USER BEST PRACTICE AND
RESULTS ON MN5

AI-FRIENDLY EUROHPC SYSTEMS

NEXTMOL

 | 25.09.2024

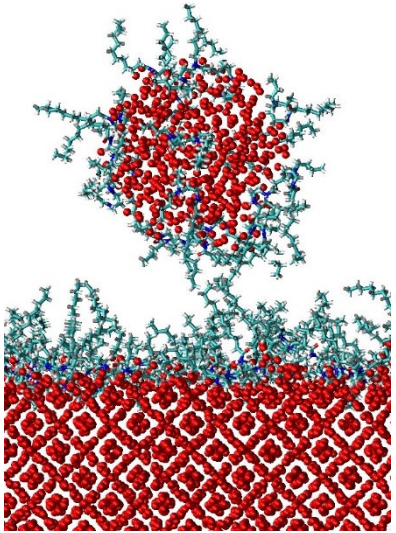
Dr. Monica de Mier, CEO

About us

- Spin-off company of the Barcelona Supercomputing Center
- Specialized in **computational chemistry**
- Develop a Software-as-a-Service platform to **accelerate the R&D** of best-in-class and more sustainable **specialty chemicals** based on **molecular modeling** and **AI**
- **Mission:** Help the chemical industry in its green and digital transition
- Specialty chemicals: Polymers and surfactants
- Modeling: Molecular Dynamics (Gromacs)
- AI: Machine Learning (scikit-learn)
- ISO27001 certified on information security

Use cases

- Migration of additives in polymer matrices (packaging, plastics) | *diffusion*
- Additives for improved performance of detergents (home care) | *critical micelle concentration, surface tension, interfacial tension*
- Agglomeration inhibitors for flow assurance (O&G) | *adsorption, agglomeration barrier*
- Cooling resins (electronics) | *thermal conductivity*
- Encapsulation of active ingredients or fragrances (personal care) | *solubility*
- Biobased polymers to replace fuel-based ingredients in cosmetics (personal care) | *glass transition temperature, mechanical properties*

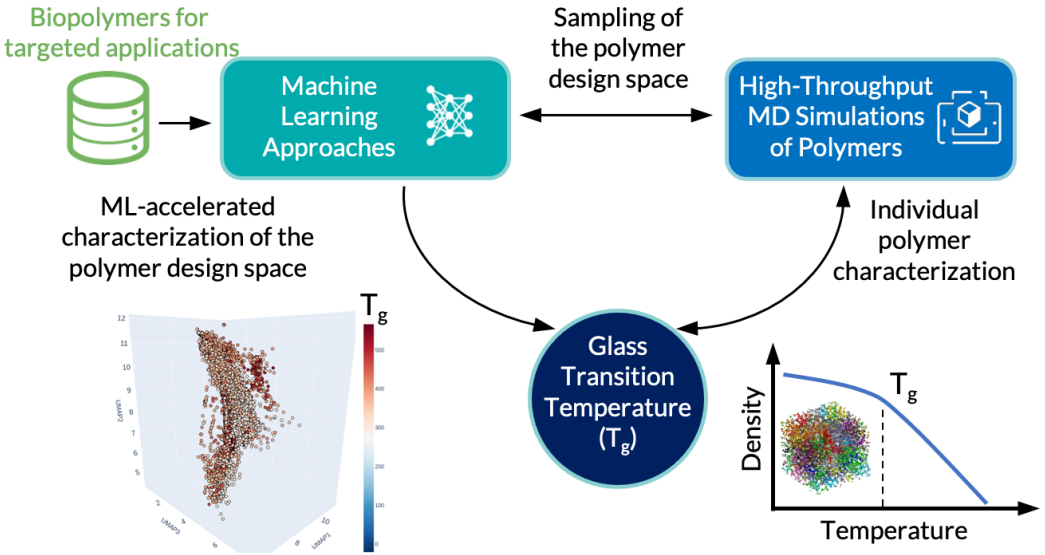


Supercomputing access

- 10.4 million core hours on JUWELS (Jülich Forschungszentrum, Germany), MeluXina (LuxProvide, Luxembourg) and MN5 ACC (Barcelona Supercomputing Center)
- Open R&D
- PRACE Project Access and EuroHPC JU Call for Proposals for Extreme Scale Access Mode
- The call is open to all fields of science, industry and public sector justifying the need for and the capacity to use extremely large allocations in terms of compute time, data storage and support resources
- Offers three distinctive application tracks:
  - Scientific Access, intended for applications from the academia and public research institutes
  - **Industry Access**, **intended for applications with Principal Investigator (PIs) coming from industry**
  - Public Administration Access, intended for applications with PIs coming from the public sector

High-Throughput Molecular Dynamics and Machine Learning

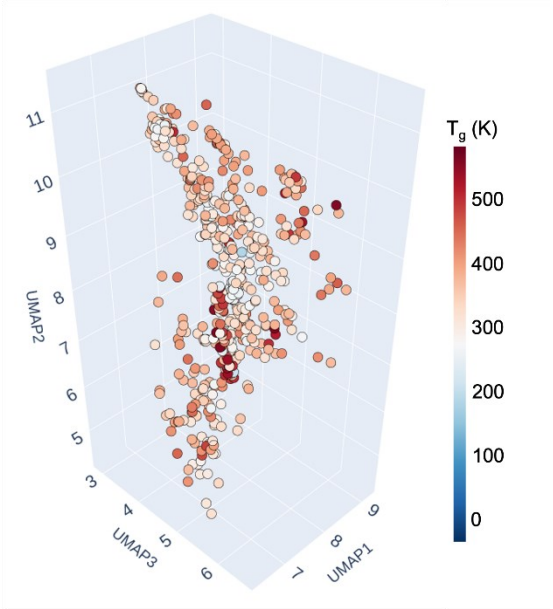
Predicting the Glass Transition Temperature of Biopolymers via High-Throughput Molecular Dynamics and Machine Learning



Publication (ACS Applied Polymer Materials): https://pubs.acs.org/doi/full/10.1021/acsapm.3c03040

High-Throughput Molecular Dynamics and Machine Learning

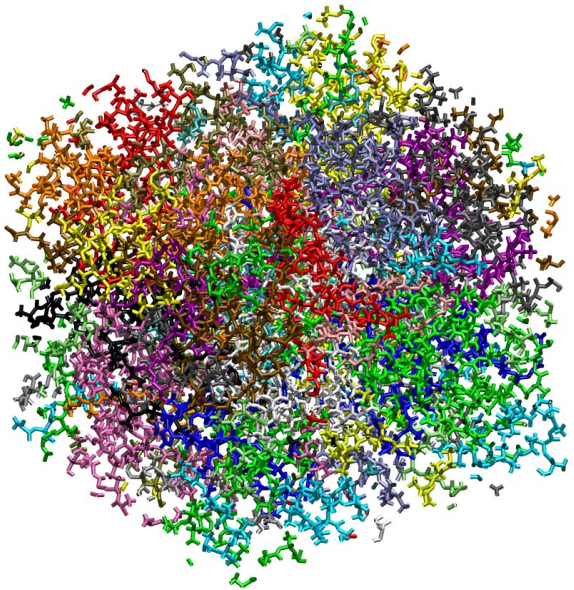
- Combination of ML and high-throughput MD to efficiently sample and characterize the relevant chemical space
- Reliable simulation protocols have been implemented to evaluate the Glass transition temperature (Tg) of a series of 58 homopolymers (in good agreement with experiments) and 488 copolymers
- 2,184 simulations (four replicas per polymer) were performed, for a total simulation time of 143 μs
- This dataset was then used to train a ML model for the prediction of the MD-calculated Tg with a mean absolute error of 19 K and an R^2 score of 0.83



ML model: https://biopolymer-ml-pub.nextmol.com/

High-Throughput Molecular Dynamics and Machine Learning

- 58 homopolymers and 488 copolymers
- Simulation boxes filled with 10 polymer chains of ~2,000 atoms each
- Own polymer builder for homopolymers and copolymers (both block and random) of any size, well pre-equilibrated
- Box size is chosen such that the final system has a density of 0.5 g/cm^3
- GAFF and GLYCAM06 (polysaccharides) force fields



Polymer melt generated with NEXTMOL Builder

Let's HPC

NEXTMOL

- EuroHPC JU Calls are a great opportunity for industry (including SMEs) to access supercomputing resources
- Open R&D
- Your code(s) need to be ready for HPC
- Helpdesk support is excellent
- Good planning of the calculations, uniformly distributed in time

NEXTMOL

The next molecules that the world needs!

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