Term project

Objective: To get experience in designing and performing computer simulations.

Parts of the project:
- Design (or adapt an idea from literature) a simulation that is of scientific or computational interest to you.
- Choose and justify computational approach that is appropriate.
- Write the code (or add parts to MSE627-MD or MSE627-MC codes)
- Perform simulations and analyze the results.
- Prepare a report/paper.
- Make a short presentation to the class (mini-symposium).

Timeline:
- September 25th – decide on the topic/title of your project, inform the instructor
- November 1st – prepare the first draft of the introduction (with references to relevant papers) and discuss progress with instructor (optional)
- End of November or early December (dates TBD) – turn in report; give presentation to the class at a mini-symposium

Below are several examples of possible term projects. These are just examples, you can propose your own project that is relevant to your thesis research or just seems interesting to you. If the intention is to continue computational work in the future, the term project may be a well-defined part of a larger research project.
Cluster formation and disintegration in a vapor


Research Project: Microcanonical molecular dynamics simulation of a gaseous system with presence of clusters. Potential can be the Lennard-Jones for argon. Perform simulations for different densities and temperatures. Choose $P$ and $T$ based on known phase diagram for Ar. Analyze velocity distributions of atoms. Relate simulation data to Homogeneous Nucleation Theory, e.g. [F. F. Abraham, Homogeneous Nucleation Theory (Academic, New York, 1974)]

An example of MD simulation of cluster birth-death processes in a vapor:

Computational challenges: Choosing the initial velocities of atoms based on the desired temperature; Identification of clusters; Changing volume/density; Visualization, making animations; Statistical analysis.
Strain relief mechanisms in lattice mismatched heterostructures


**Research Project:** Simulation of interfacial fracture due to the lattice mismatch between the overlayer and substrate. Calculate stress distributions, Analyze the mechanisms of stress relief (crack propagation, dislocation nucleation). Discuss the final defect configuration.

**Computational challenges:** Choosing parameters of Lennard-Jones potential for two lattices; Calculation of stress distribution, Structural analysis; Visualization, making animations.
MD simulation of human crowds, bumper car rides, etc.

Simulations based on a hypothesis that humans in a crowd interact with their neighbors through some form of “social potential,” analogous to the repulsive potential energies between physical particles.

**Computational challenges:** Designing “social potentials” and laws of motion; Setting up a 2D model, boundary conditions, *etc.*; Analysis of snapshots and dynamics; Visualization.


Experiments at the rides at the amusement park of Barselona TIBIDABO are compared with analogous hard disks system: radial distribution functions of cars’ coordinates are calculated.
Reactive mixing in multilayers, self-propagating reactions

fcc atoms (Ni or Al) are **green** B2 NiAl is **blue**

unclassified (amorphous or grain boundary atoms) are **translucent orange**

M.J. Cherukara, T.P. Weihs, A. Strachan, Molecular dynamics simulations of the reaction mechanism in Ni/Al reactive intermetallics, Acta Mater. 96, 1-9, 2015

V. Turlo, O. Politano, and F. Baras, Alloying propagation in nanometric Ni/Al multilayers: A molecular dynamics study, J. Appl. Phys. 121, 055304, 2017

MD simulation of thermally ignited samples of reactive core/shell Ni/Al wires or multilayers

**Computational challenges:** Implementation of interatomic potential for binary system, generation of initial systems, structural analysis (identification of phases and defects), visualization.

*University of Virginia, MSE 4270/6270: Introduction to Atomistic Simulations, Leonid Zhigilei*
Structure of small atomic clusters

**Research Project:** Search for energetically favorable atomic configurations for small Lennard-Jones clusters of atoms. Compare non-crystalline icosahedral clusters with face-centered cubic clusters for small numbers of atoms. Which ones have lower energy? What is the role of surface and interior energies? What is the critical size when the crystalline structure becomes more stable? Compare with experimental electron diffraction data and other simulations. This study can be performed for metals as well (EAM potential).


Huang et al., RSC Adv. 4, 7528, 2014 - single-crystalline and multiple-twinned gold nanoparticles

**Computational challenges:** Making initial configurations with fcc and non-crystalline structure; Adding EAM potential in case of metal clusters; Structural analysis; Choosing and adding to the MD code an algorithm for energy minimization; Visualization.
Stability and evolution of nanoscale features on surfaces

http://www.lassp.cornell.edu/cooper_nanoscale/nanofeatures.html

**Research Project:** Investigate the stability and evolution of nanoscale features on Si or metal surface. Modeling of the decay of islands and pits can be performed by Monte Carlo or Molecular Dynamics method. Choose a system for which experimental data is available or which is of potential technological interest. Compare simulation results with available experimental data or discuss potential implications of the results.


**Computational challenges:** Adding interatomic interaction potential appropriate for the system of interest to the MD/MC code; Adding/modifying algorithm for MD/MC simulation; Creating initial configuration; Visualization, making animations.
Melting of small atomic clusters or core-shell structures

Research Project: Simulation study of melting of small Lennard-Jones clusters. Where does melting start, how it proceeds, what are the driving forces? Is there a region of coexistence of melted surface and solid core? Is there desorption from the surface at temperatures close to the melting point? Define the onset of melting through the visual inspection and analysis of the atomic mobility. Compare with results from other simulations.

K.-C. Fang and C.-I. Weng, Nanotechnology 16, 250 (2005) - Si clusters

Computational challenges: Choosing the initial velocities of atoms based on the desired temperature; Performing simulations at constant energy or constant temperature conditions; Structural analysis; Visualization, making animations.

University of Virginia, MSE 4270/6270: Introduction to Atomistic Simulations, Leonid Zhigilei
Melting – Crystallization - Amorphization

Research Project: Simulation of melting, crystallization, and/or amorphization of a model material (e.g. Lennard-Jones Ar, Stillinger – Weber Si, EAM metal). Many papers have been published on this subject. A big variety of questions can be addressed.


V. A. Likhachev et al., Phil. Mag. A 69, 421-436, (1994) - Quenching of nickel from the melt leading to its amorphization or crystallization.


Computational challenges: Code Nosé-Hoover constant temperature and pressure algorithm. Analysis of structural changes, dynamic properties; Visualization.
Coexisting liquid and solid phases, kinetics of melting and solidification

**Research Project:** Determine the melting temperature of a system (Lennard-Jones, EAM metal, Stillinger-Weber Si) by examining coexistence of a liquid and solid at a fixed pressure. Discuss various approaches that have been used to determine the melting temperature for a given potential.

What is the dependence of the velocity of melting/solidification on the degree of overheating/undercooling above/below the equilibrium melting temperature?


**Computational challenges:** Choosing appropriate boundary conditions; physics of melting and how to study it computationally; structural analysis, animations.
Simulation of atomic structure of interfaces, dislocations, vacancies, and interstitials in two-dimensional crystals


Examples of 2D MD simulations:

Computational challenges: Making initial atomic configurations for defects; Choosing correct periodicity for grain boundaries; Structural analysis; Calculation of atomic level stresses; Visualization, making animations.
Simulation of dynamic processes in two-dimensional crystals


**Research Project A.** Test a theory for melting in two dimensions that was developed by Kosterlitz, Thouless, Halperin, Nelson, and Young (the KTHNY theory, after the initials of its authors' last names).

B. Study generation of a dislocation cloud screening the elastic field of a disclination introduced into a finite-size crystallite.


**Computational challenges:** Preparing initial atomic configurations; Analysis of structural changes; Calculation of atomic level stresses; Visualization, making animations.
Collision of small atomic clusters

Research Project: Simulation study of the dynamics of colliding clusters, study the development of temperature, potential energy, transformation of the shape of the resulting particle. What are the energy transformations during the collision? What is driving the subsequent reshaping of the resulting particle? Is temperature increasing or decreasing in this processes?


Computational challenges: Choosing the initial velocities of atoms; Quantitative analysis should be inspired by structural analysis, visualization, and animations.
The Tethered Membrane - a Model of Random Surface

Research Project: A simple model of polymerized membranes, the tethered membrane, has been proposed as a model to study the large-scale properties of random surfaces (microemulsions, lipid bilayers, vesicles, and suspensions of monolayers of exfoliated layered crystals). You can reproduce some of the results of this study and extend the model to address new questions.


Computational challenges: Development (based on MSE627-MD) of a computer code for the tethered membrane model; Temperature control; Structural analysis; Visualization, making animations.
Dynamics of Coulomb explosion of identical charged particles

E. B. Kolomeisky, *Coulomb Universe in a Jellium droplet*,

**Research Project:** Simulation of evolution of a system of $N \gg 1$ identical charged particles repelling each other according to the $1/r$ Coulomb law from various compact initial configurations. The goal is to verify recently developed theory that addresses dynamics of Coulomb explosion from macroscopic standpoint. It is predicted that evolution of this system has a lot in common with that of the physical Universe with hallmarks such as Hubble’s law present. Calculate density distributions as well as evolution of relative velocities of the particles versus their separation. Test sensitivity of the outcome to initial conditions.

**Computational challenges:** Choosing initial configurations; Dealing with long-range Coulomb interactions; Visualization, making animations.
Research Project: Modify molecular dynamics algorithm for a two-dimensional space of constant curvature. Perform simulations of a close-packed system in the curved space. What is the structure? Why? This project is suitable for a physicist with a taste for mathematics.


Computational challenges: Modification of molecular dynamics code to reproduce a curved space; Structural analysis of a two-dimensional system; Visualization, making animations.
2D Monte Carlo modeling of microstructural evolution (grain growth, recrystallization, precipitation, coarsening)

http://cmpweb.ameslab.gov/cmsn/microevolproj.html

**Research Project:** Develop a computer code for the Monte Carlo Potts model that can be used to study kinetic evolution of the system towards thermodynamic equilibrium. Perform 2D simulation of grain coarsening or recrystallization. The description of the method and references can be found in [Dierk Raabe, Computational materials science: the simulation of materials, microstructures and properties (Wiley-VCH: Weinheim, 1998) pp. 223-232].

**Computational challenges:** Developing a computer code for the Monte Carlo Potts model; Preparing initial structure; Visualization, making animations.
Oscillatory surface segregation of Si-Ge alloys

**Research Project:** There is a study by P. C. Kelires & J. Tersoff, Phys. Rev. Lett. 63, 1164-1167 (1989) in which they incorporate two kinds of Monte Carlo moves – small atomic displacements and interchange of atom type) to investigate surface segregation vs temperature in Si-Ge alloys. You can investigate similar effects for the Stillinger-Weber Si-Ge system, and/or investigate segregation of Si and Ge atoms in small clusters…

**Computational challenges:** Coding potentials; Varying types of MC moves; Making the initial atomic configuration; Choosing boundary conditions; Structural analysis; Visualization.


Computational challenges: Implementation of new computational methods; Large number of simulations; Data analysis and fitting
**Calculation of the Critical Point**

**Research Project:** Calculation of critical point in MD is not a straightforward task and requires reconstruction of a liquid-vapor coexistence curve (binodal line). The project may involve calculation of equilibrium liquid and vapor densities for LJ potential (or other systems) and fitting the binodal line to the analytical dependence.


**Computational challenges:** Density averaging over a simulation; Calculation of the time for density equilibration; Temperature control; Building the initial system; Large number of long simulations; Data analysis and fitting.
Heat conductance of interfaces


**Research Project**: Perform calculation of heat flux through an interface. Investigate the effect of interface sharpness, material properties mismatch, interfacial film thickness, or other factors on the interfacial conductance.

**Computational challenges**: Calculation of heat flux in MD simulation; Building the initial system; Temperature control; Data analysis and fitting.