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High Throughput Modelling of Polymers with Computational Chemistry and Machine Learning

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Problems with Polymer Discovery

- Slow development cycle
- Random trial and error
- High financial and environmental cost
- Composites complicates research further

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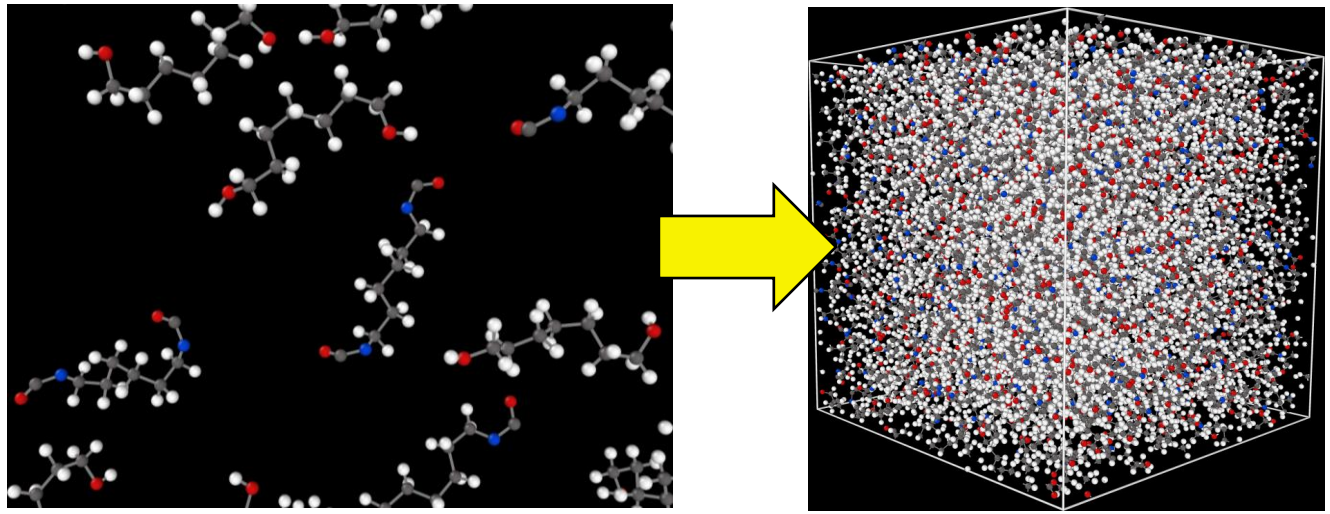
Molecular Dynamics

- Modelling chemistry using classical mechanics
- Model large repeating structures like polymers
- Enable rapid exploration of material design space



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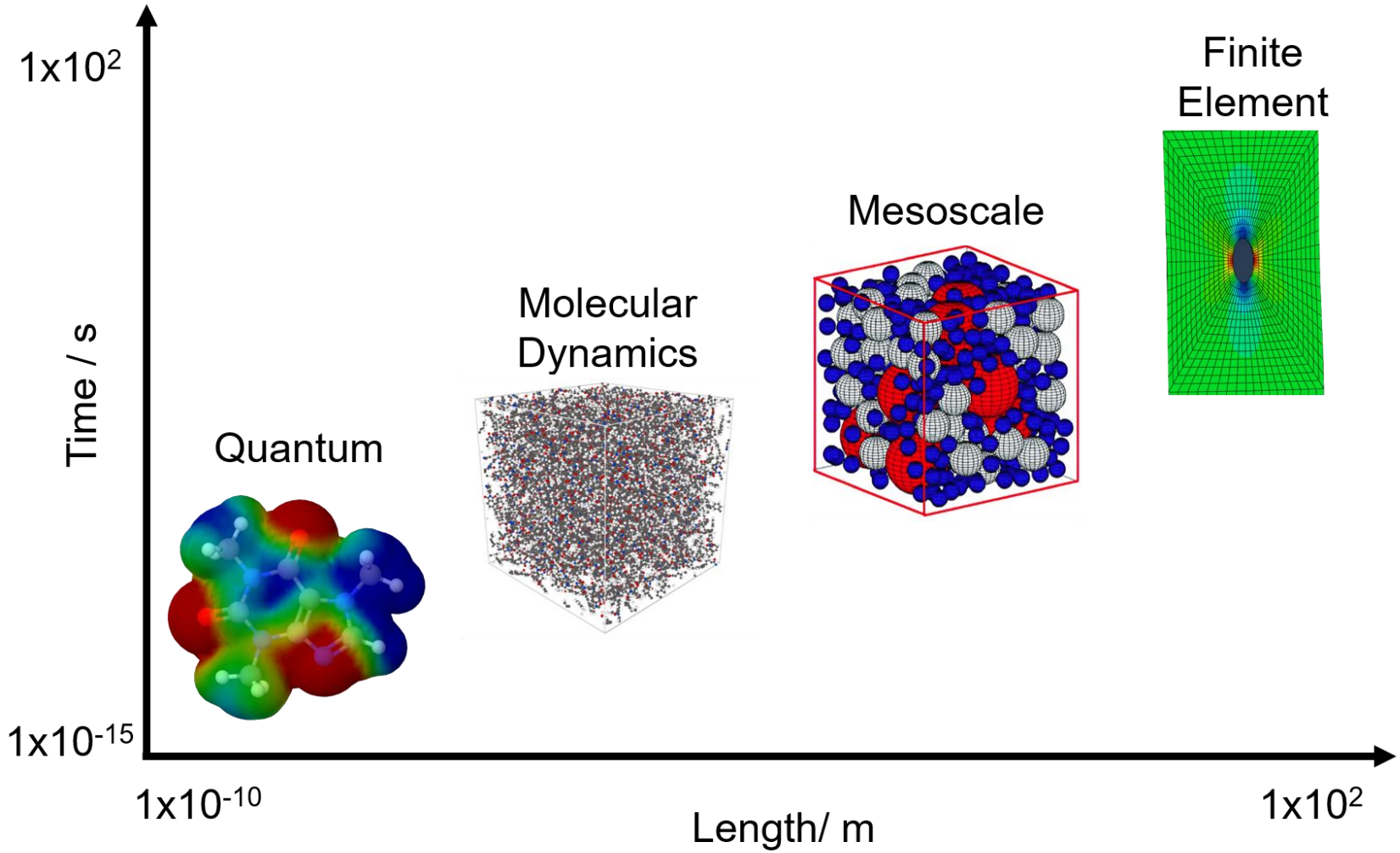
MD Scale

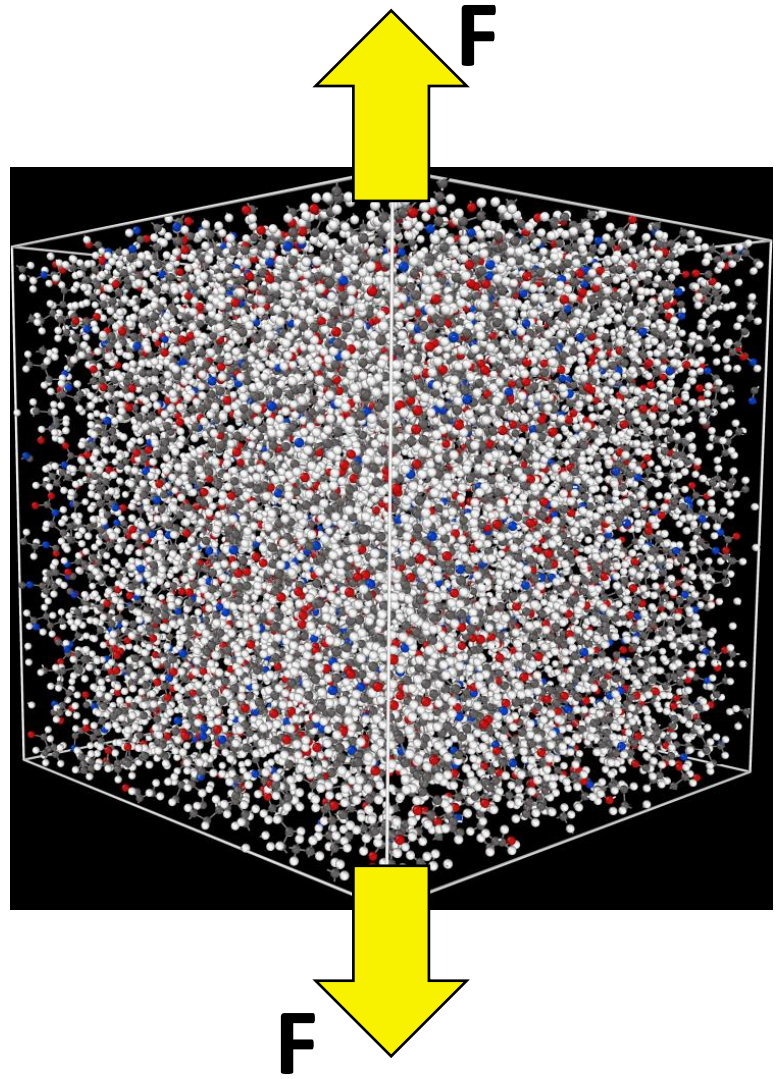
- Faster than quantum
- Don’t render microscale
- Feed into longer scales



Mesoscale Figure: *X. Du and L. Jin, Methodology: Meso-Scale Simulation Approach, 2021*

MD Predictable Properties

- Glass Transition Temperature (T_g)
- Storage & Loss Modulus
- Density and Free Volume
- Degree of Crosslinking
- Coefficient of Thermal Expansion (CTE)
- Young's Modulus
- Shear Modulus
- Poisson's Ratio
- Yield Stress



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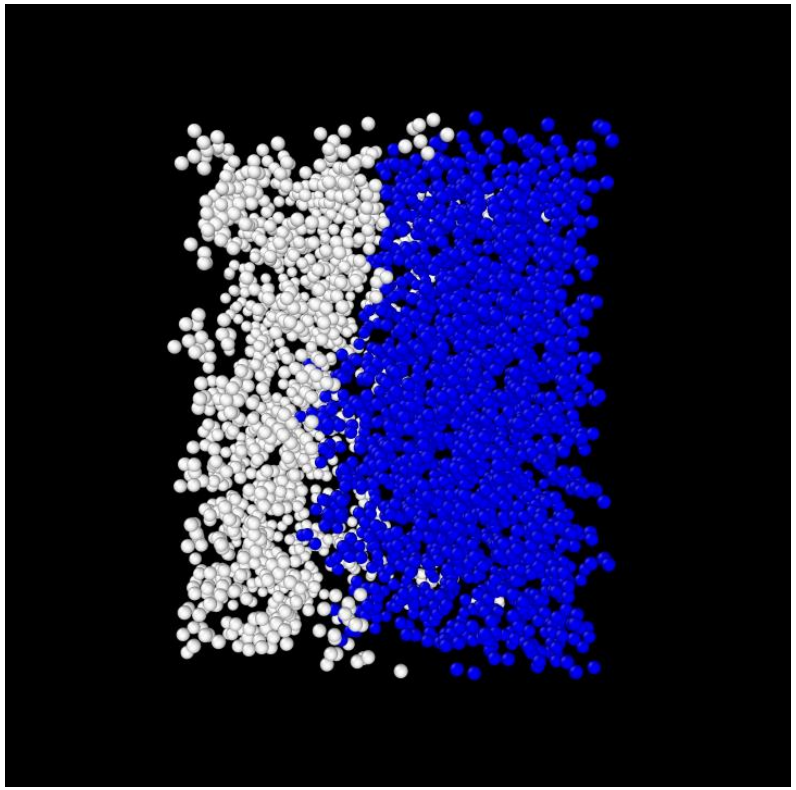
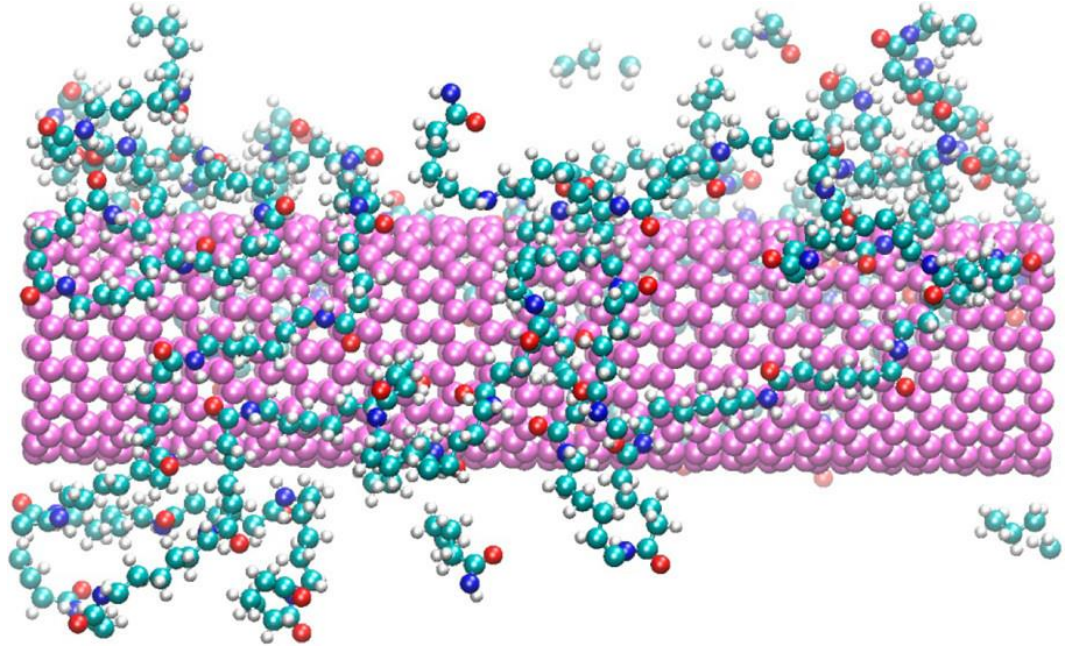
Atomistic Visualisation

Polymer/Solvent Phase Separation



Polymer/CNT Interface



J. Phys. Chem. C 2014, 118, 18, 9841–9851

MD Software

- Range of commercial and open-source tools
- Limited programming needed to get started
- Small but well established ecosystem

Processing

OVITO

RDKit
Open-Source Cheminformatics and Machine Learning

Simulation

LAMMPS

MATERIALS STUDIO

GROMACS
FAST. FLEXIBLE. FREE.

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Welcome to Computational Chemistry!

This sounds too good to be true?

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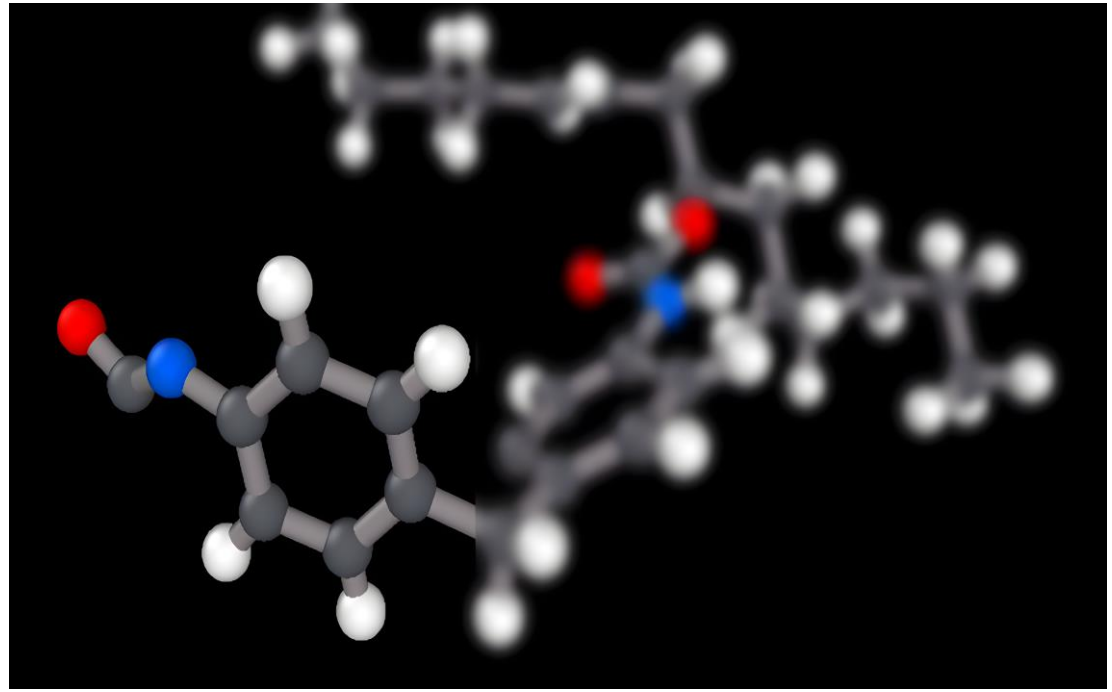
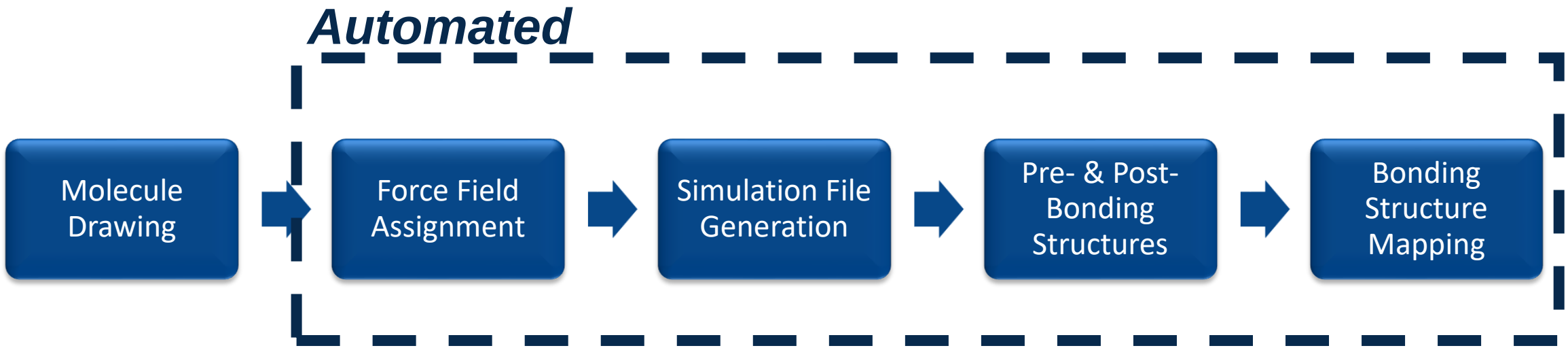
Problems with Computational Chemistry

- Significant barrier to entry
- Difficult and tedious pre-processing
- High computational cost prohibits high-throughput

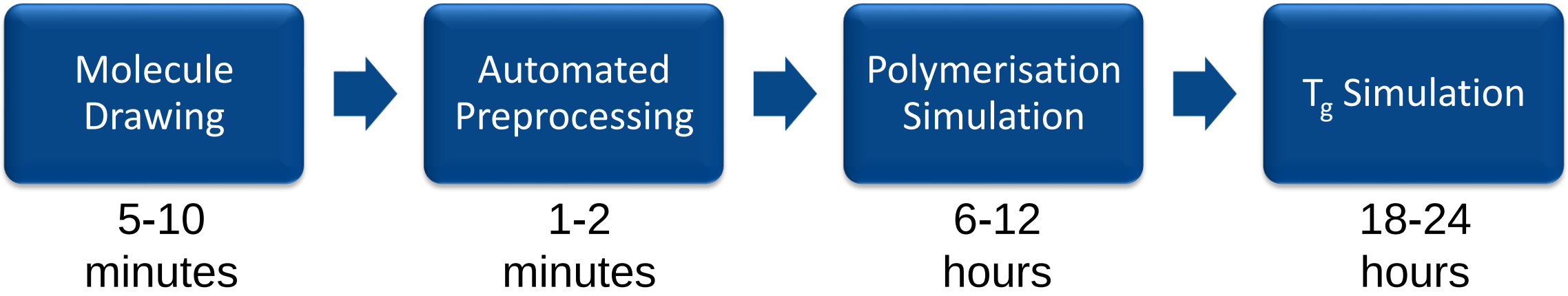


Automated Pre-Processing

- Developed an automated pre-processing workflow
- Polymer models easily parameterised and built
- Only requires the user to draw the molecule



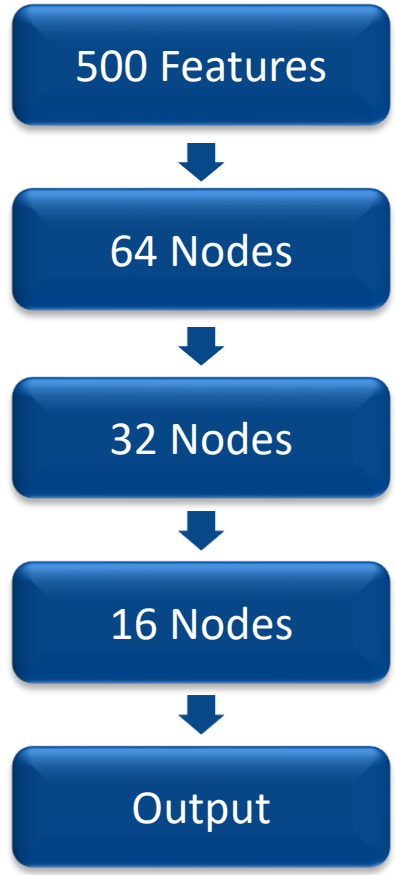
Polymer Characterisation



- Practical tasks are now simple and fast
- However, extensive simulation time is required
- Limits high-throughput simulation

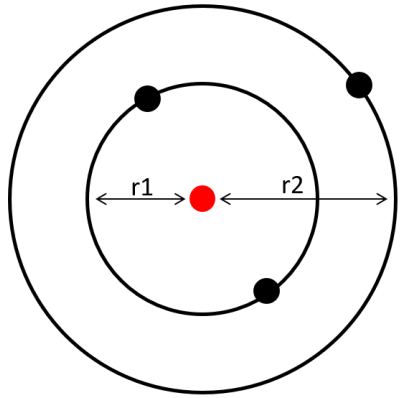
Fast Simulations - Machine Learning Surrogates

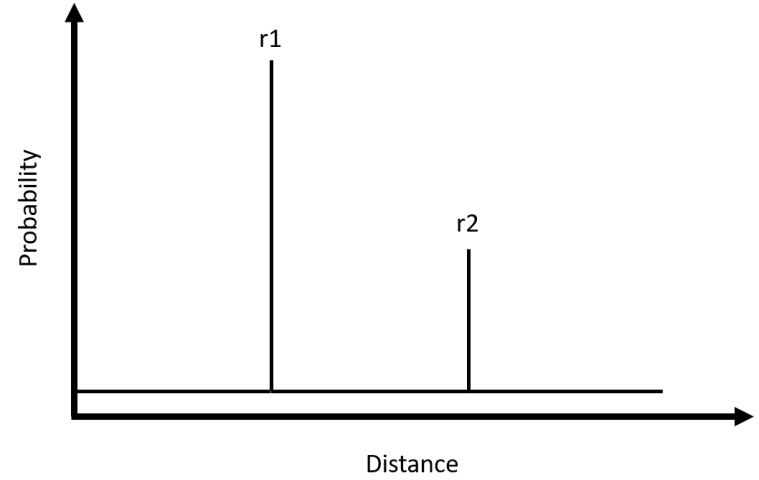
- Current MD simulations: 24 – 36 hours
- Eliminate MD simulation through prediction
- Using small neural network architecture
  - Low computational cost to train

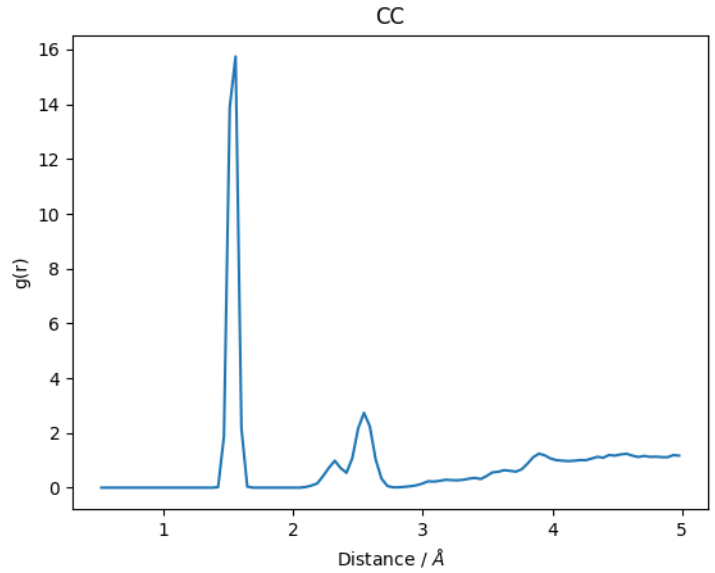


Features – Radial Distribution Function

- Using radial distribution as features
  - Probability of an atom being found at a given distance
  - Powerful way of condensing topology data







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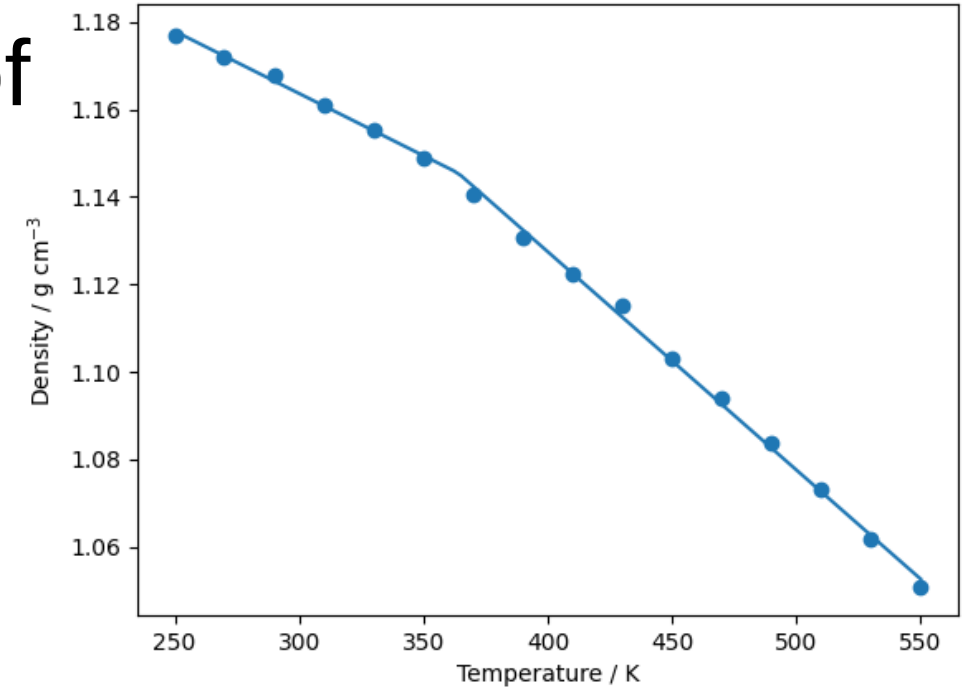
Glass Transition Temperature in MD

- 96 characterised polyurethane models
- Validated models via comparison of liquid density
- T_g range 320 – 450 K



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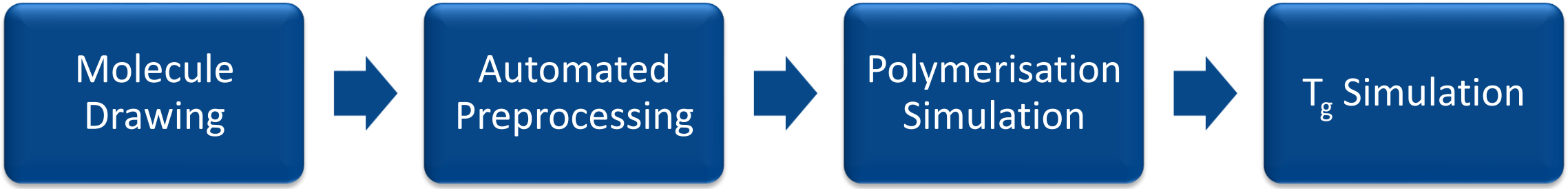
Glass Transition Temperature in ML

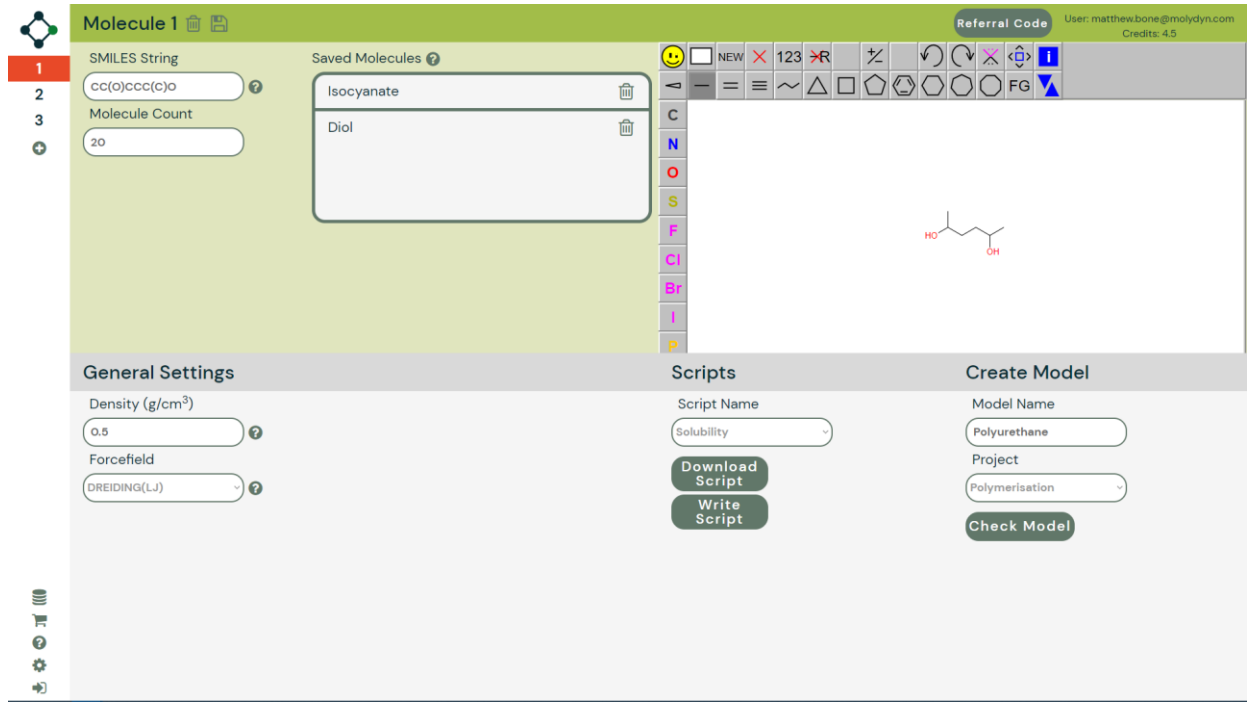
- Close prediction from simple feature
  - MAE: 10-20 K; RMSE: 20-30 K
- Modern form of Quality Structure Property Relationship
- ML use significantly reduces runtime - 80% reduction



Commercialisation

- Accessible chemical simulation for everybody
- 90% reduction in pre-processing time
- Developing total simulation solution

Molydyn



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Questions?

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Acknowledgements

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