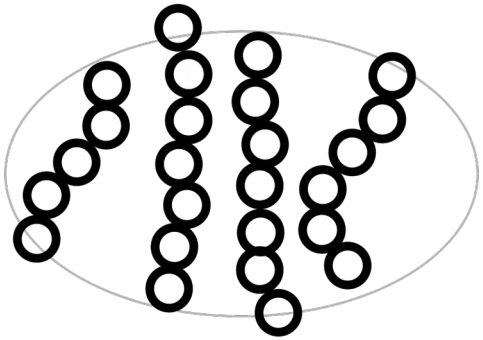
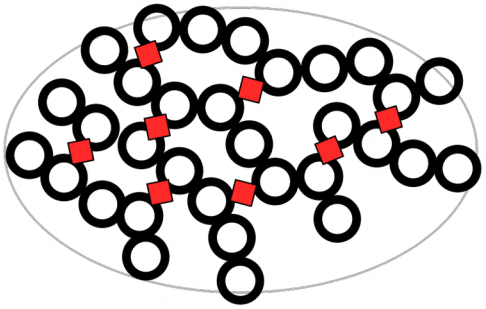
Thermoset Polymers

are polymers that are forming irreversible and well-defined 3D networks either via heating or the addition of a curing agent. The resulting materials are very strong and rigid.

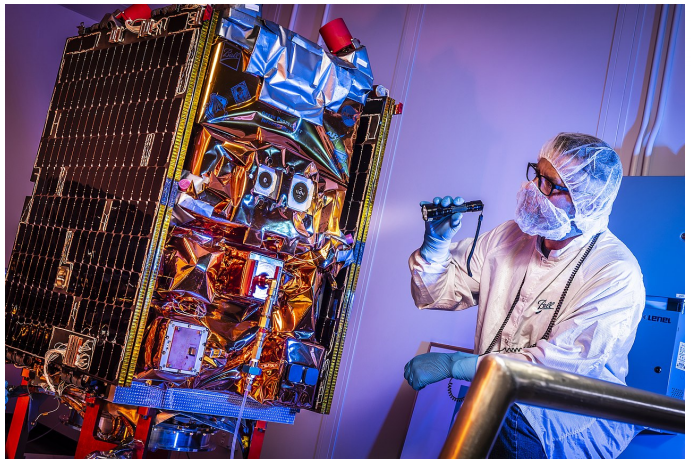


Individual polymer chains



Cross linked 3D thermoset polymer

Construction Industry



Aerospace Engineering & Military

5-minute Epoxy

Thermosets: Epoxide resins cured with amine hardeners

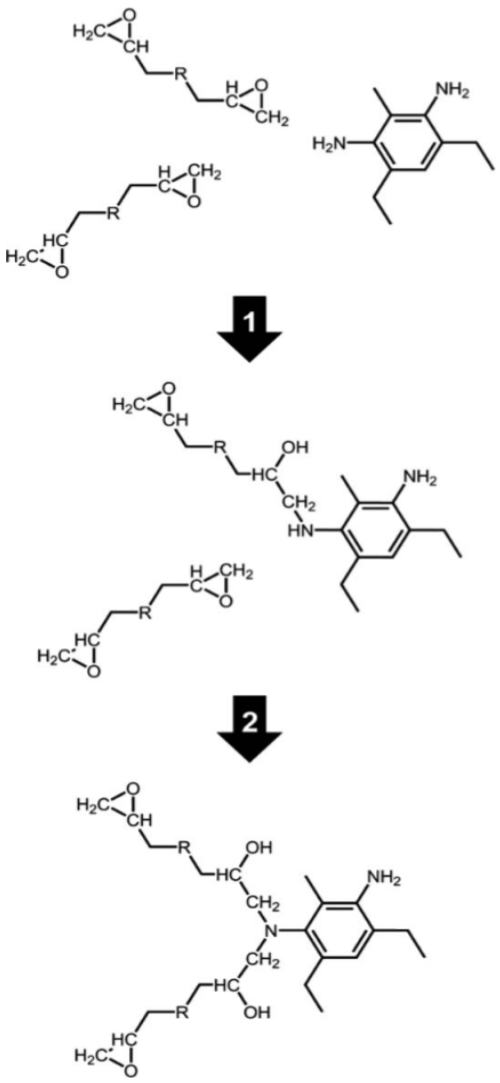
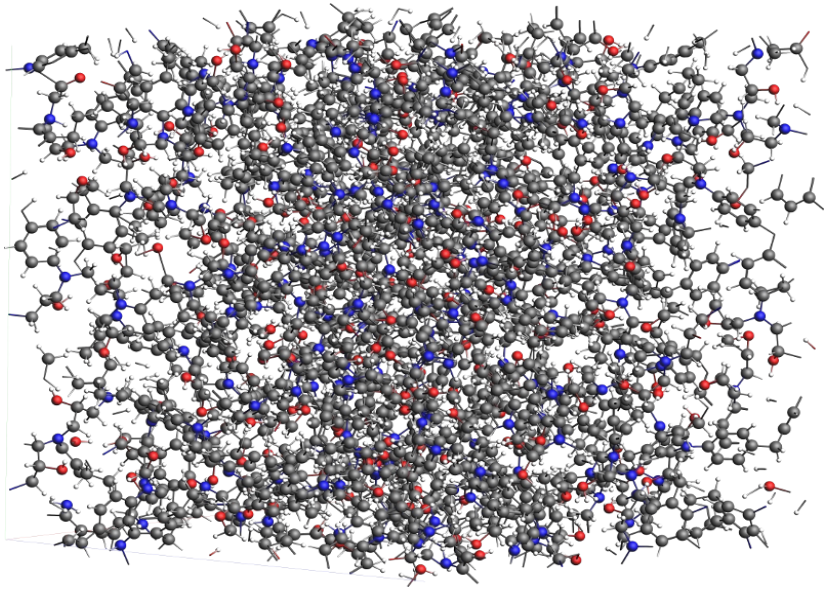


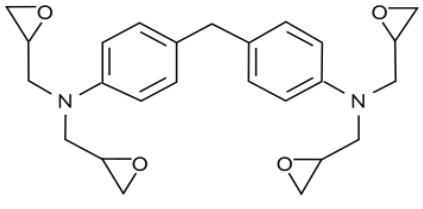
FIGURE 2 Epoxide-amine crosslinking reactions.

Objective

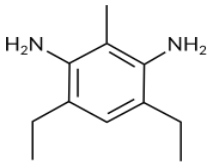
- Study effect of crosslinking on mechanical properties

- **Exp.** very slow, ~ 5h to reach 77% cross-linking
- **Sim.** time scale for MD calculations typically nanoseconds





TGDDM
Resin



DETDA
Hardener

TGDDM-DETDA polymer
- xlink density = 0.78
- 5244 atoms

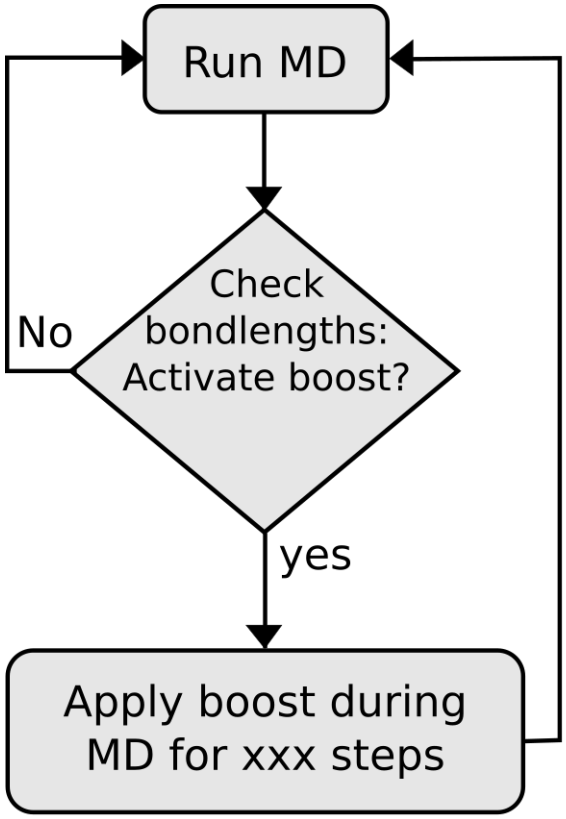
How to generate these structures?

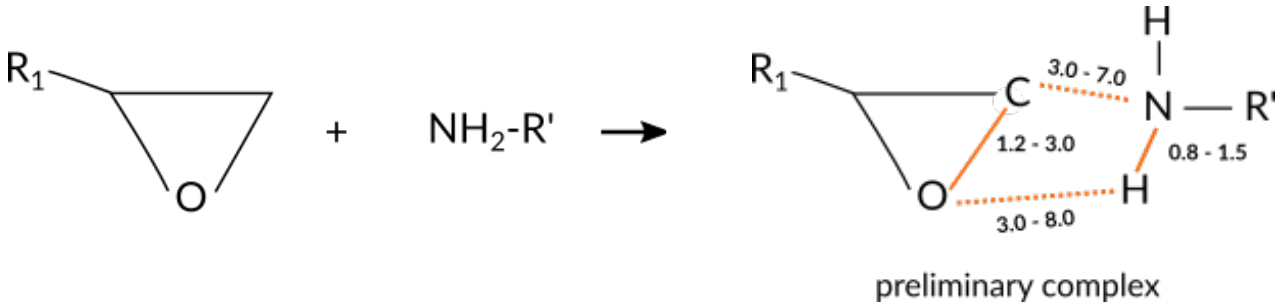
Generating highly cross-linked Epoxies

Generating Polymer Structures

Local bond boost ansatz

A. Vashisth, *et al*. J. Phys. Chem. A 2018, 122, 32, 6633-6642 (2018).



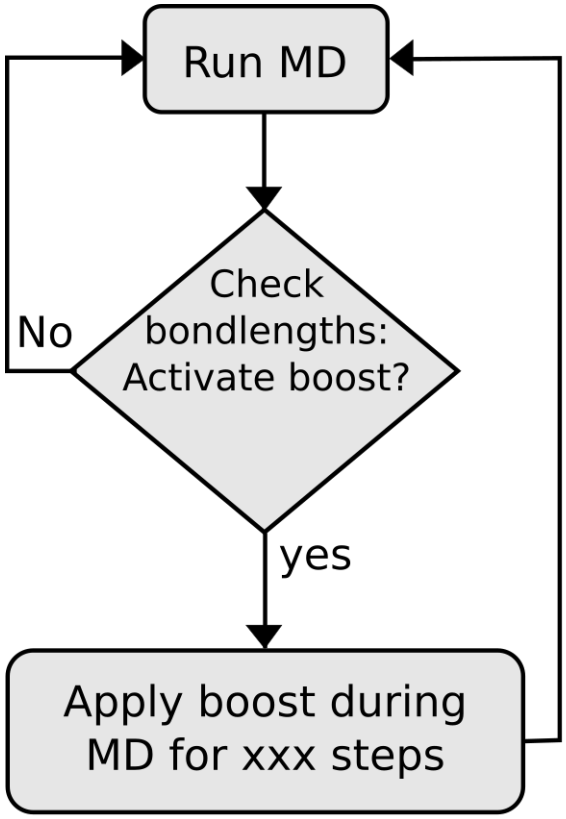


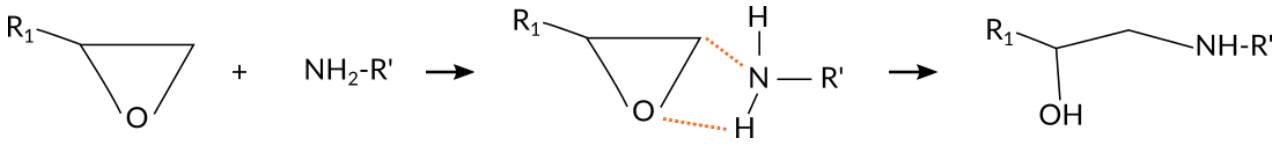
Once reactants satisfy bond length criteria the Bond Boost is switched on:

Generating highly cross-linked Epoxies

Generating Polymer Structures

Advanced SCM tutorial online:
Polymer structures with the bond boost acceleration method





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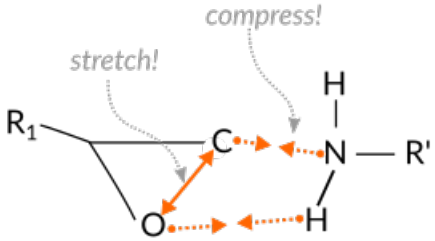
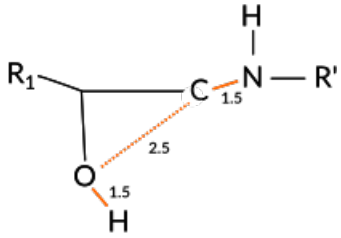


bond boost



target bond lengths

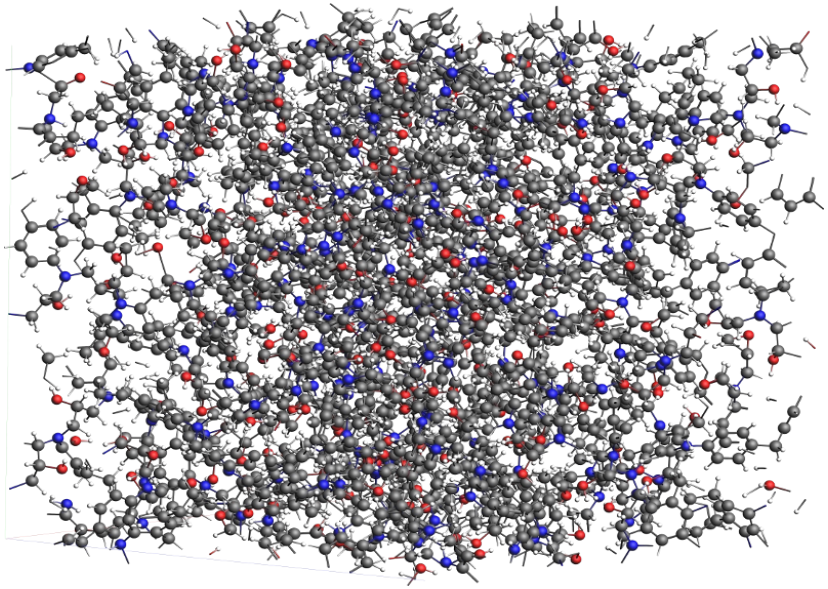
$$E_{rest} = F_1\{1 - \exp(-F_2(R_{ij} - R_{12})^2)\}$$

DEMO

Mechanical Properties of highly cross-linked Epoxies

Calculating mechanical properties

Advanced SCM tutorial online:
Mechanical properties of epoxy polymers



- Strain one lattice vector while allowing the others to relax
- Average over all directions and several different polymer structures
- Stress response calculated from atomic stresses
  (Thompson, Plimpton, Mattson, J Chem Phys, 131, 154107 (2009))

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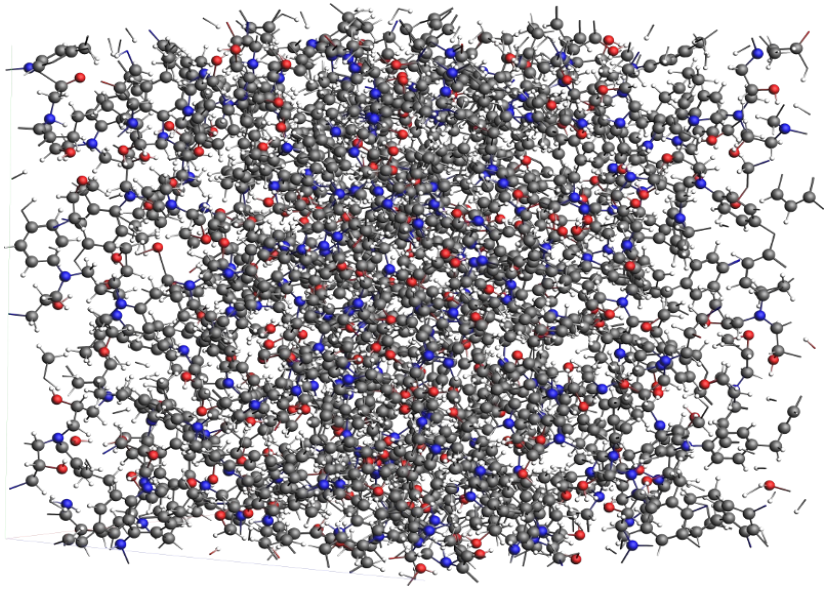

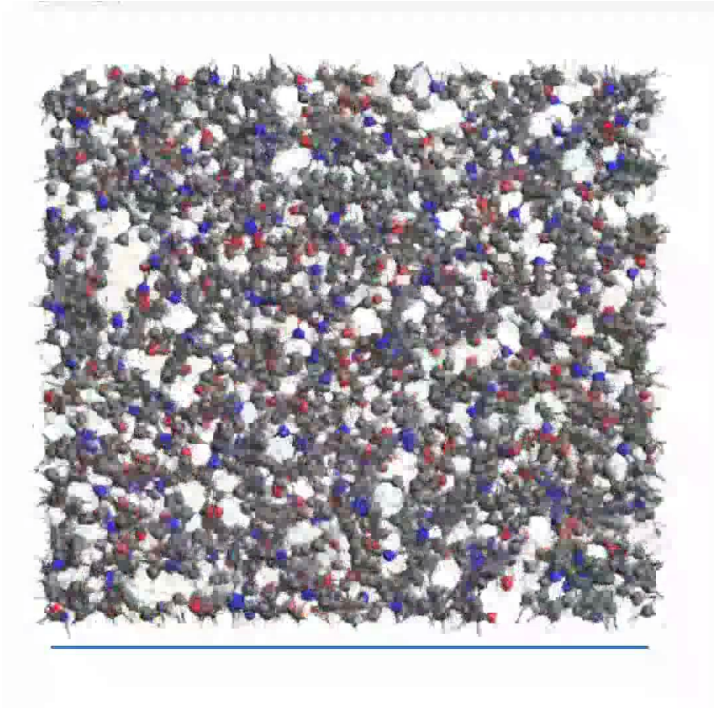

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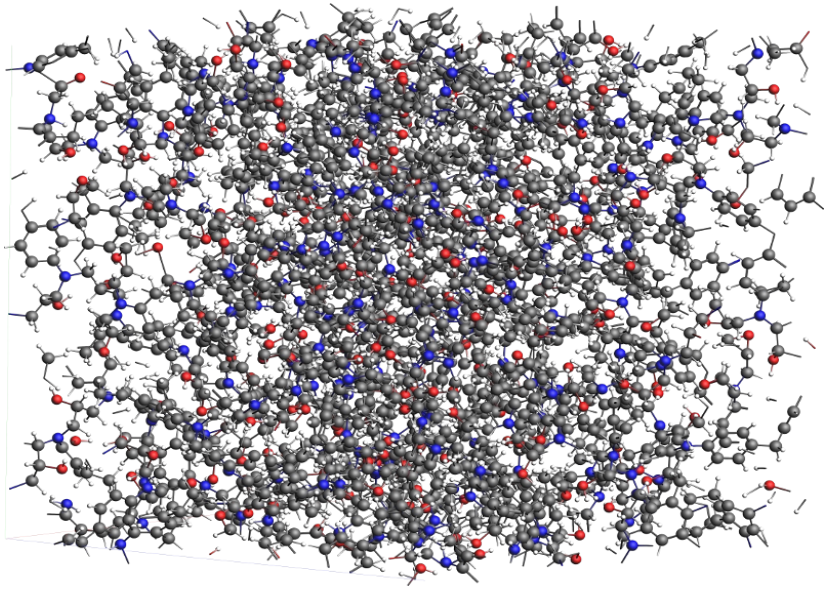

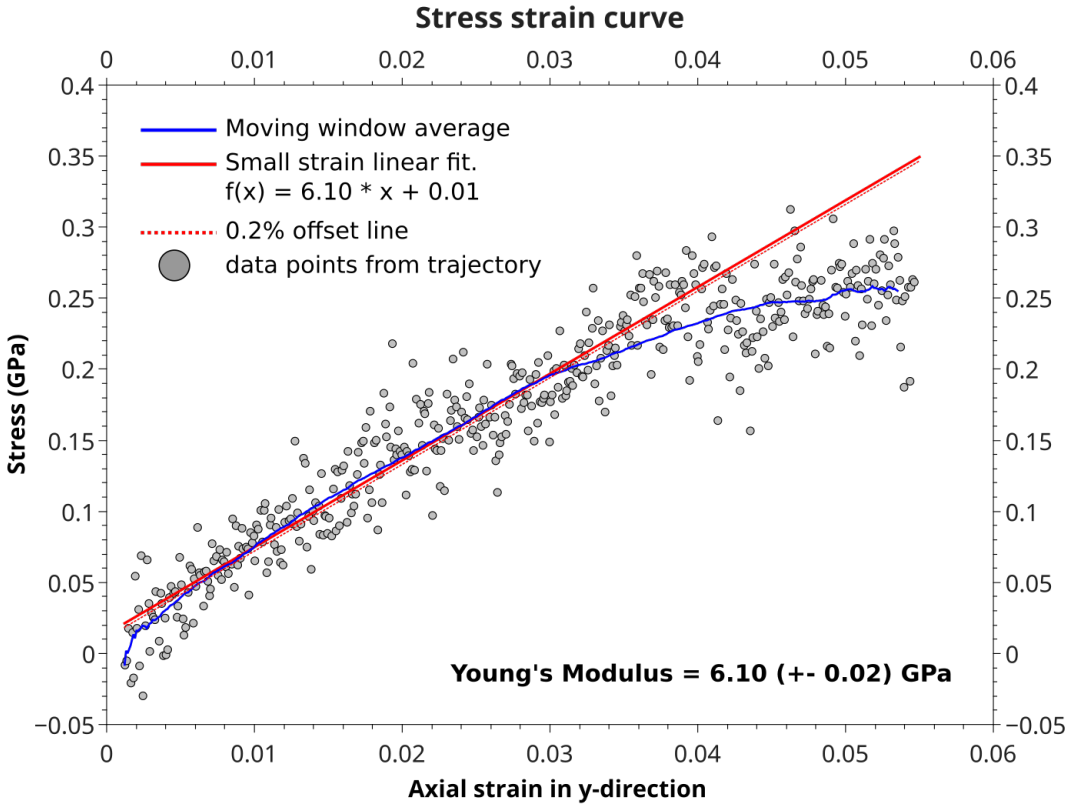

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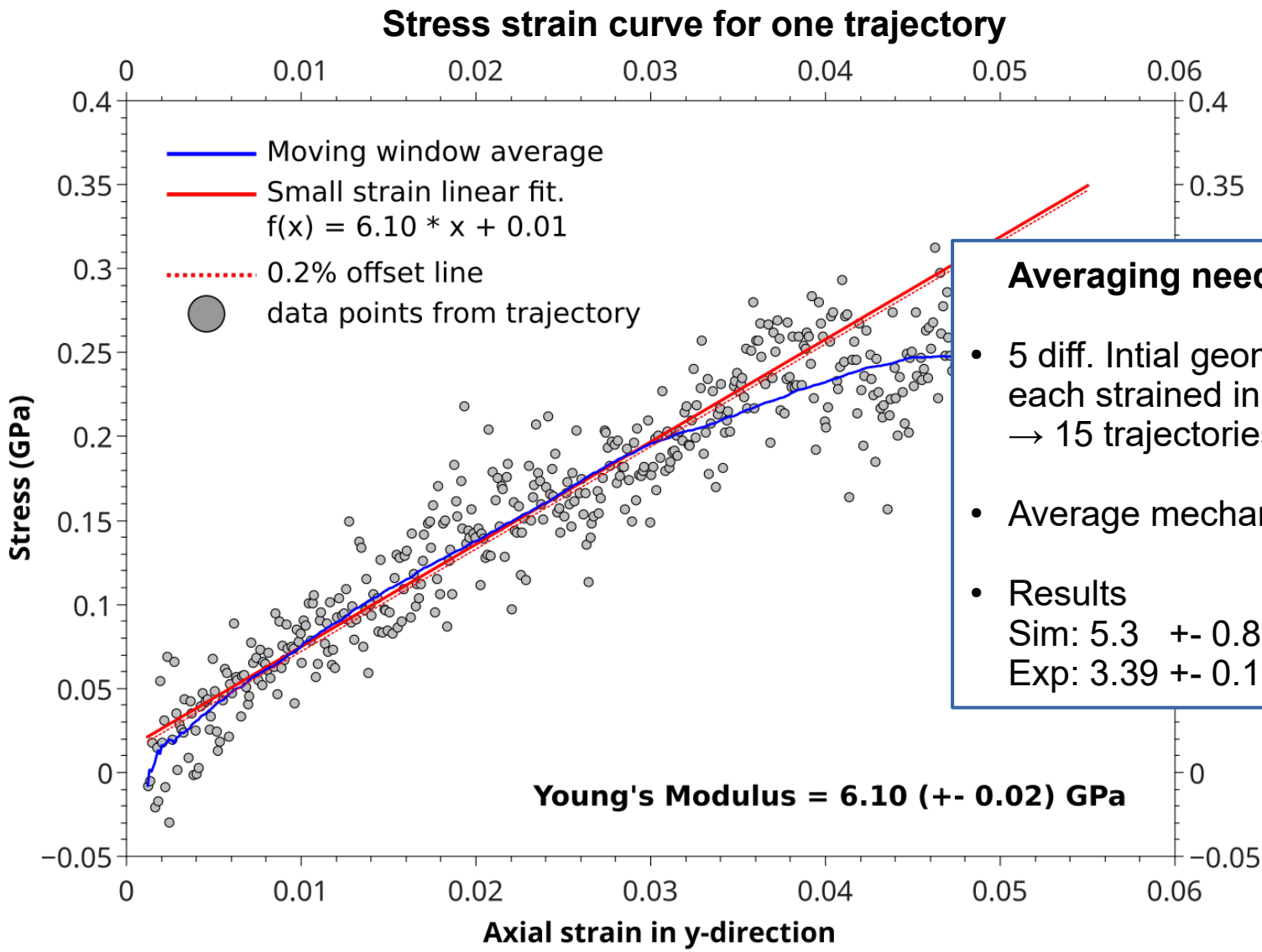
Results: Young's Modulus

workflow based on M.S. Radue,*et al.* J. Polym. Sci. B 2018, 56, 255–264.

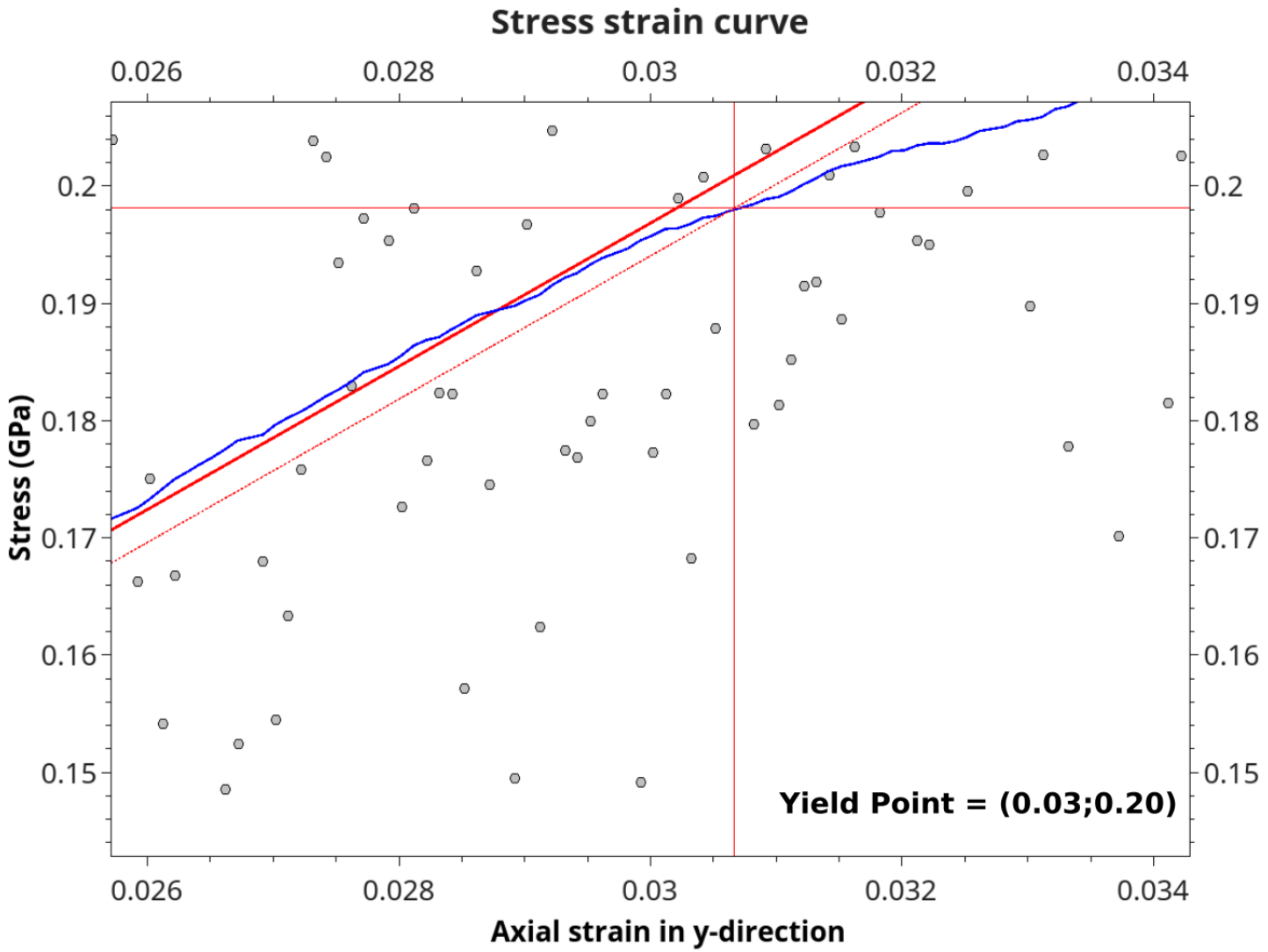


Averaging needed!

- 5 diff. Intial geometries each strained in x,y,z
  → 15 trajectories
- Average mechanical properties
- Results
  Sim: 5.3 +- 0.81 Gpa
  Exp: 3.39 +- 0.11 GPa

Results: Yield Points

workflow based on M.S. Radue,*et al.* J. Polym. Sci. B 2018, 56, 255–264.



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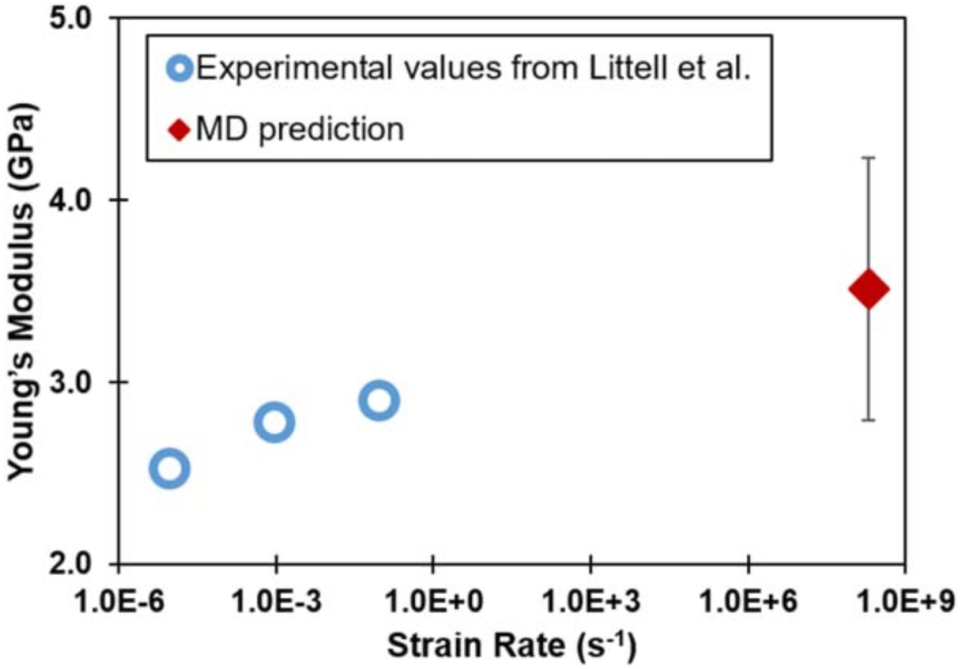
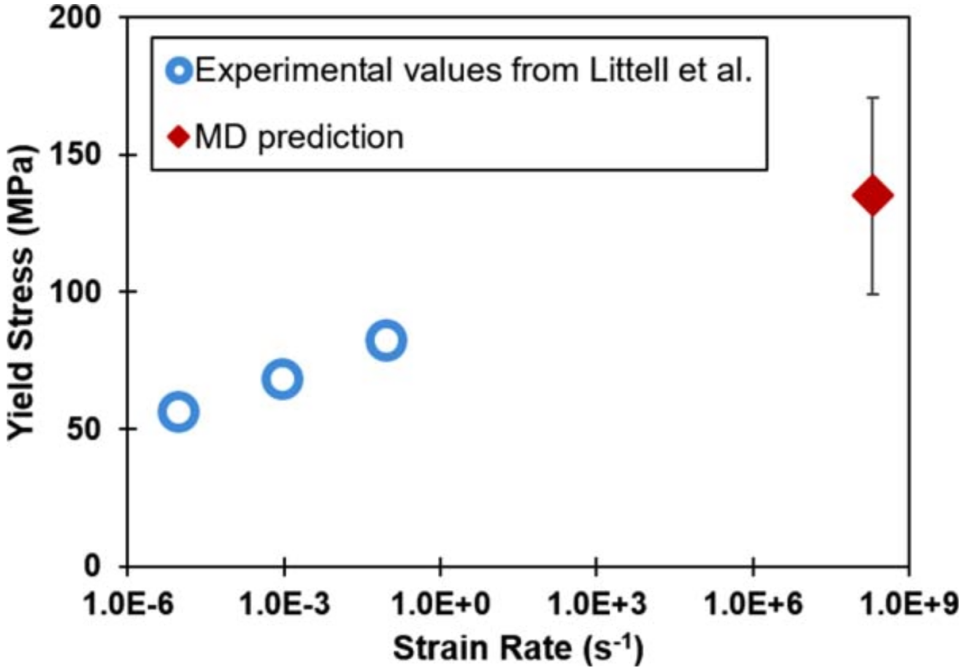
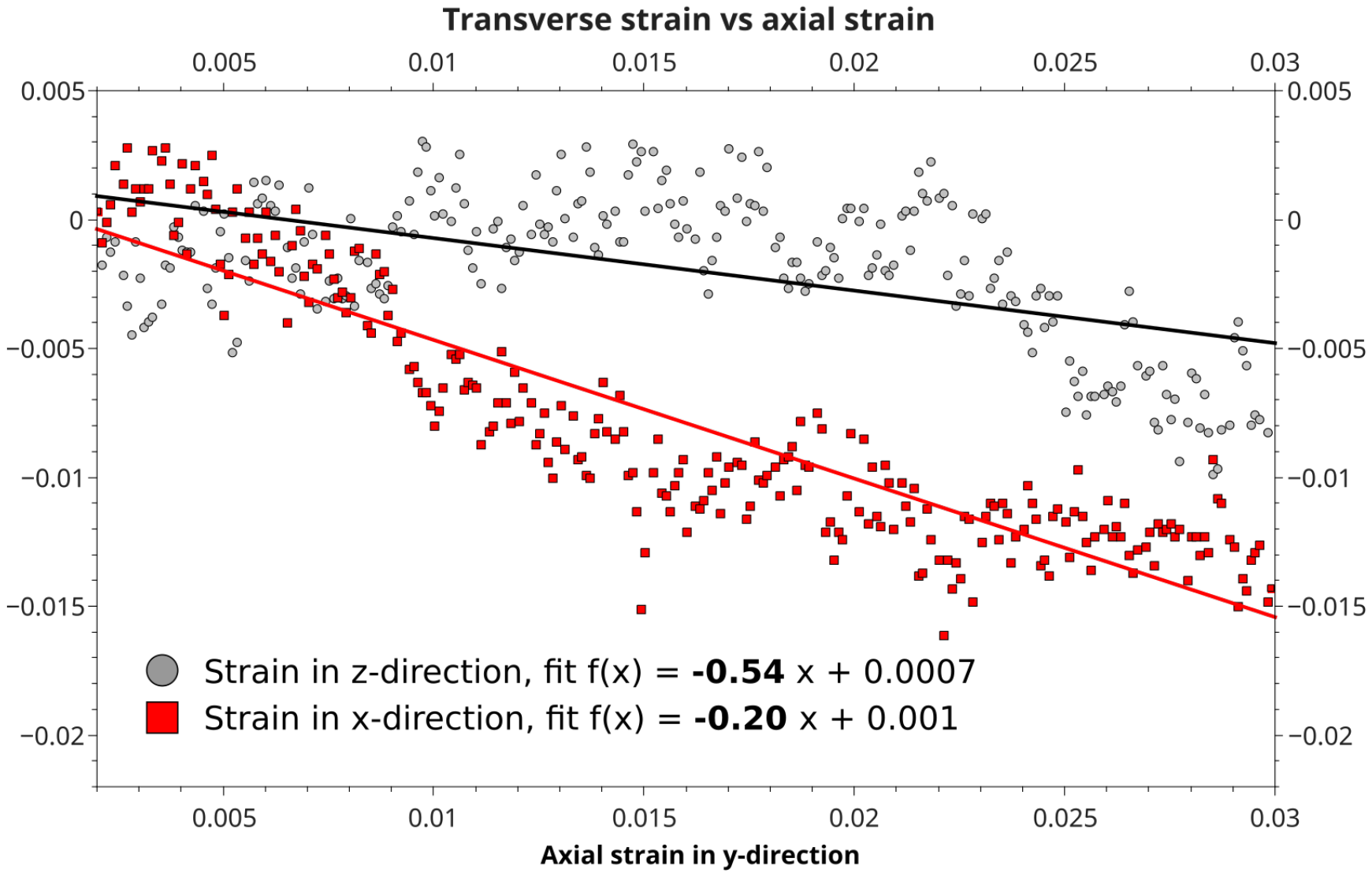


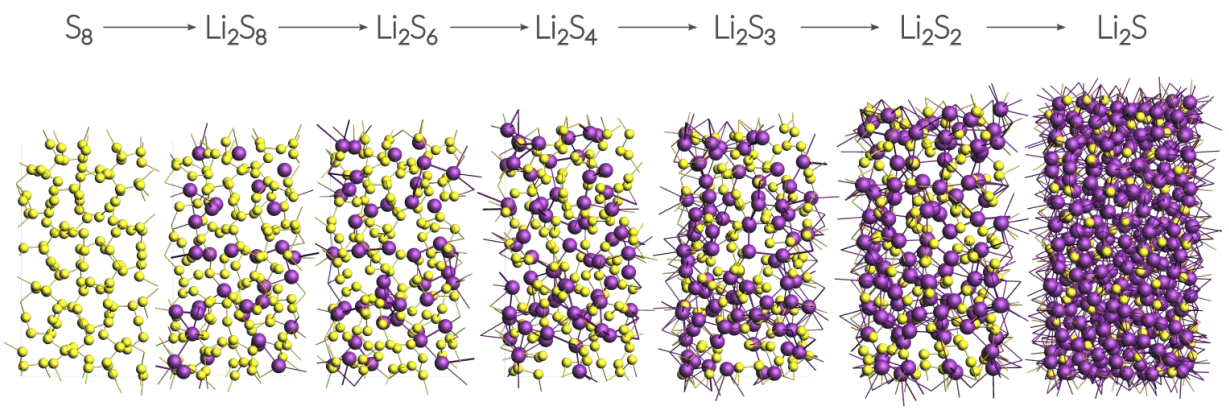


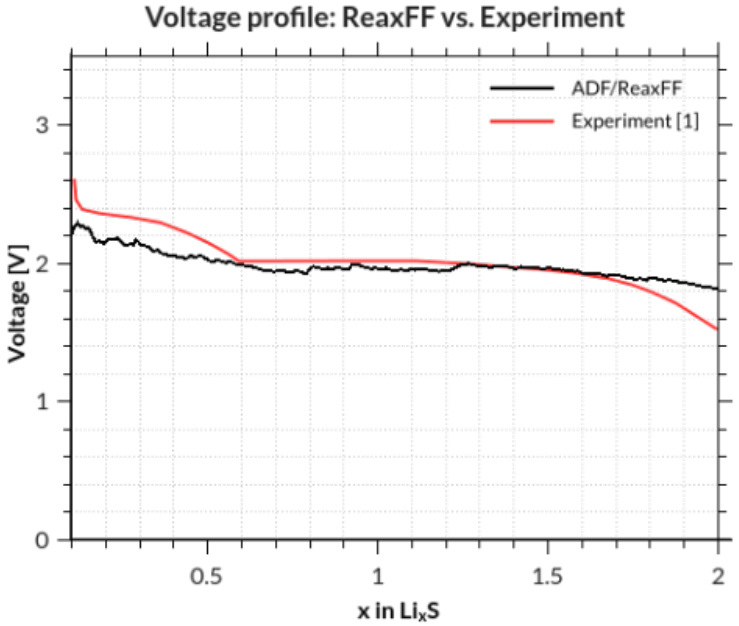
Results: Poisson's Ratio

calculations based on M.S. Radue,*et al.* J. Polym. Sci. B 2018, 56, 255–264.

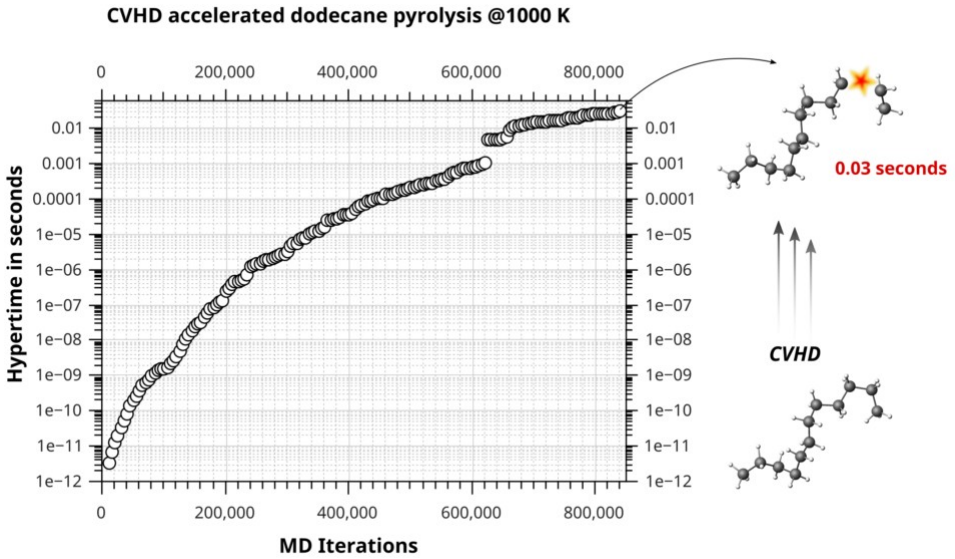


More Advanced ReaxFF (AMS Tutorials)

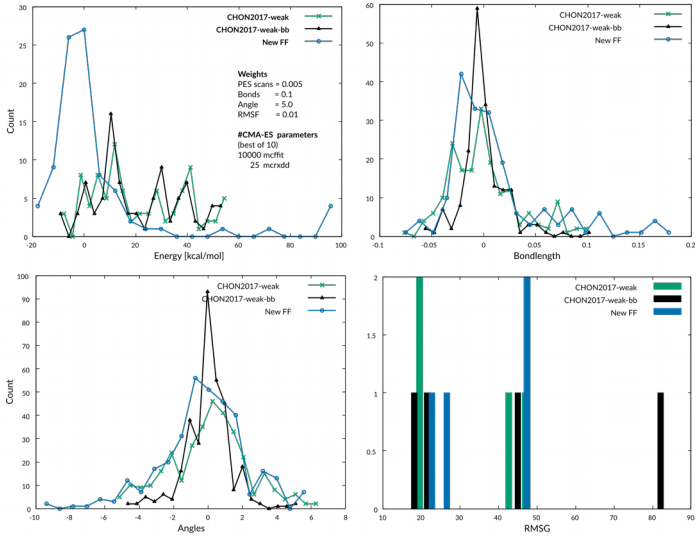




LiS Battery Discharge Simulation w. Grand Canonical MC



Collective variable driven hyperdynamics



Reparametrizing ReaxFF