Basic principles of molecular and coarse-grained simulations

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Concepts covered:

- Computer simulations in polymer physics
- Molecular dynamics and Monte Carlo approach
- Periodic boundary conditions
- Open-source codes
- Non-equilibrium molecular dynamics
- Coarse-grained molecular dynamics. Brownian dynamics
- Smoluchowski and Langevin approaches
- Systems with one or many degrees of freedom
- Dumbbell model
- Finite extensibility
- Rouse chains
- Coarse-grained simulations for unentangled and entangled polymers.