Multiscale Modeling & Design of Shape-memory Polymers, PSED Cluster 2011-12

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Academic Disciplines: **Mechanical Engineering, Civil Engineering, and Theoretical & Applied Mechanics**

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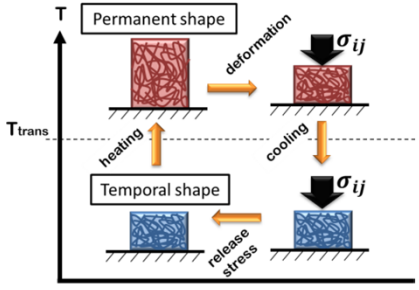
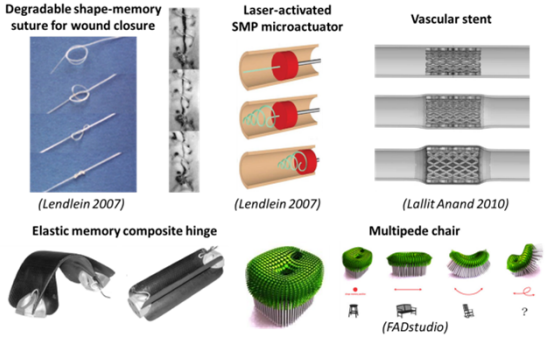
RESEARCH OBJECTIVE

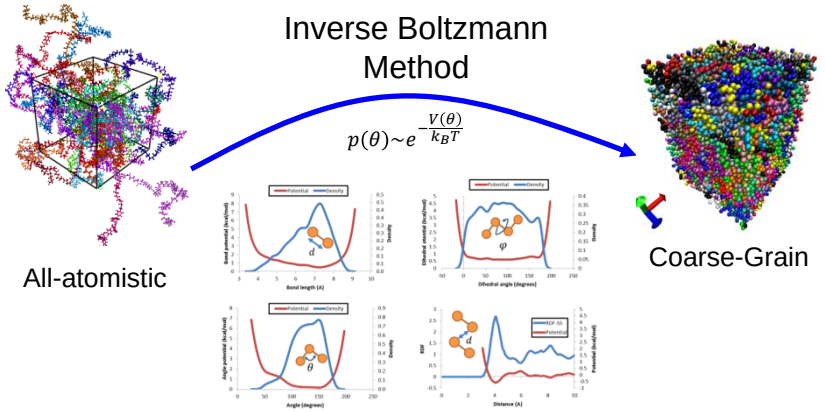
Shape memory polymers (SMP) are a promising class of responsive polymeric materials that can be programmed to adopt a temporal shape and upon application of an external stimulus, such as heat, can recover their permanent shape. In this work we propose a **hierarchical multiscale modeling approach to reach a deeper understanding and adequate quantification of the thermo-mechanical response of SMP**. This modeling and characterization effort is of capital importance for the design and implementation of SMP in current technological applications.

Shape memory cycle and applications

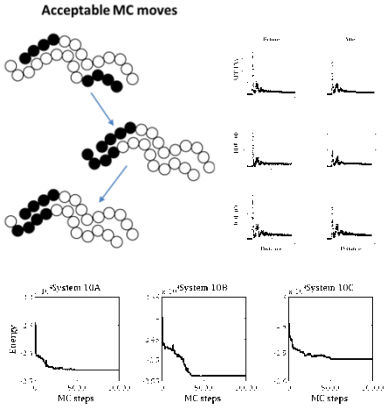




Multiscale modeling methodology



Generation of phase segregated Coarse-Grain systems

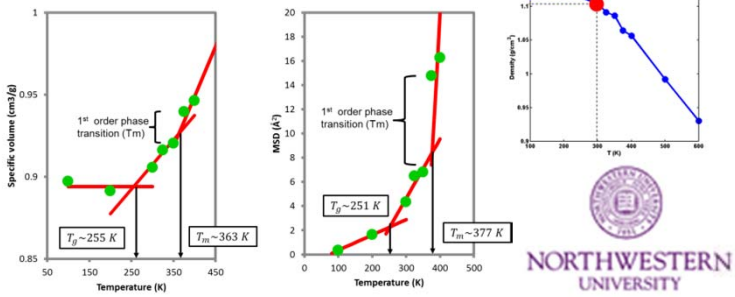


Methodology: Kinetic Monte Carlo (KMC)

- for $t = 0, \ldots, t_{end}$; for $i = 1, \ldots, N_c$
- Step 1: Generate two uniformly distributed random numbers, $u_i^d \in [-1,1]$ and $u_i^b \in [0,1]$.
- Step 2: Use u_i^d to determine the direction in which to attempt a MC move.
- Step 3: Calculate the change in energy ΔU associated with the attempted move.
- Step 4: If $\Delta U \leq 0$, accept the move and skip step 5. If $\Delta U > 0$, go to step 5.
- Step 5: Calculate the Boltzmann factor $b = e^{-\frac{\Delta U}{k_B T}}$. If $u_i^b < b$, accept the move.

Atomistic model validation

Selected properties, namely glass transition and melting temperatures and density, have been calculated using the atomistic model and compared to experimental results of macroscopic systems.



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