Purdue MSE597G Lectures on Molecular Dynamics simulations of materials

Lecture 1:
Classical Mechanics

Alejandro Strachan
School of Materials Engineering and Birck Nanotechnology Center
Purdue University
strachan@purdue.edu

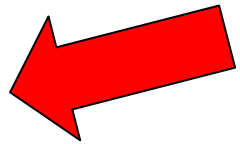
PURDUE UNIVERSITY

Lectures on Molecular Dynamics simulations

Introduction

- What is molecular dynamics (MD)? Examples of current research
- Why molecular dynamics?

Part 1: the theory behind molecular dynamics



- Basic ideas & algorithms
- Brief introduction to the physics necessary to run & understand MD

Part 2: total energy and force calculations

- Quantum mechanical origin of atomic interactions
- Inter-atomic potentials: “averaging electrons out”

Part 3: advanced techniques, mesodynamics, verification and validation

- MD in under isothermal and isobaric conditions
- Coarse grain approaches and dynamics with implicit degrees of freedom
- Before you perform production runs

What is molecular dynamics?

Follow the dynamics (motion) of all the atoms in your material

Numerically solve classical equations of motion (Newton's):

Approximation

$$\vec{F}_i = m_i \vec{a}_i \qquad \text{or} \qquad \begin{cases} \dot{\vec{r}}_i = \dfrac{\vec{p}_i}{m_i} \\ \dot{\vec{p}}_i = \vec{F}_i \end{cases}$$

Forces on atoms come from the interaction with other atoms:

$$\vec{F}_i = -\vec{\nabla}_{r_i} V\left(\{r_j\}\right)$$

Total potential energy

Approximated
(in almost all cases)

Classical mechanics: Hamilton's picture

William Hamilton reformulation of classical mechanics (1800's)

Hamiltonian:

$$H(\{r_i\},\{p_i\}) = V(\{r_i(t)\}) + \sum_{i=1}^{3N} \frac{p_i(t)^2}{2m_i}$$

i denotes atom and Cartesian component (x, y, or z)

Equations of motion can be derived from the Hamiltonian:

- These equations can only be solved analytically for very few cases
- MD solves the dynamics of many atoms (billions in supercomputers)

Classical mechanics: conserved quantities

$$H(\{r_i\},\{p_i\}) = V(\{r_i(t)\}) + \sum_{i=1}^{3N} \frac{p_i(t)^2}{2m_i}$$

Let's calculate the time derivative of the Hamiltonian:

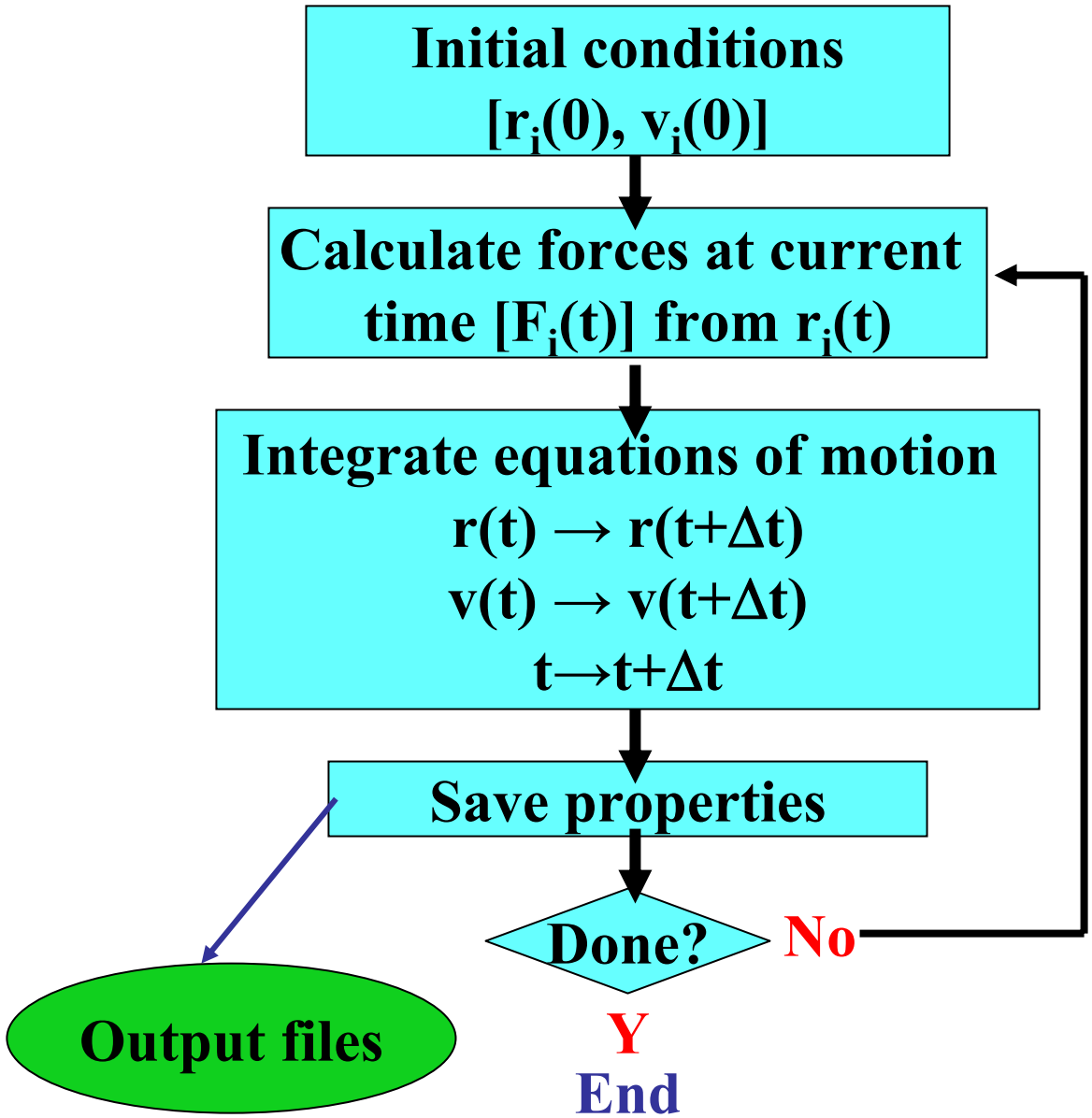
$$\frac{dH}{dt} = \sum_{i=1}^{3N} \left(\frac{\partial H}{\partial r_i} \dot{r}_i + \frac{\partial H}{\partial p_i} \dot{p}_i \right)$$

Using the equations of motion we get:

Other constants of motion are:

- Linear momentum:
- Angular momentum:

Structure of a minimalist MD code



Analysis/interpretation of MD: statistical mechanics

Goal: describe concepts that enable relating molecular dynamics with thermodynamics properties