THE UNIVERSITY of TENNESSEE KNOXVILLE

Lecture 09: Ordinary Differential Equations (ODE)

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This and that

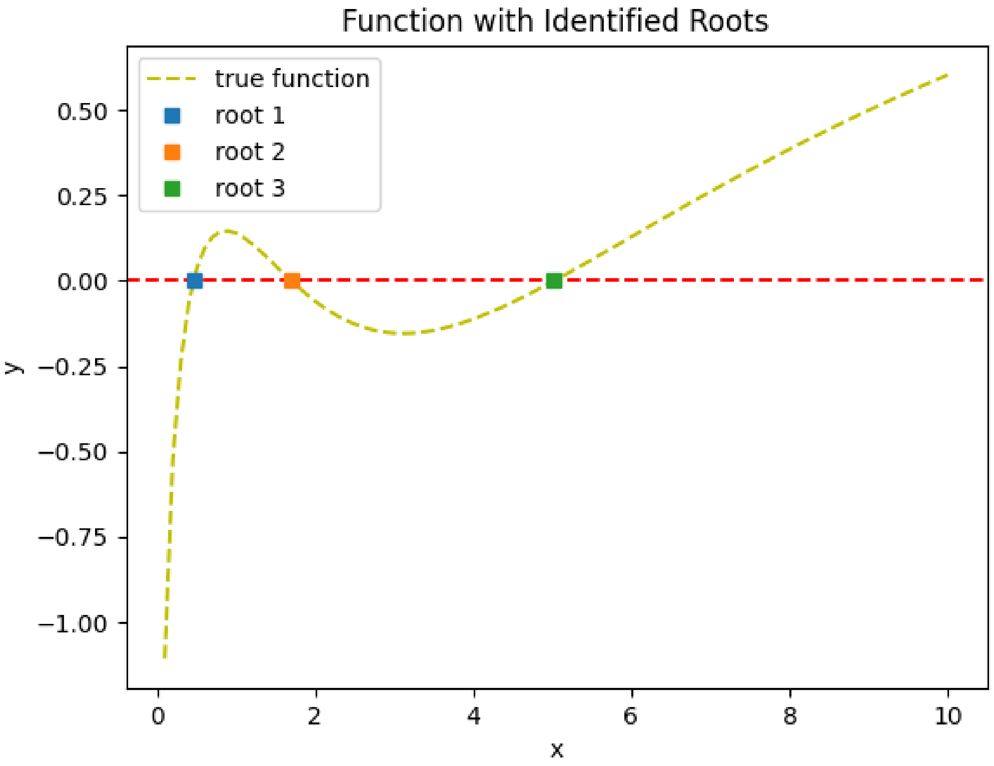
- Please share homeworks, midterms, and finals both with me (sergei2@utk.edu) and Sheryl Sanchez (ssanch18@vols.utk.edu)

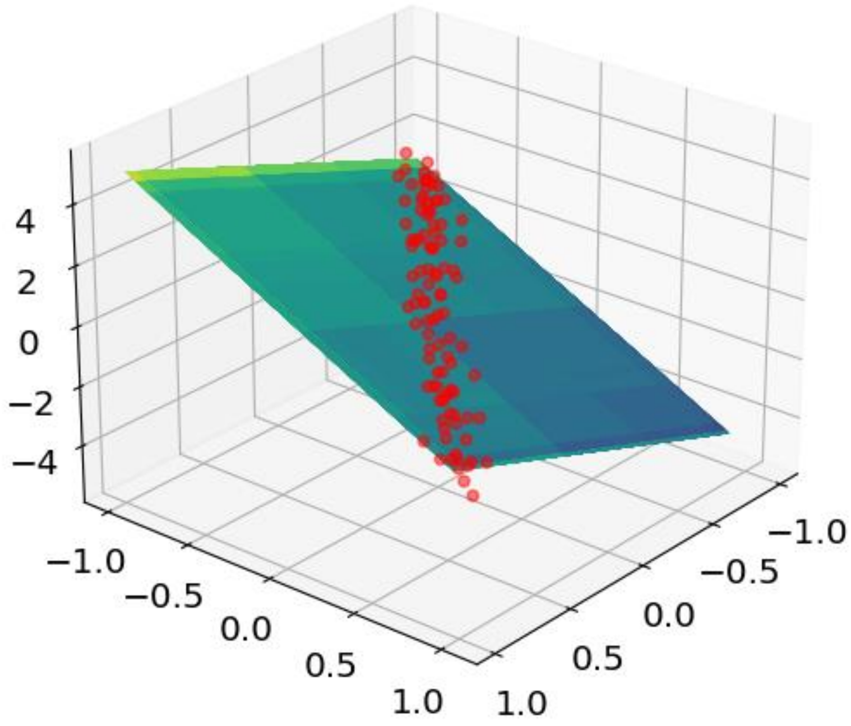
- If you do not see your grade on the Canvas for HW1-3, or if you would like to change it, please (re)submit the homework

- GitHub lecture by Rama Vasudevan - Wednesday, February 21, 2024 1:00 PM-2:00 PM. Please send me email so I forward you the invite

- For office hours, please drop me e-mail in advance if you would like to meet

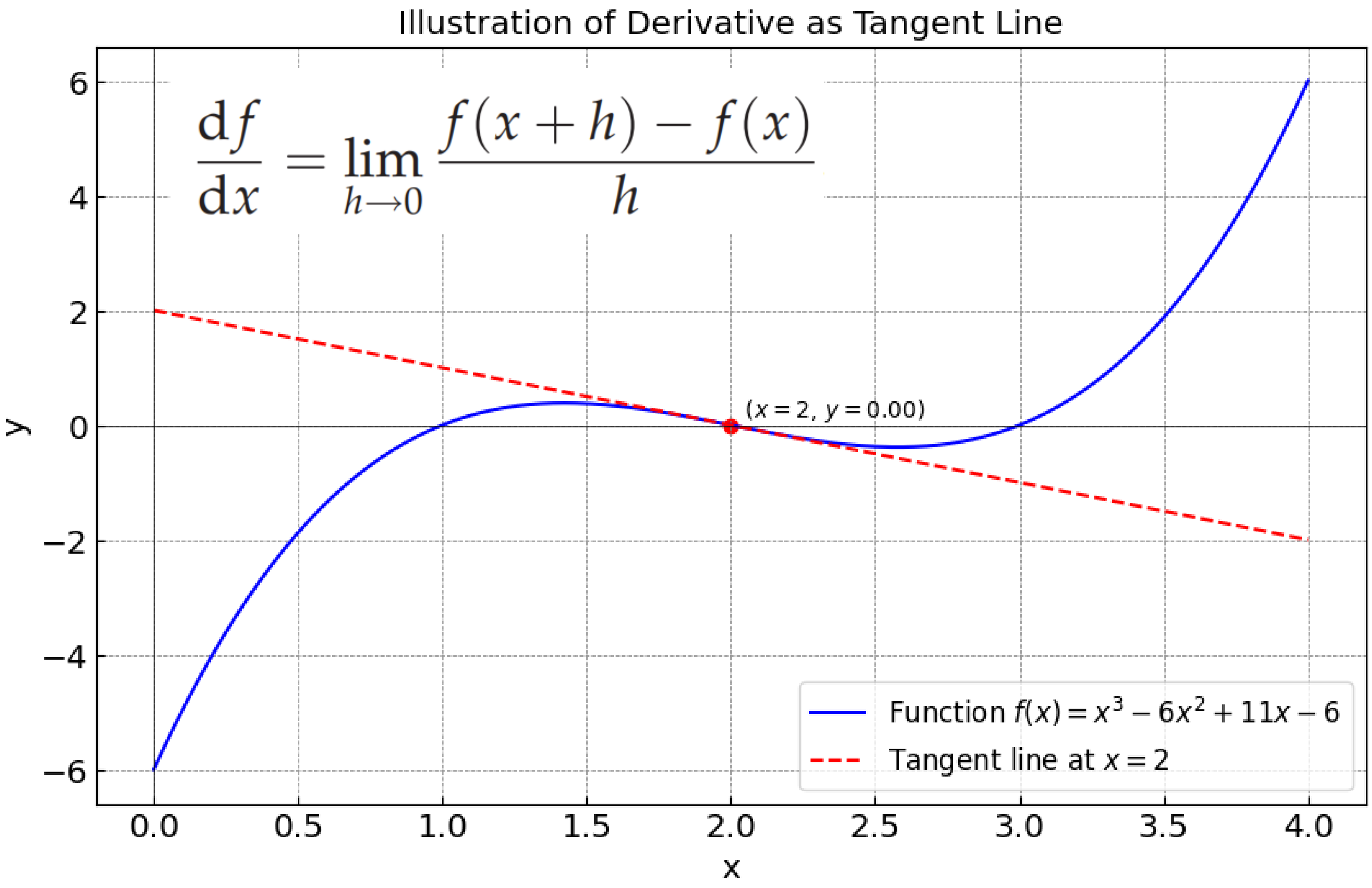
Homework 3





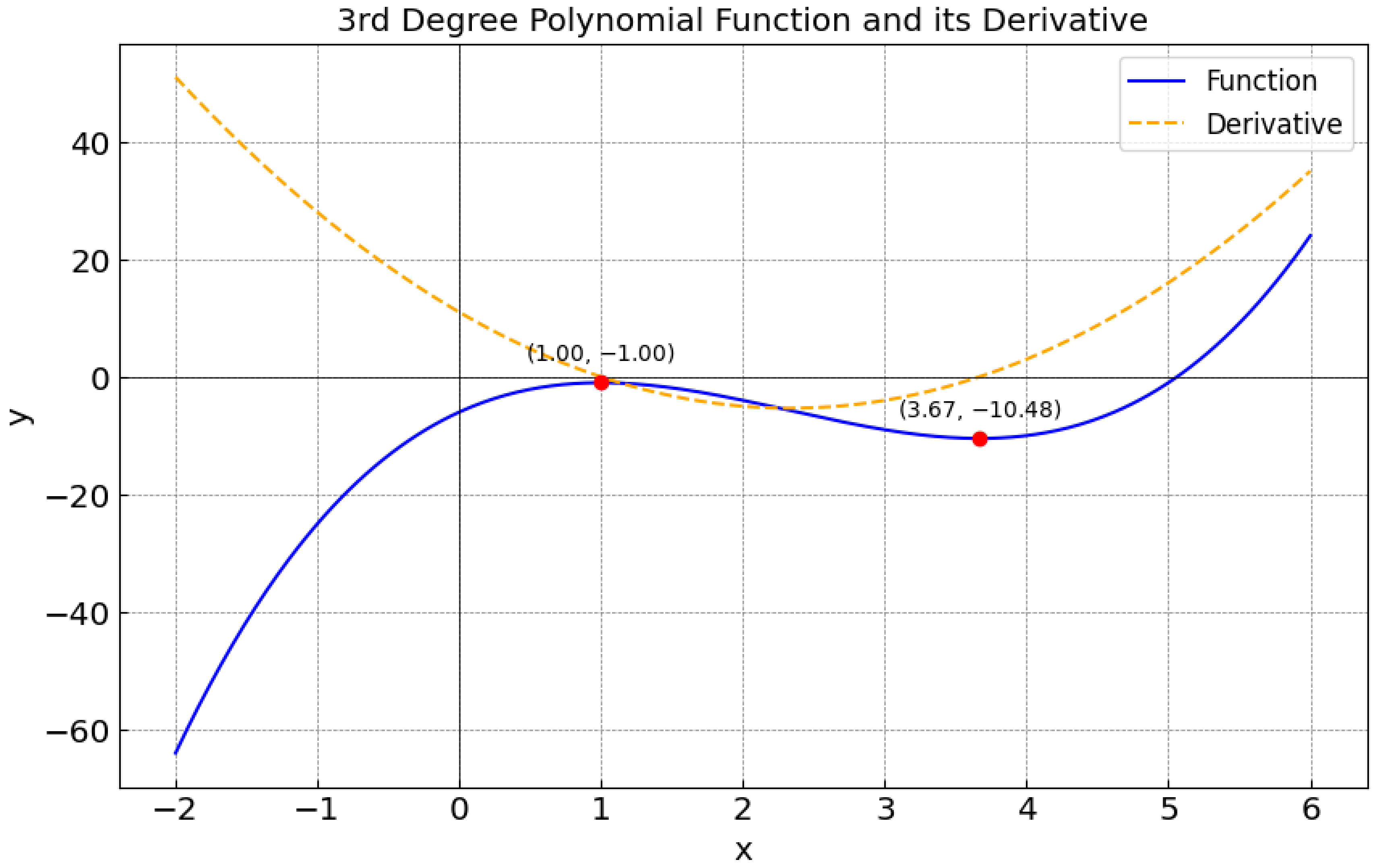
- Generally, done well!
- Some of the solutions on complexity were really impressive!
- Note that the equation has 3 roots!
- V(t) is infinite dimension
- Noted multicollinearity!

Derivative at a single point



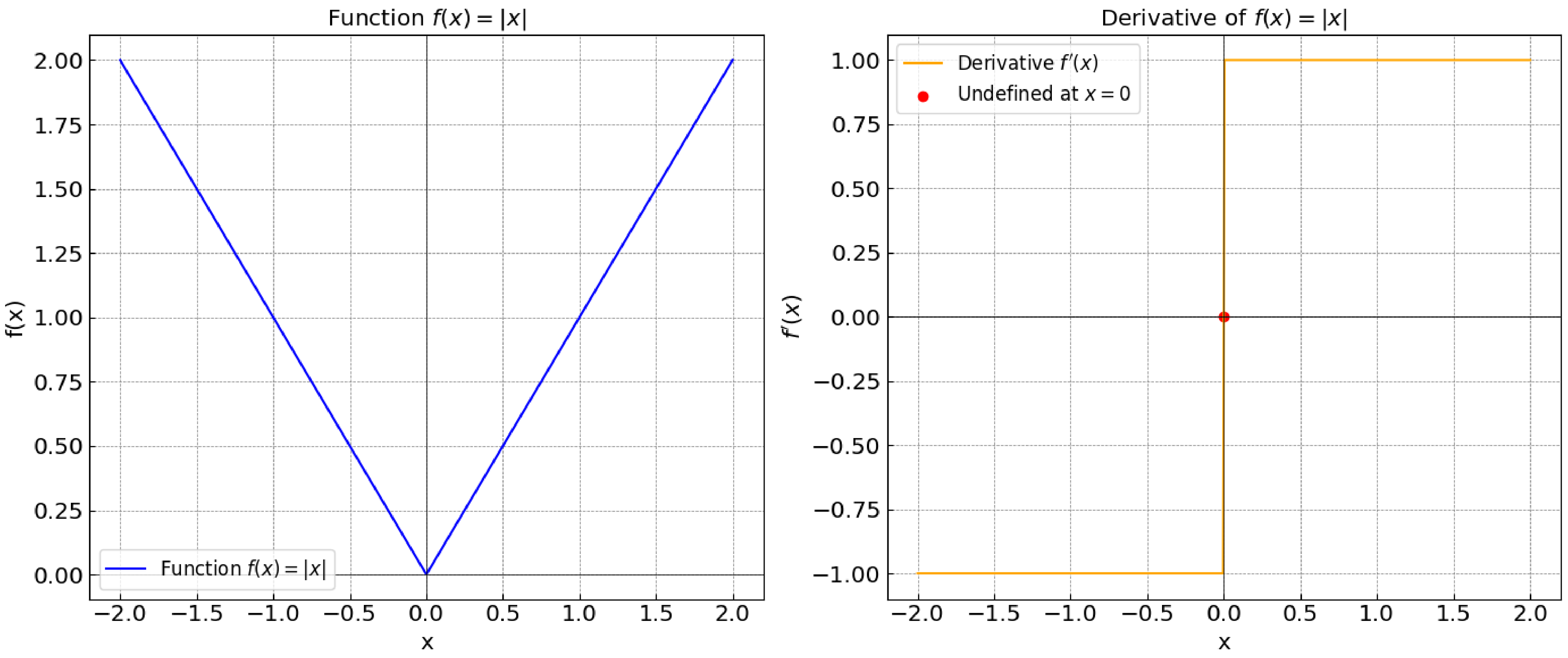
We need to define an arbitrary small step in space to define derivative

Derivative of a function

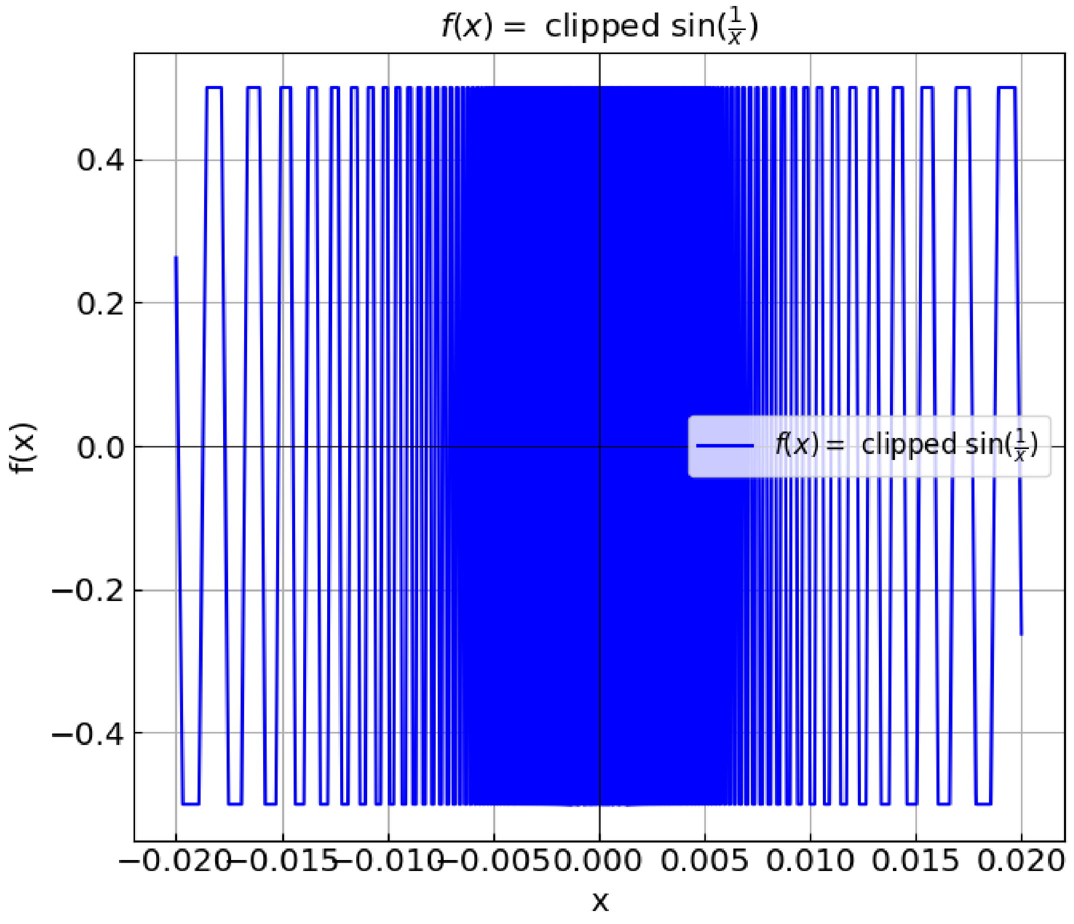


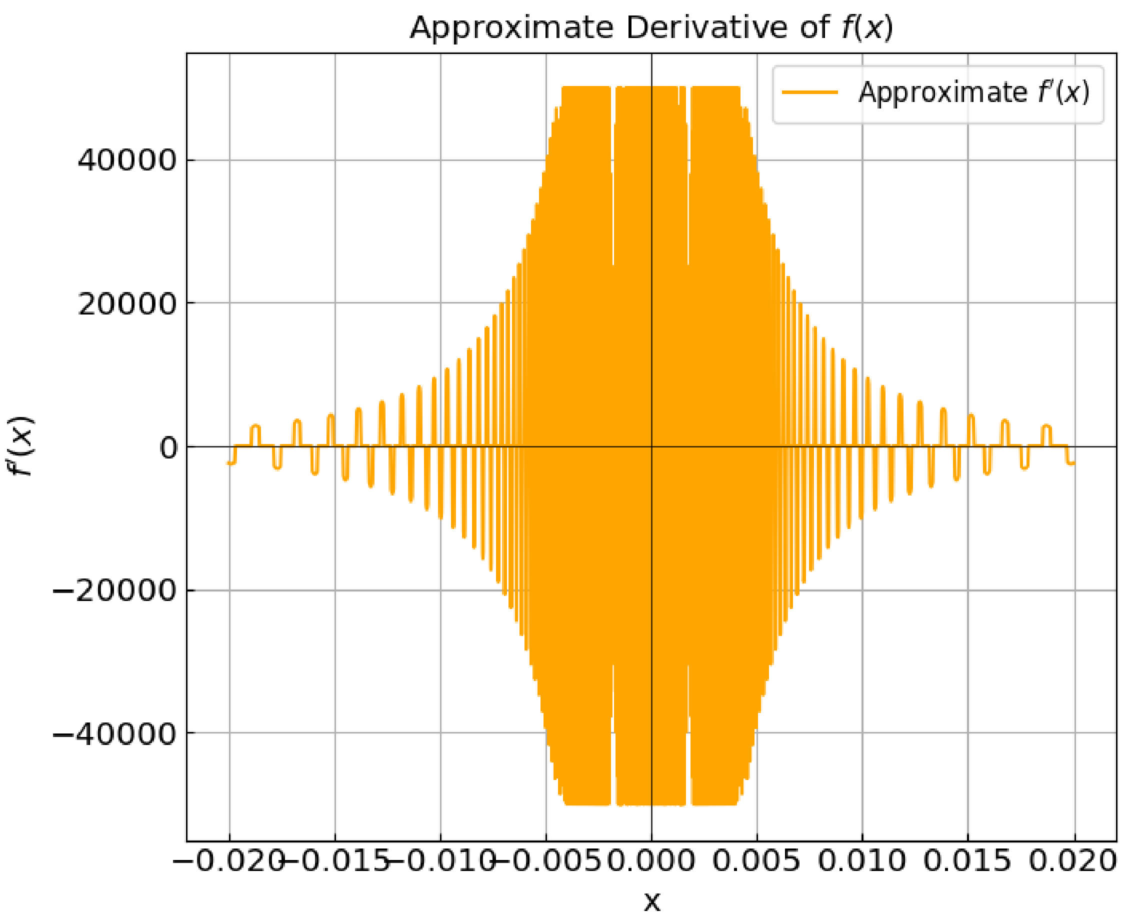
Zeroes of derivative are the extrema of the function

Not all functions are differentiable



Not all functions are differentiable





From derivatives to differential equations

1.Newton's Laws:

1. **First Law (Inertia)**: An object remains in uniform motion unless acted upon by a force.
2. **Second Law (Force and Acceleration)**: The force acting on an object is equal to the mass of that object times its acceleration (*F=ma*).
3. **Third Law (Action and Reaction)**: For every action, there is an equal and opposite reaction.

2. Acceleration (*a*) is the second derivative of position (*x*) with respect to time (*t*)

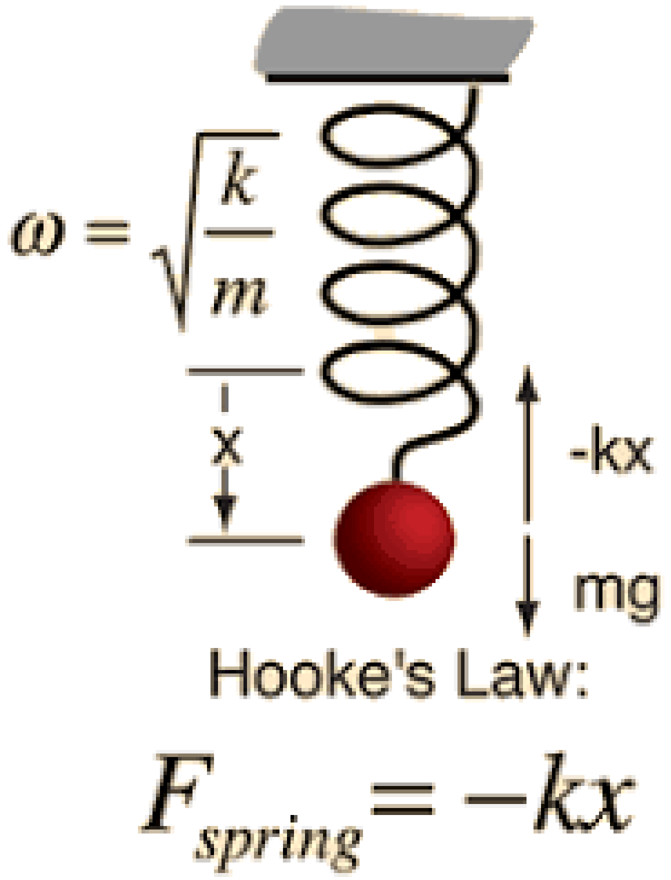
3.Equation of motion: $F= m\, dt^2/d^2x$.

4. Example: Simple Harmonic Motion (SHM):

1. Mass on a spring: $F = - k\, x$
2. Differential equation for SHM:

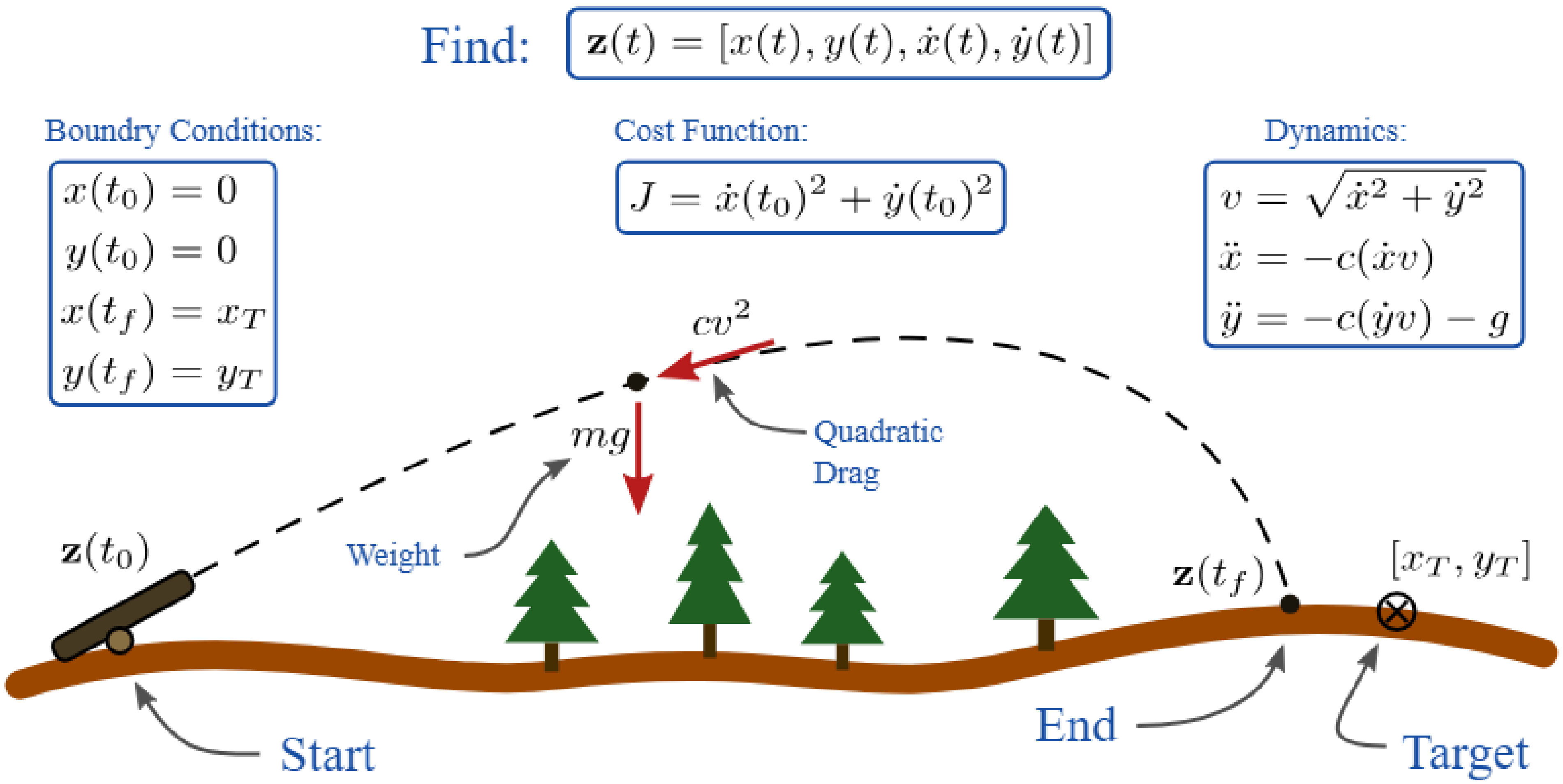
$dt^2/d^2x+\omega^2x=0$,

where ω is the angular frequency.



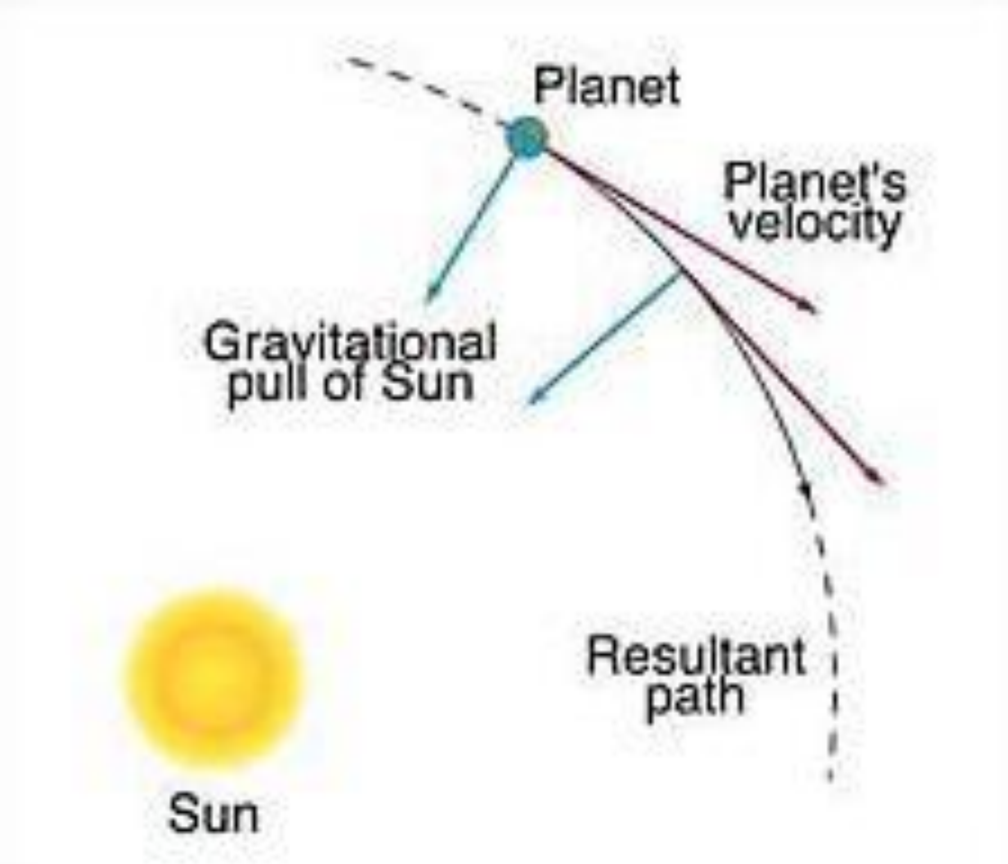
http://hyperphysics.phy-astr.gsu.edu/hbase/shm2.html

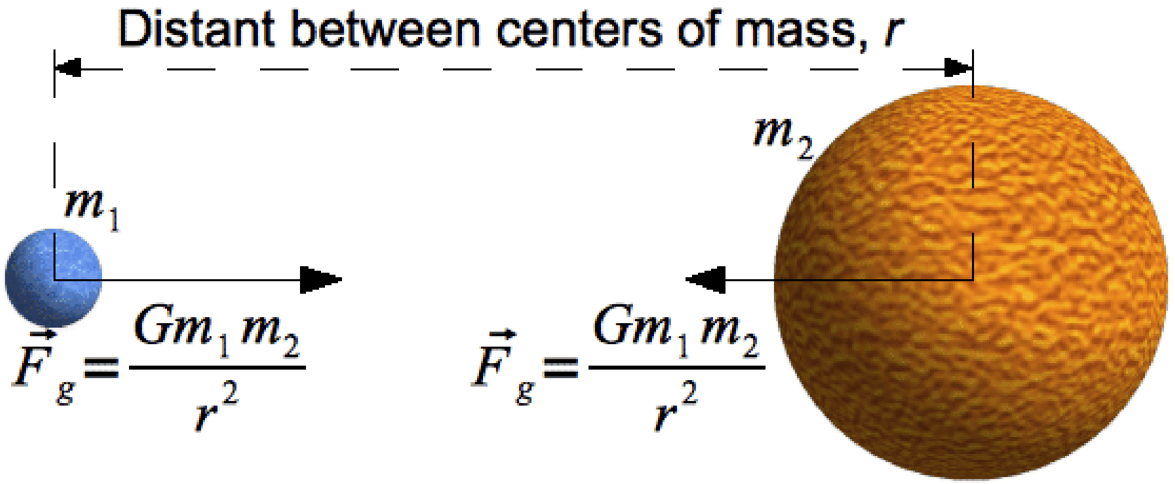
Initial and boundary value problems



https://www.matthewpeterkelly.com/tutorials/trajectoryOptimization/canon.html

Stationary solutions





https://www.phy.olemiss.edu/~luca/astr/Topics-Introduction/Newton-N.html

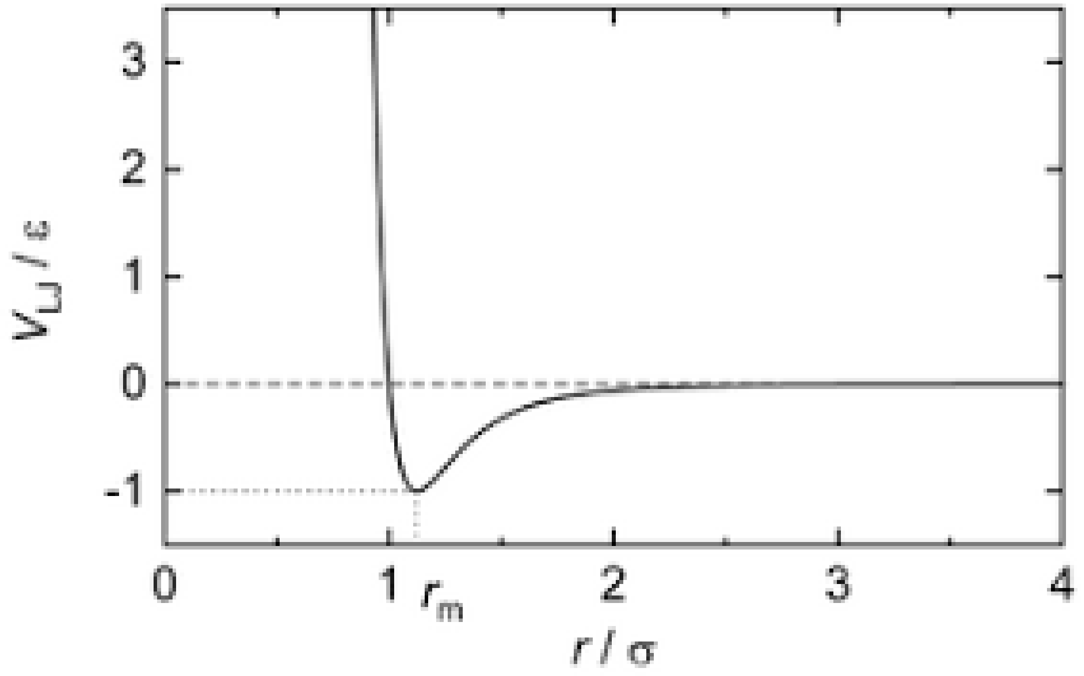
https://erikajanesite.wordpress.com/2017/09/24/225/

Molecular dynamics

- System of N particles with a pair potential
- Newton's equations of motion (classical *N*-body problem)

$$m\ddot{\mathbf{r}}_\mathbf{i} = -\sum_j \nabla_i V_{\mathrm{LJ}}^{ij}(|\mathbf{r}_\mathbf{i} - \mathbf{r}_\mathbf{j}|)$$

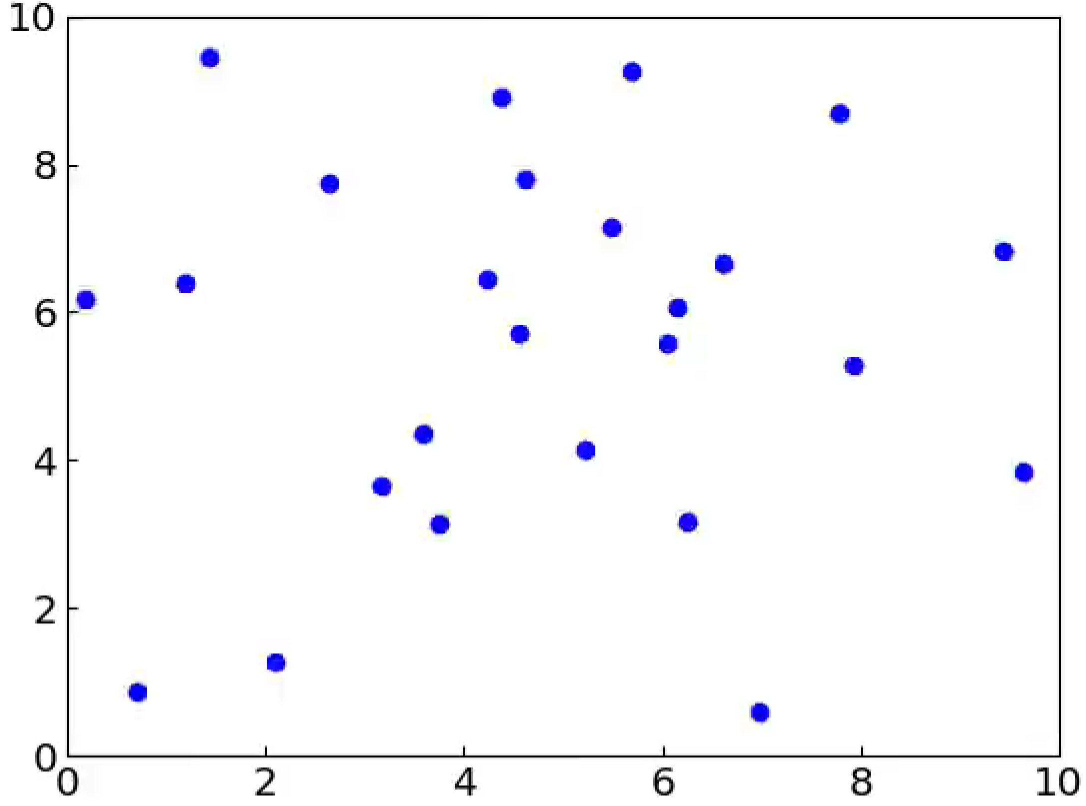
- Box simulation
  - Periodic boundary conditions
  - Minimum-image convention

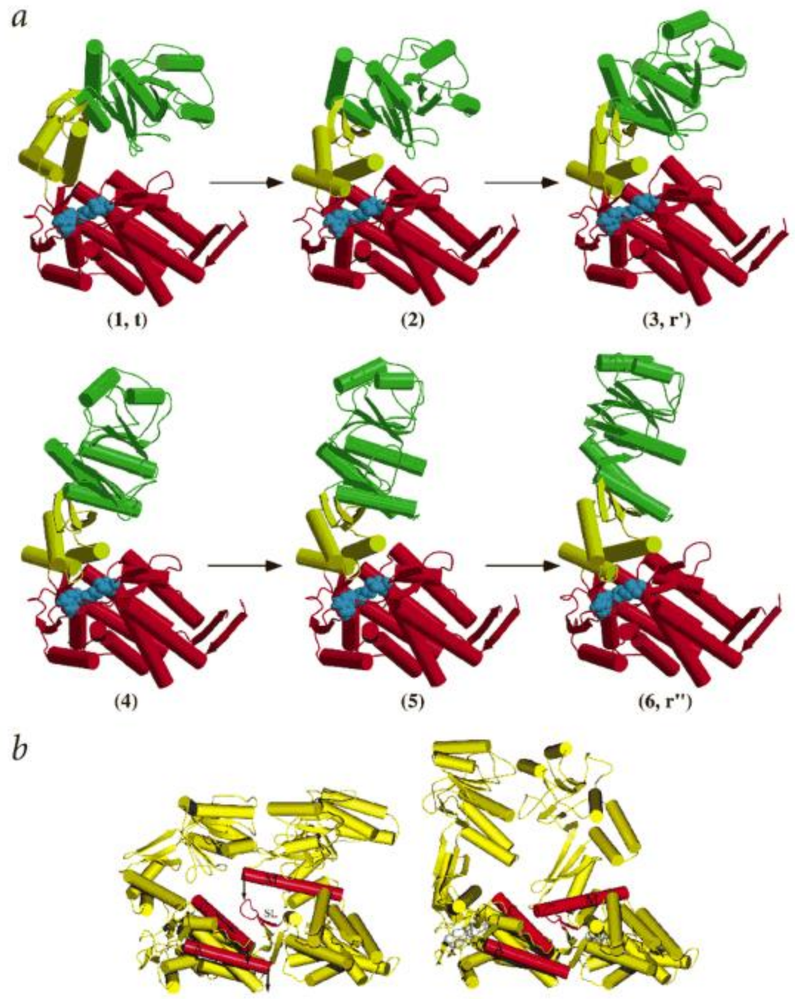


- If *N* is large enough, system can be characterized by macroscopic parameters
  - Energy-Volume-Number (UVN), microcanonical ensemble
  - Temperature-Volume-Number (TVN), canonical ensemble

- MD simulations give access to the **equation of state**

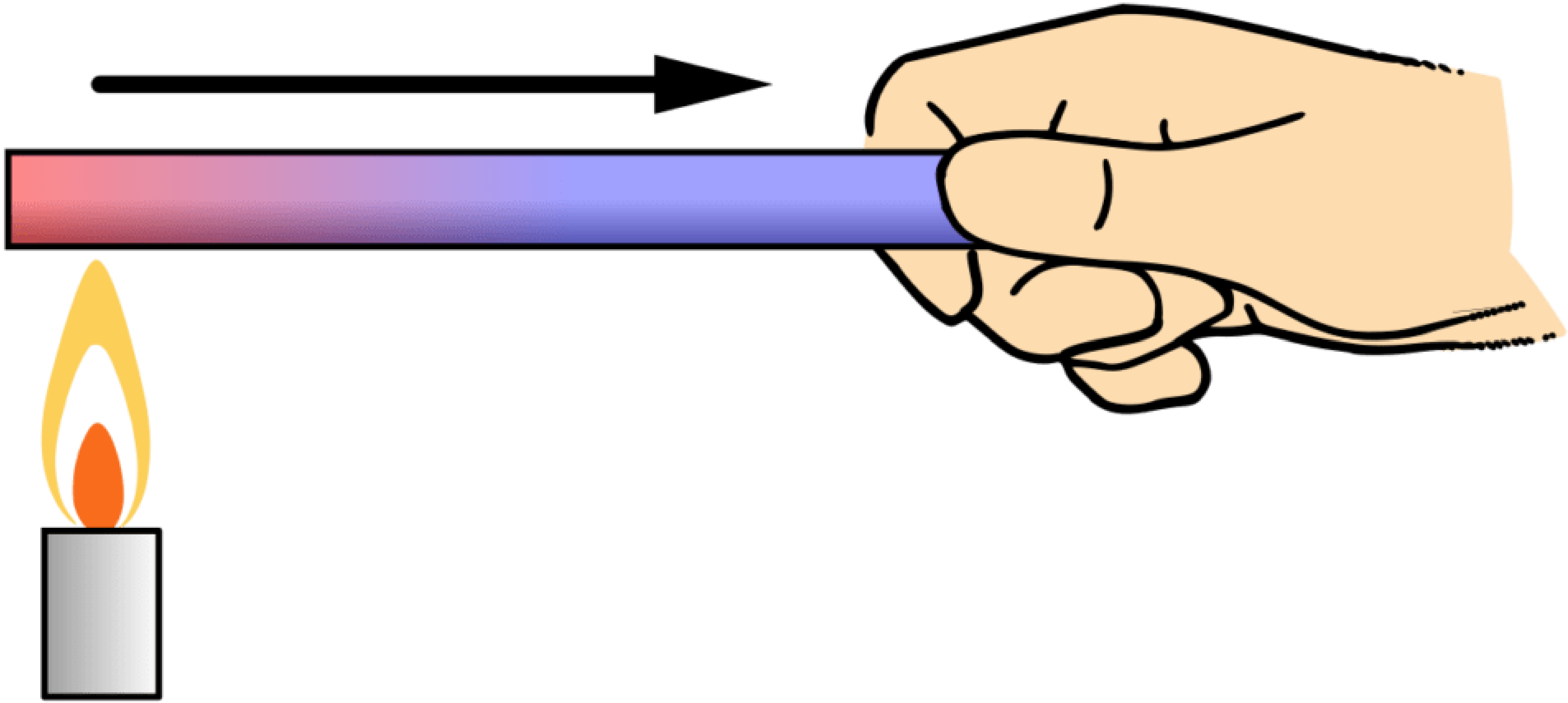
Molecular dynamics





https://www.nature.com/articles/nsb0902-646

Heat Transfer



https://chemicalengineeringworld.com/modes-of-heat-transfer/

Heat Transfer

1. Fourier's Law: The rate of heat transfer (q) through a material is proportional to the negative gradient of the temperature field (∇T) and the area (A) perpendicular to the direction of heat transfer, $q = -kA\nabla T$ where k is the thermal conductivity of the material

2. Conservation of Energy: For a given volume, the change in internal energy (U) over time (t) must equal the net heat flow into the volume minus the work done by the volume on its surroundings. In the absence of work and assuming constant density (ρ), this yields:

$$\partial U/\partial t = -\nabla \cdot q + q^{\cdot}$$

where $q^{\cdot}$ is the rate of heat generation per unit volume, and q is the heat flux vector

3. Relating Internal Energy to Temperature: Assuming the material's specific heat capacity (c_p) is constant, the internal energy change can be related to the temperature change:

$$U = \rho c_p T$$

1.Substituting this into the conservation of energy equation and using Fourier's law, we get the heat equation for a homogeneous, isotropic material without internal heat generation as:

$$\rho c_p \partial t \partial T = k\nabla^2 T$$

Colabs!