

Lecture 5. Molecular Dynamics Simulations

- Download course materials
<https://mulan.swmed.edu/lecture5.tar.gz>

To unpack the tar.gz ball, run the following command:

tar xvfz lecture5.tar.gz

A new directory, lecture5 will be created

- Read the book chapters of “Molecular Modelling: Principles and Applications (2nd Edition)” entitled “6 Computer Simulation Methods” and “7 Molecular Dynamics Simulations Methods”
- Download amber manuals from ambvermd.org
- Go through Amber tutorials from ambermd.org