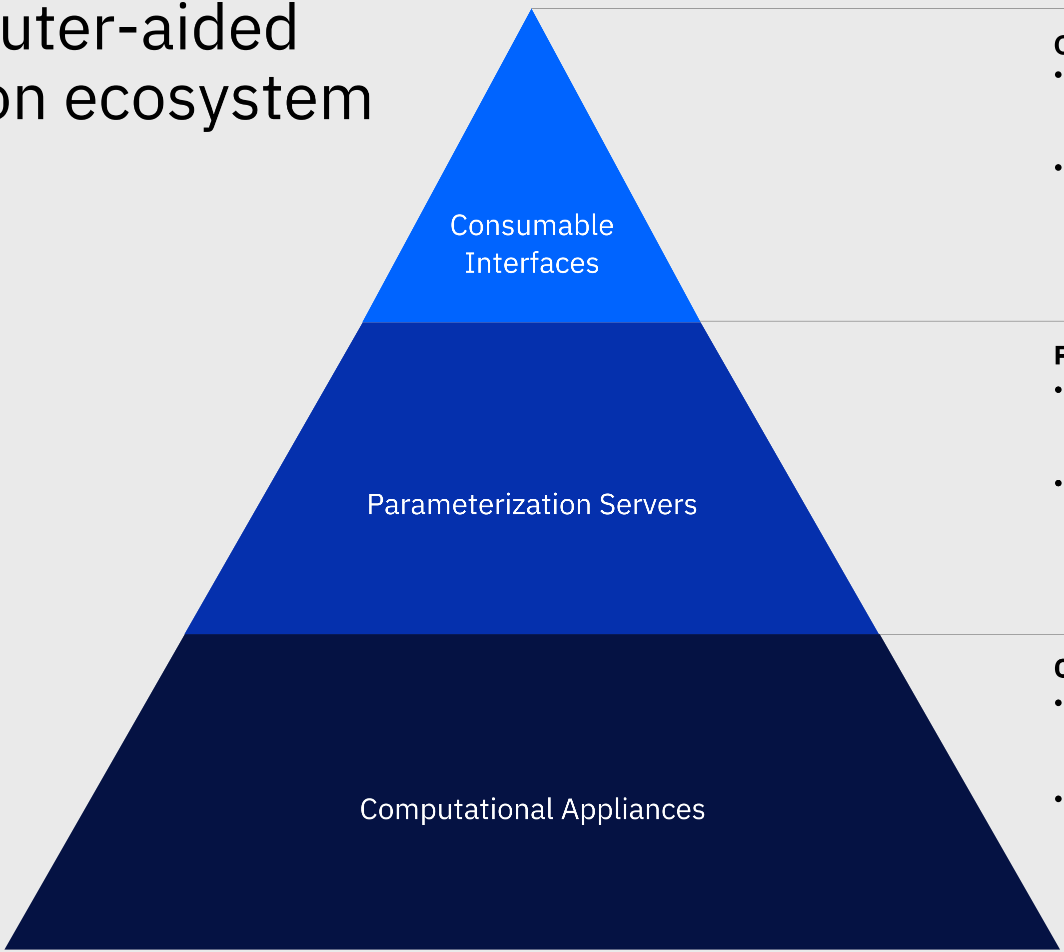

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Computational Appliances

- *Capability*: Tools and processes for creating robust ***workflows***, encoding the ***state-of-the-art***
- *Exploitation*: Computational scientists transform workflows into reusable services.

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IBM

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