THE UNIVERSITY of TENNESSEE KNOXVILLE

Lecture 08: Physics Discovery

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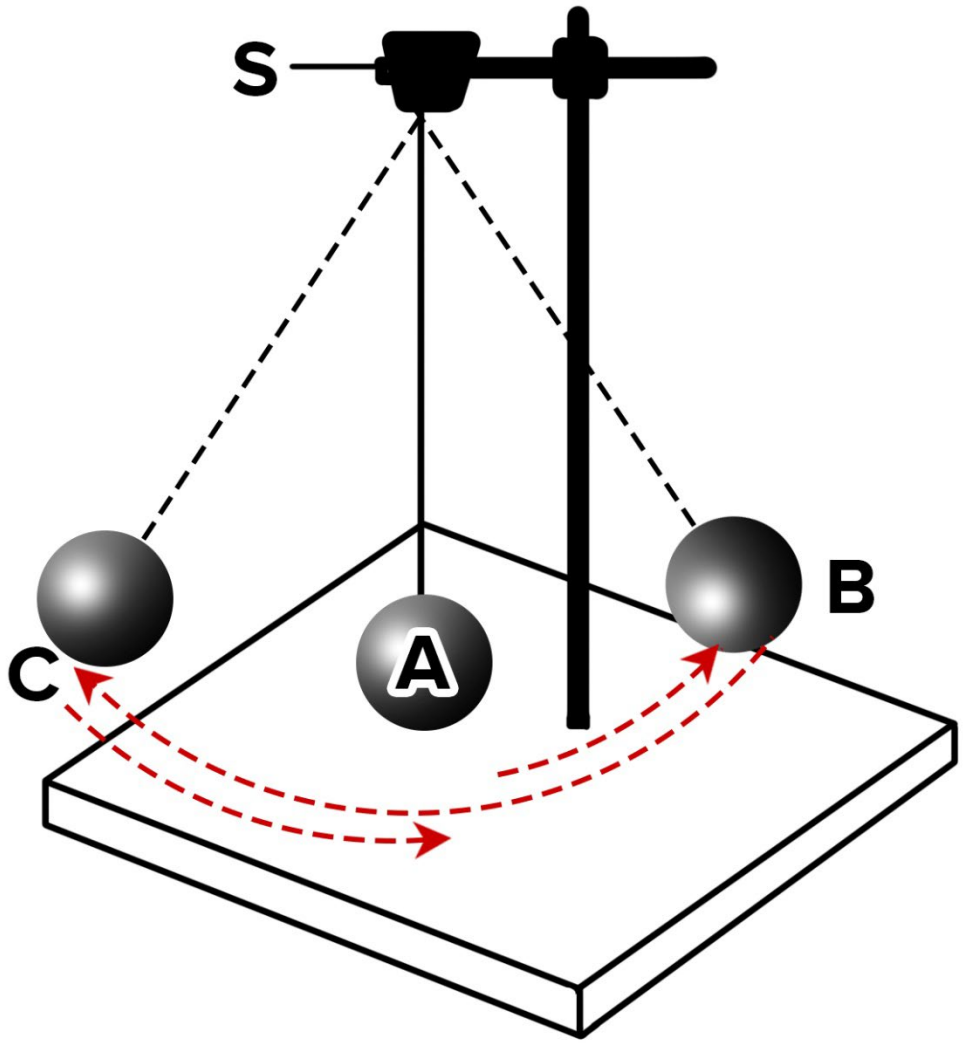
Back to functions from data

- If the function is known, we can fit it to data
- If we have several possible functions, we can fit all of them and compare the quality of fits
- We can also make some judgements based on the parameter values
- But what if we do not know the functions?



Overall, its not all about formulae!

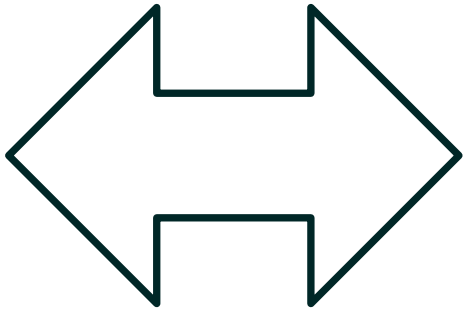
Short-Form Physical Laws (Symbolic Expressions)

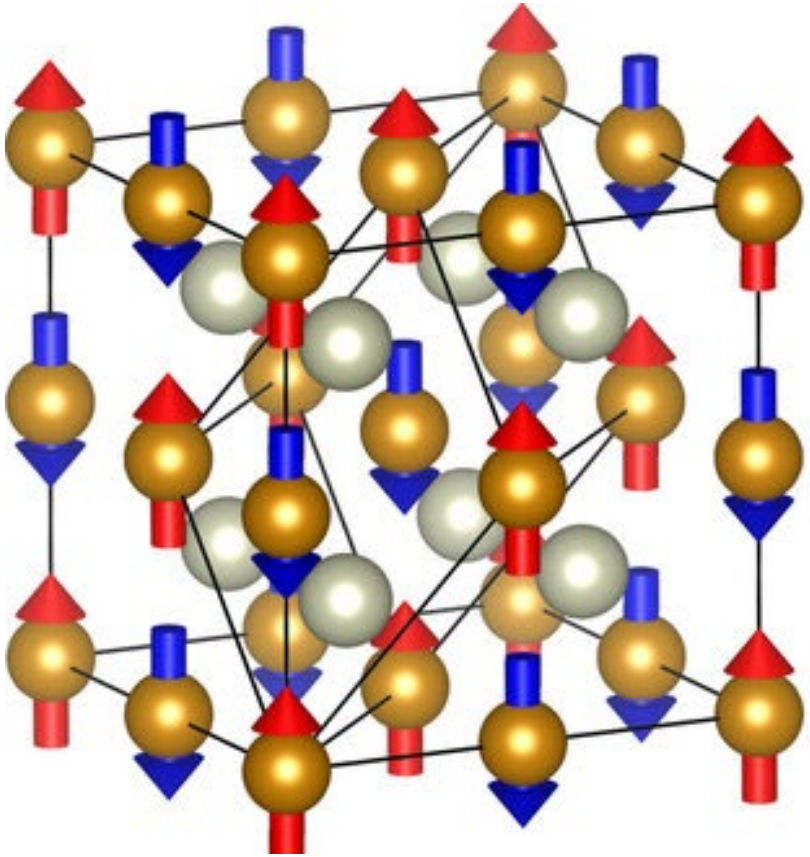
- Many fundamental physical laws can be compactly written as mathematical equations.
  - **Newton's Laws**: F=ma (simple equation but powerful predictive capability).
  - **Maxwell's Equations**: Compact set of equations describing electromagnetism.
  - **Schrödinger Equation**: Governs quantum mechanics with relatively few terms.
- Often derived from symmetry principles, conservation laws, or variational principles.
- Easily generalizable and applicable across different systems.

Emergent Complexity from Simple Models

- Some models have very few parameters but give rise to complex behavior.
  - **Ising Model**: Defined by simple spin interactions but exhibits phase transitions.
  - **Navier-Stokes Equations**: Governing fluid dynamics, but leading to turbulence.
  - **Cellular Automata** (e.g., Conway's Game of Life): Simple update rules create highly complex patterns.
- No compact symbolic equation fully describes emergent behavior.
- Understanding often requires numerical simulations, renormalization group theory, or statistical mechanics

How Can we Model Magnetism?





- Each atom has a localized spin
- Spins interact with their nearest neighbors
- All dynamics can be represented via spin interactions

https://www.researchgate.net/publication/306187646_Impact_of_lattice_dynamics_on_the_phase_stability_of_metamagnetic_FeRh_Bulk_and_thin_films/figures?lo=1

Ising Model?

Ising model represents a system of spins (magnetic dipoles) on a lattice.

Without external magnetic field, the energy reads

$$E = -J \sum_{<ij>} s_i s_j$$

J > 0: ferromagnetic, sum over neighbors only

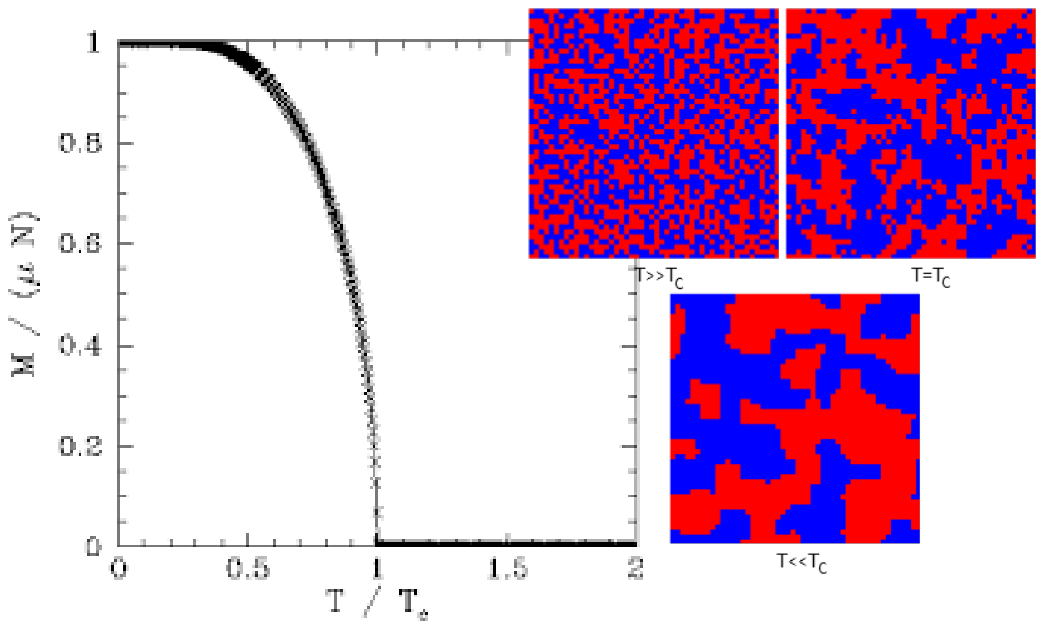
Magnetisation:

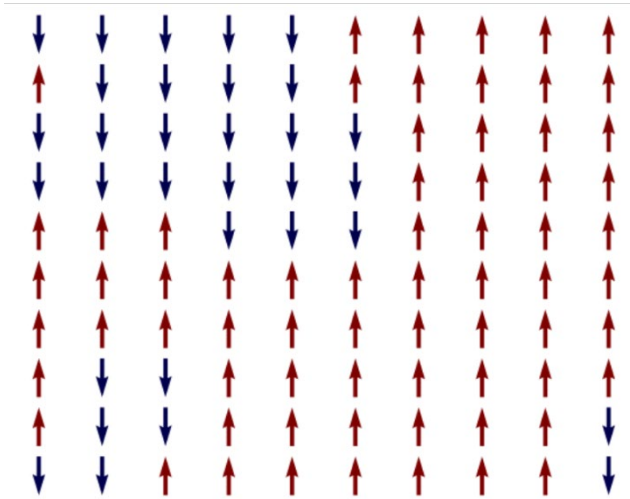
$$M = \sum_i s_i$$

Below the Curie temperature

$$\frac{k_B T_C}{J} = \frac{2}{\ln(1+\sqrt{2})}$$

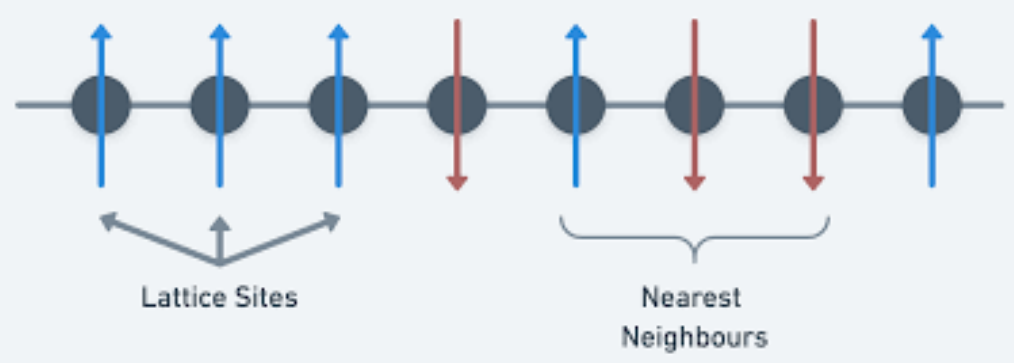
exhibits spontaneous magnetization |M|>0





From the course by Volodymyr Vovchenko,
https://github.com/vlvovch/PHYS6350-ComputationalPhysics

Ising model



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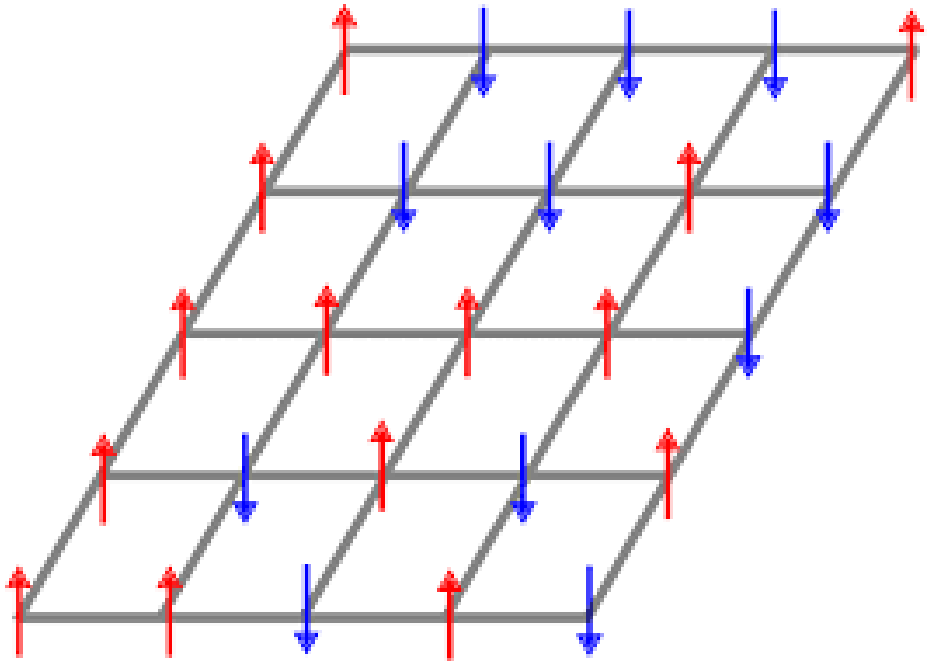

https://www.researchgate.net/figure/Schematic-representation-of-a-configuration-of-the-2D-Ising-model-on-a-square-lattice_fig2_321920877

2D Ising model

Ising model represents a system of spins (magnetic dipoles) on a lattice.

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$$E = -J \sum_{<ij>} s_i s_j$$

J > 0: ferromagnetic, sum over neighbors only

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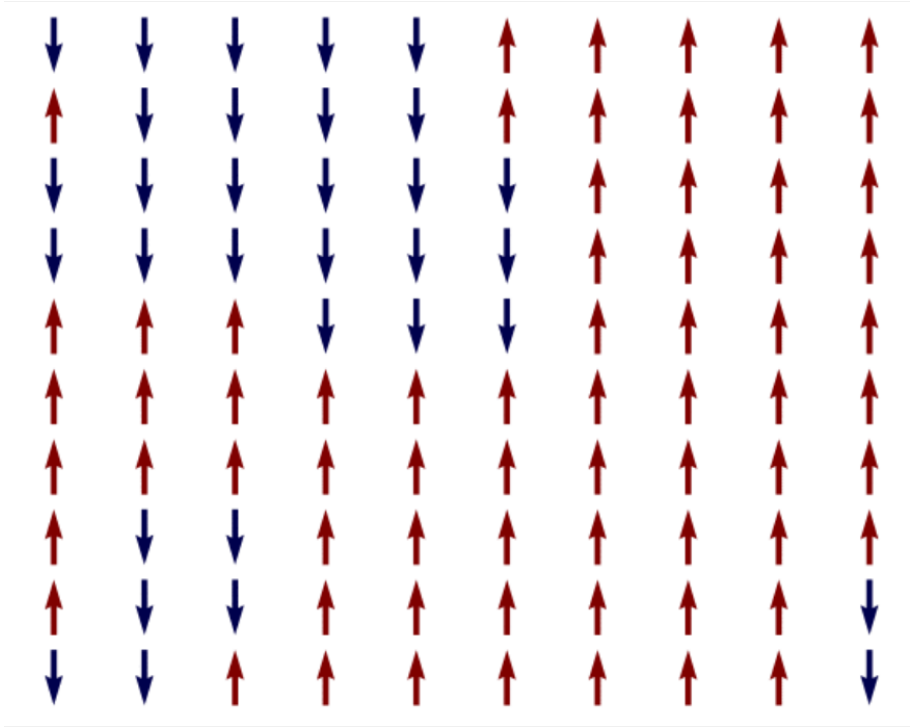

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2D Ising model

Metropolis algorithm for 2D Ising model:

- At each step have spin configuration s_i
- Randomly pick a spin i and flip its orientiation, $s_i \rightarrow -s_i$
- Calculate the energy difference

$$\Delta E = 2J \sum_j s_i s_j$$

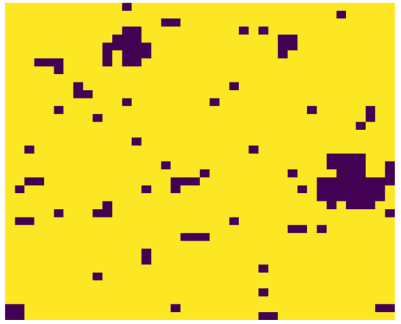
- Accept the new state with probability

$$P_a = e^{-\Delta E/T}$$

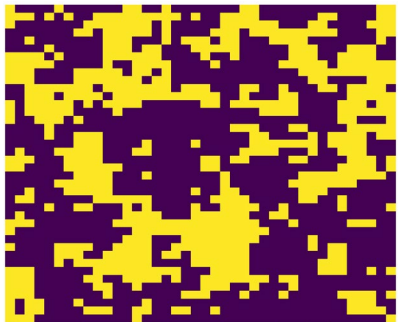
From the course by Volodymyr Vovchenko,
https://github.com/vlvovch/PHYS6350-ComputationalPhysics

NN and NNN Ising model with Disorder

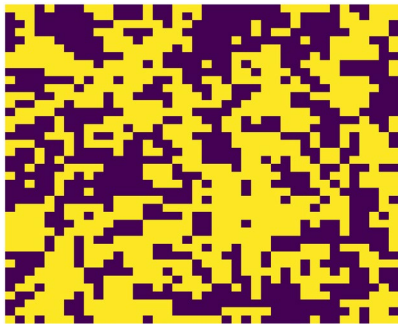
- **Hamiltonian:** $H(\sigma) = -\sum_{<i,j>}(J_1+\Delta J_1)\sigma_i\sigma_j - \sum_{<i,k>}(J_2+\Delta J_2)\sigma_i\sigma_k$,
  - The simulations are run on a square lattice of size $N = 40$
  - Where σ is the spin at a lattice site i that can assume +1 or -1.
  - J_{ij} is the interaction parameter between sites i & j
- **Monte Carlo simulation using metropolis algorithm**
  - $P_\beta(\sigma_m) = \frac{e^{-\beta H(\sigma m)}}{\sum_n e^{-\beta H(\sigma n)}}$, β is the inverse temperature
  - At each of the MC, each spin is reversed based on the probabilities determined by ratios of probabilities of microstate
- **The macroscopic properties are calculated using**
  - Energy = $< E >$, Magnetization = $< M >$
  - Specific Heat = $(< E^2 > - < E >^2)/(k_B T)^2$
  - Magnetic Susceptibility = $(< M^2 > - < M >^2)/k_B T$



$J_1 = 1$, T = 2.2

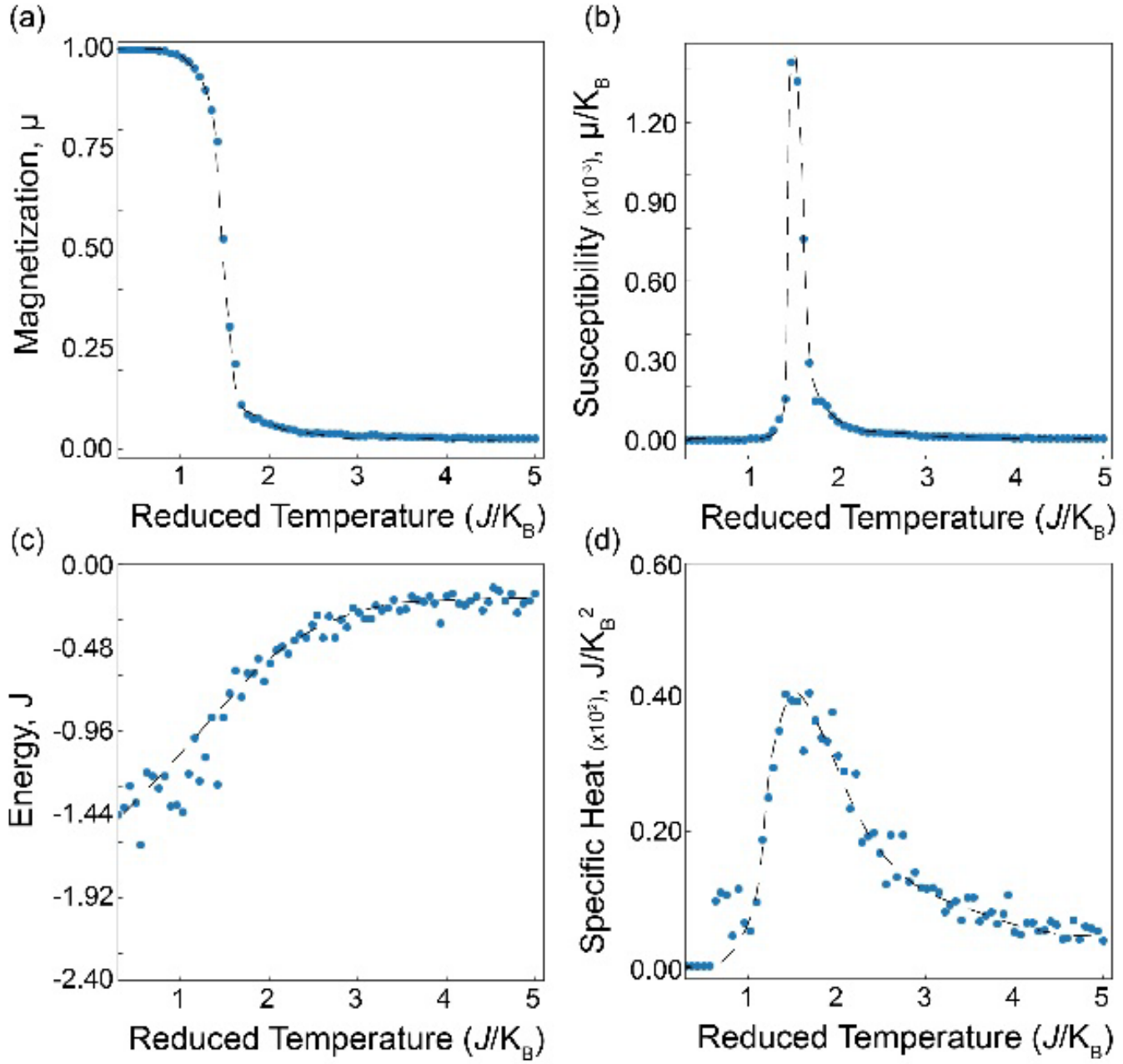


$J_1 = 1$, T = 2.8

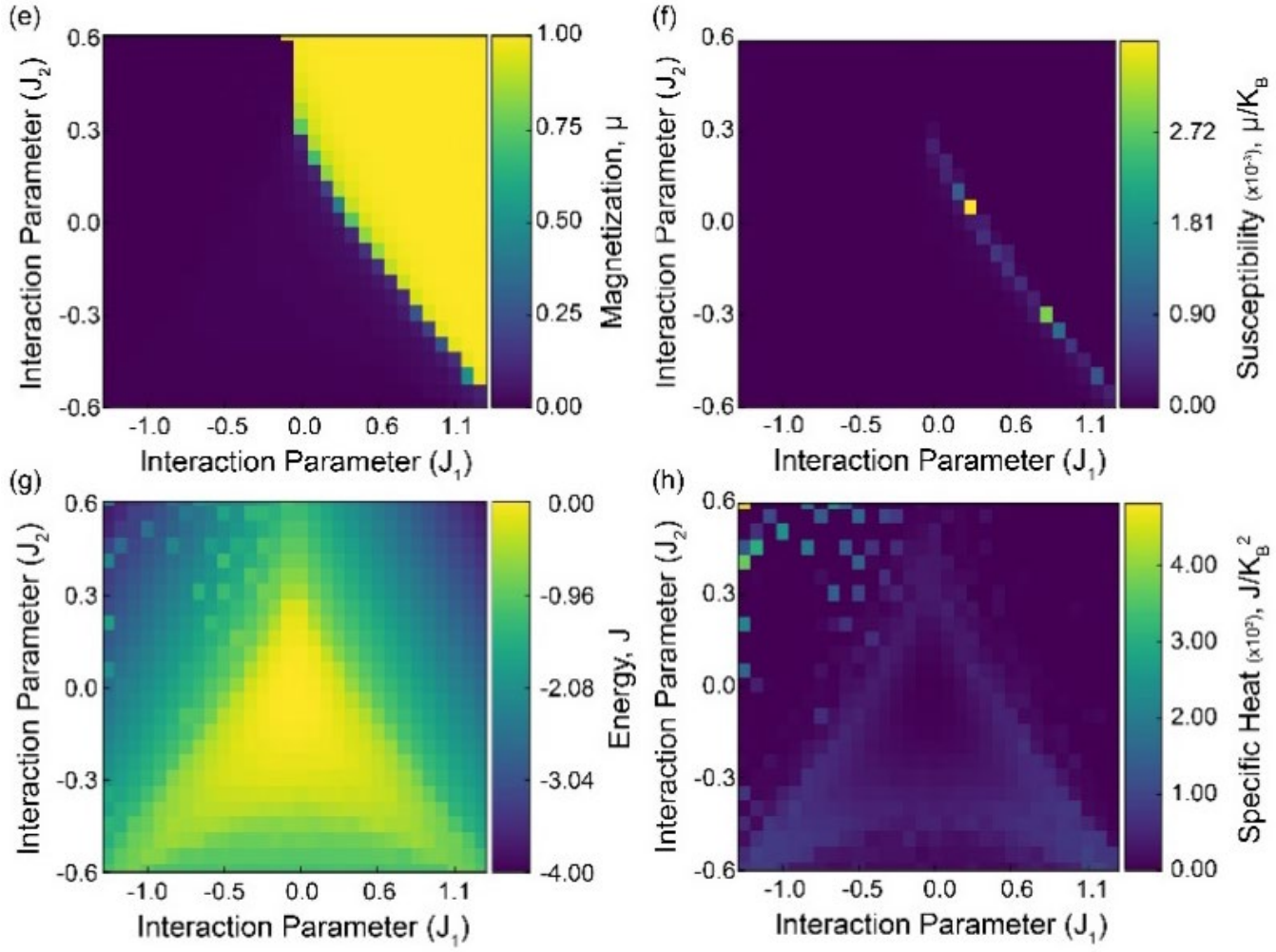


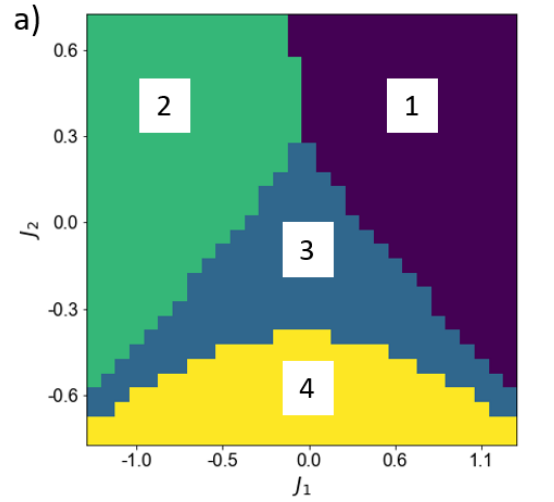
$J_1 = 1$, T = 4

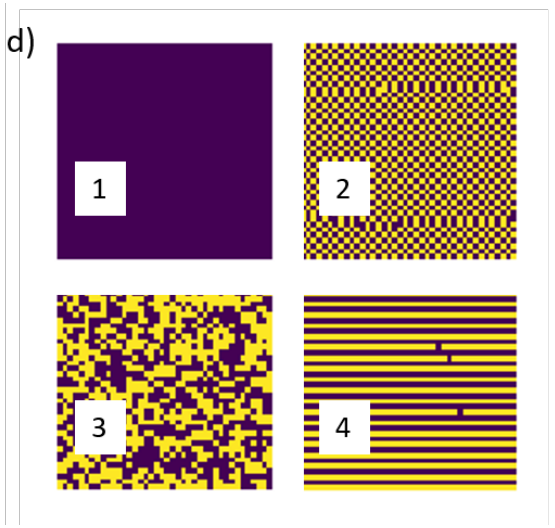
Ising model with NN interactions



Ising model with NNN interactions

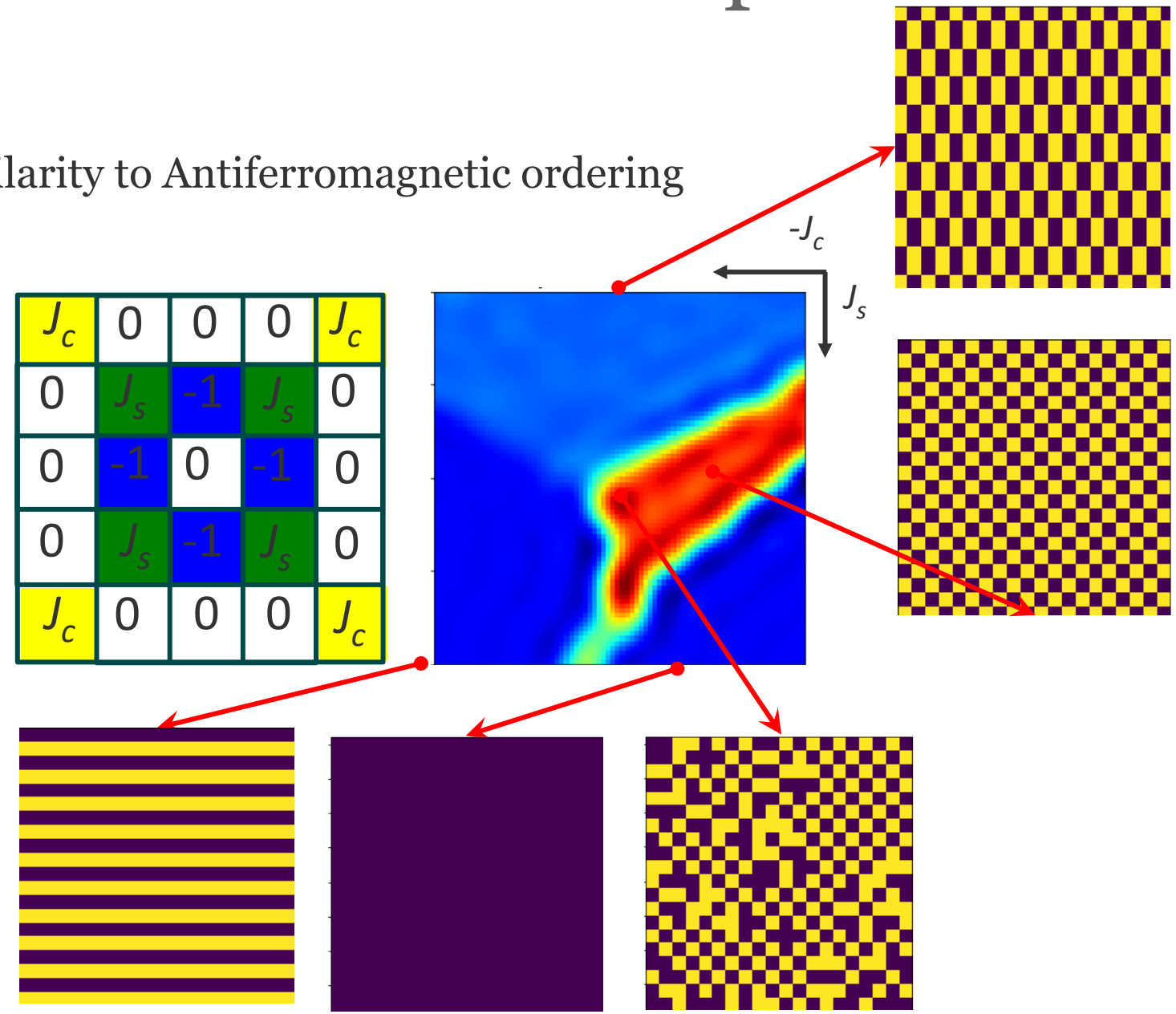




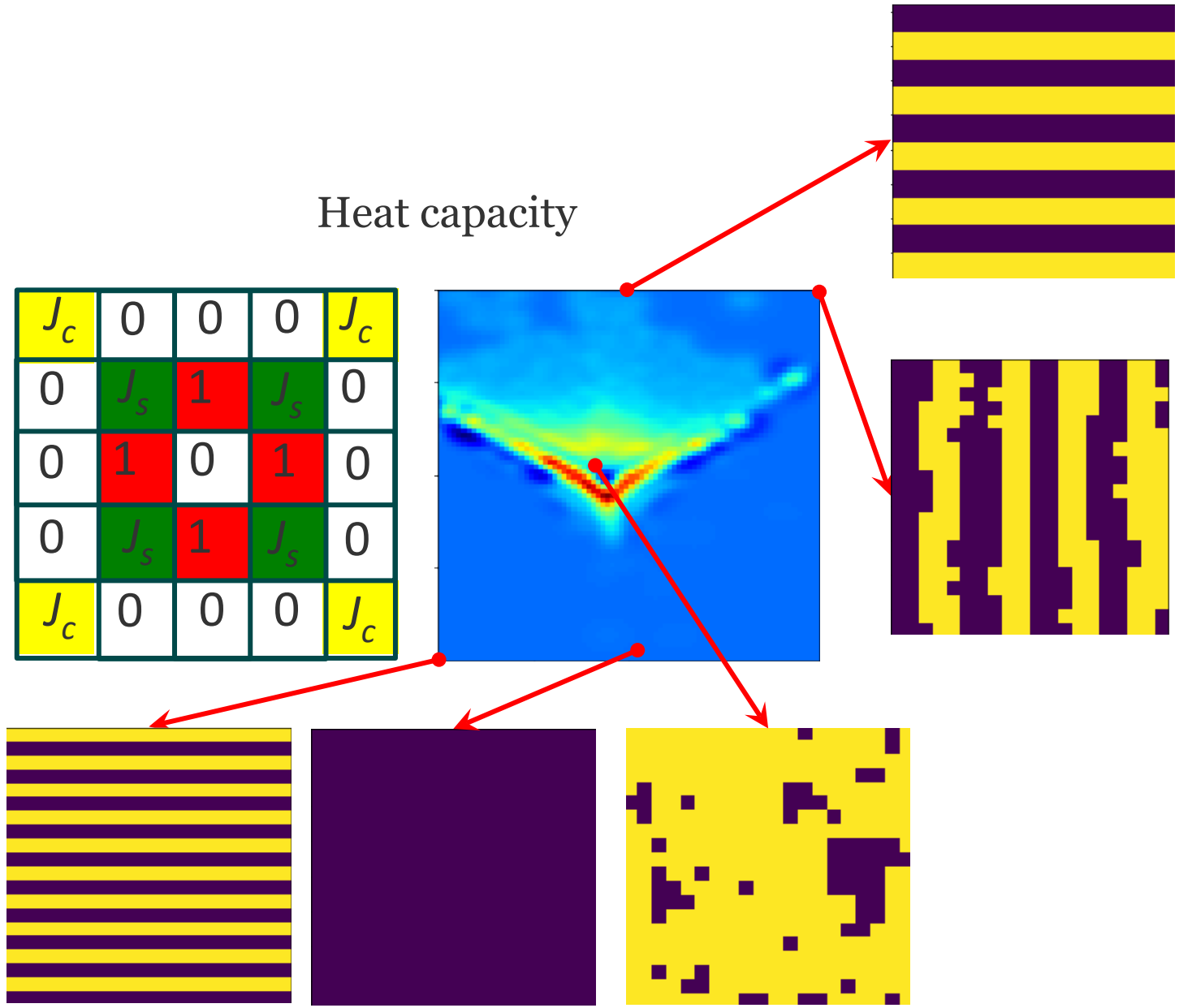


Ising model with more complex interactions

Similarity to Antiferromagnetic ordering

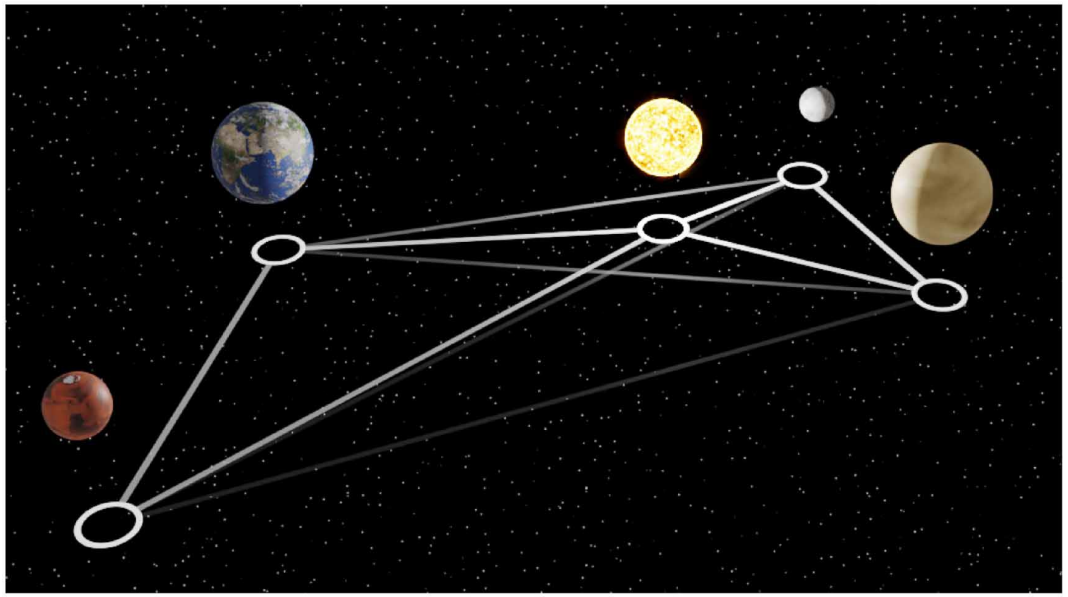


Ising model with more complex interactions

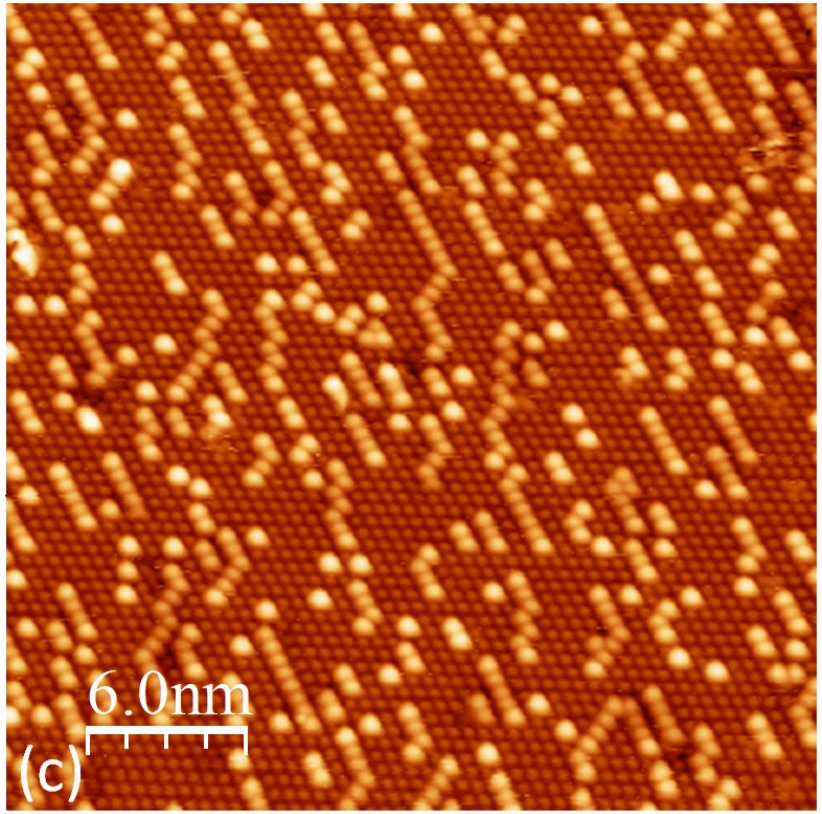


Learn Ising Model from Data?

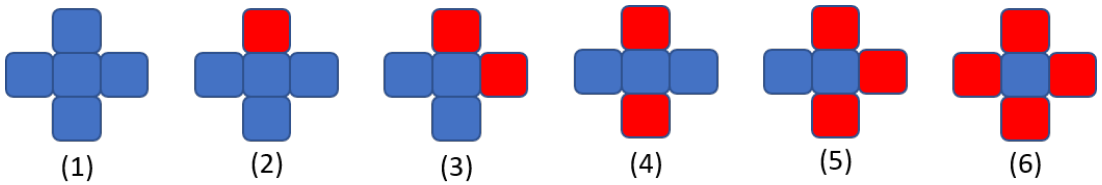
Rediscovering orbital mechanics with machine learning



Pablo Lemos *et al* 2023 *Mach. Learn.: Sci. Technol.* **4** 045002



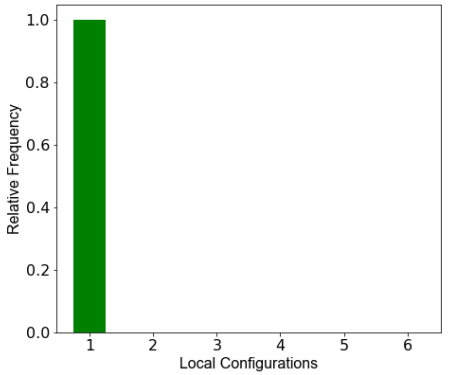
Build Descriptors



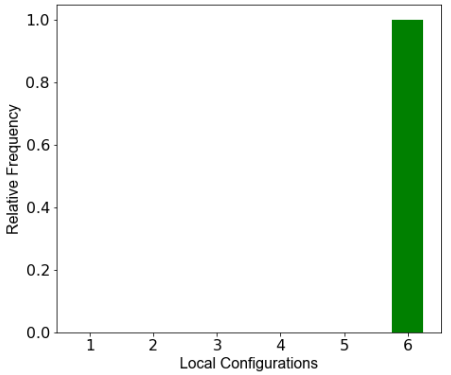
Blue and red represent opposite spins

Each simulation is now represented as a six-dimensional vector

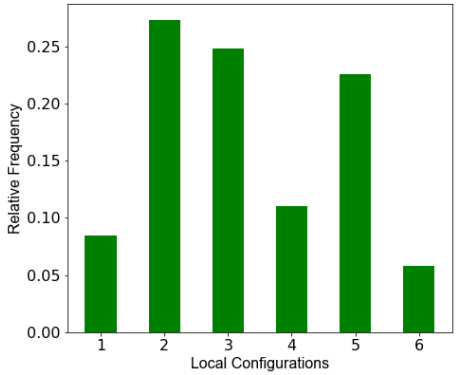
$J_1 = 1.25$
$J_2 = 0.75$



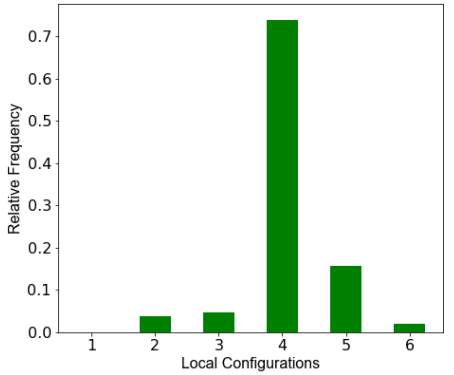
$J_1 = -1.25$
$J_2 = 0.75$



$J_1 = 0.04$
$J_2 = 0.02$

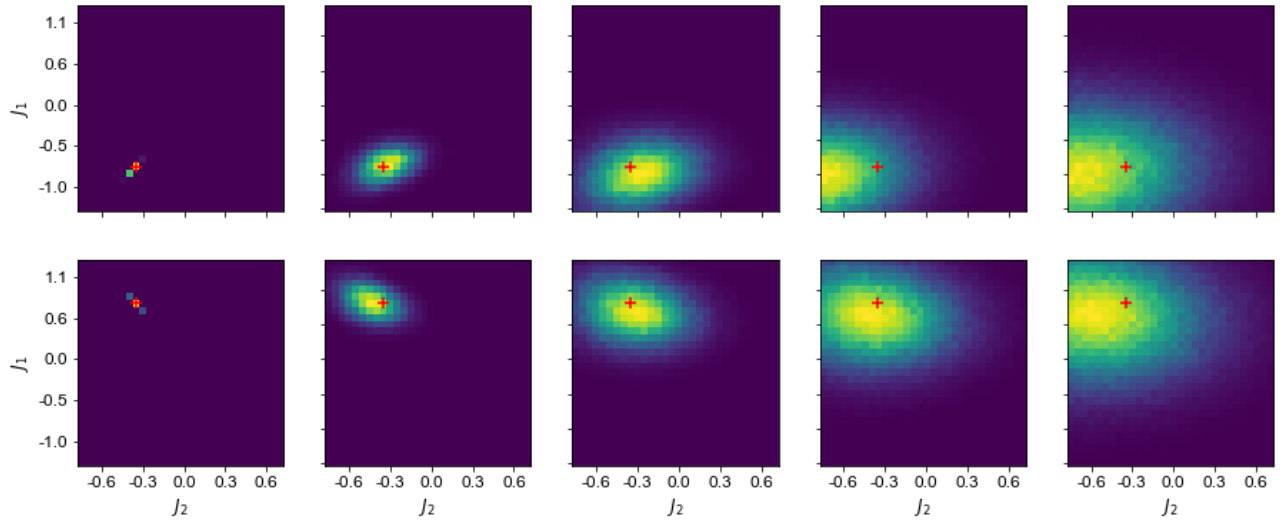


$J_1 = -1.0$
$J_2 = -0.6$

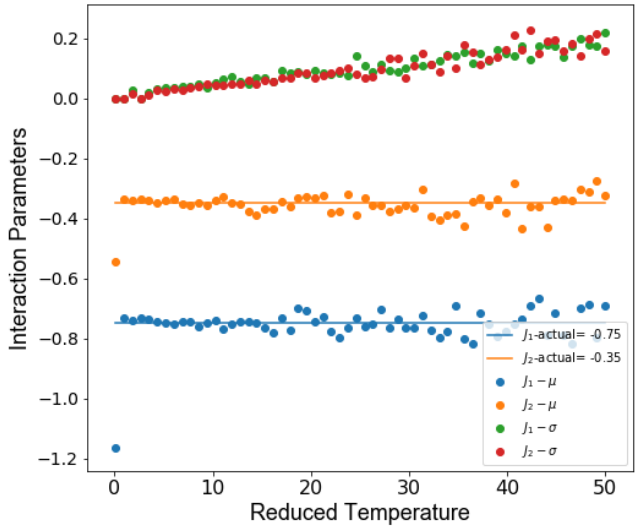


Validate against ground truth

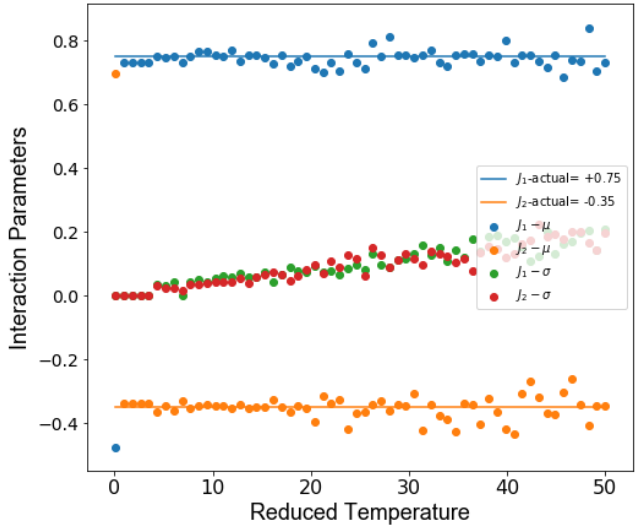
Bayesian Likelihood Estimation



$J_1 = -0.75, J_2 = -0.35$



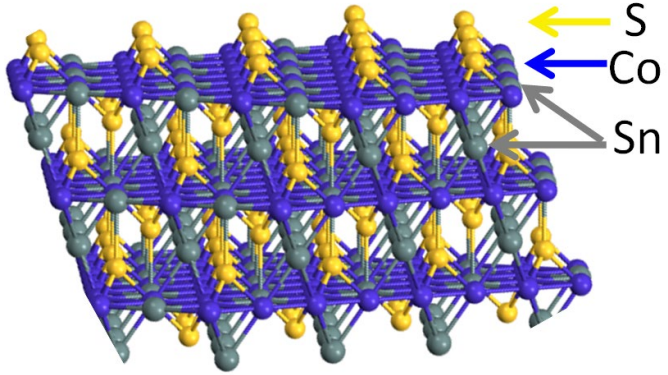
$J_1 = 0.75, J_2 = -0.35$

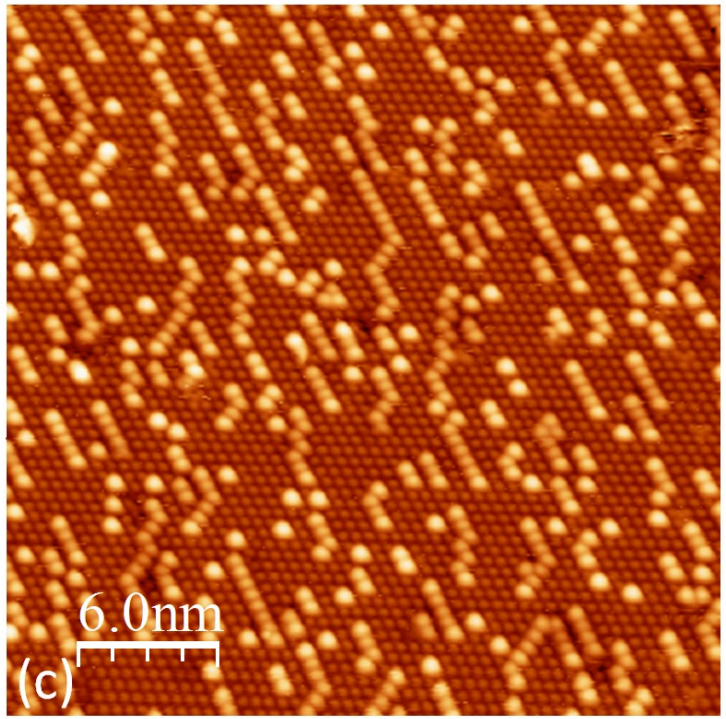


Apply to Experiemntal data

- Shandite family $A_3M_2X_2$ crystallizes in a rhombohedral structure, with a CoSn Kagome lattice sandwiched by S and Sn layers.
- we explore S adatom features on top of a CoSn subsurface of a $Co_3Sn_2S_2$ single crystal.
- A large amount of S adatoms scatter on top of the flat hexagonal subsurface of CoSn in many forms, including monomers, dimers, long 1D adatom chains, or zigzag chains.
- We aim to model the distribution of adatoms using a triangular Ising model.
- An as initial step, we need to quantify the spots available for the adatoms.

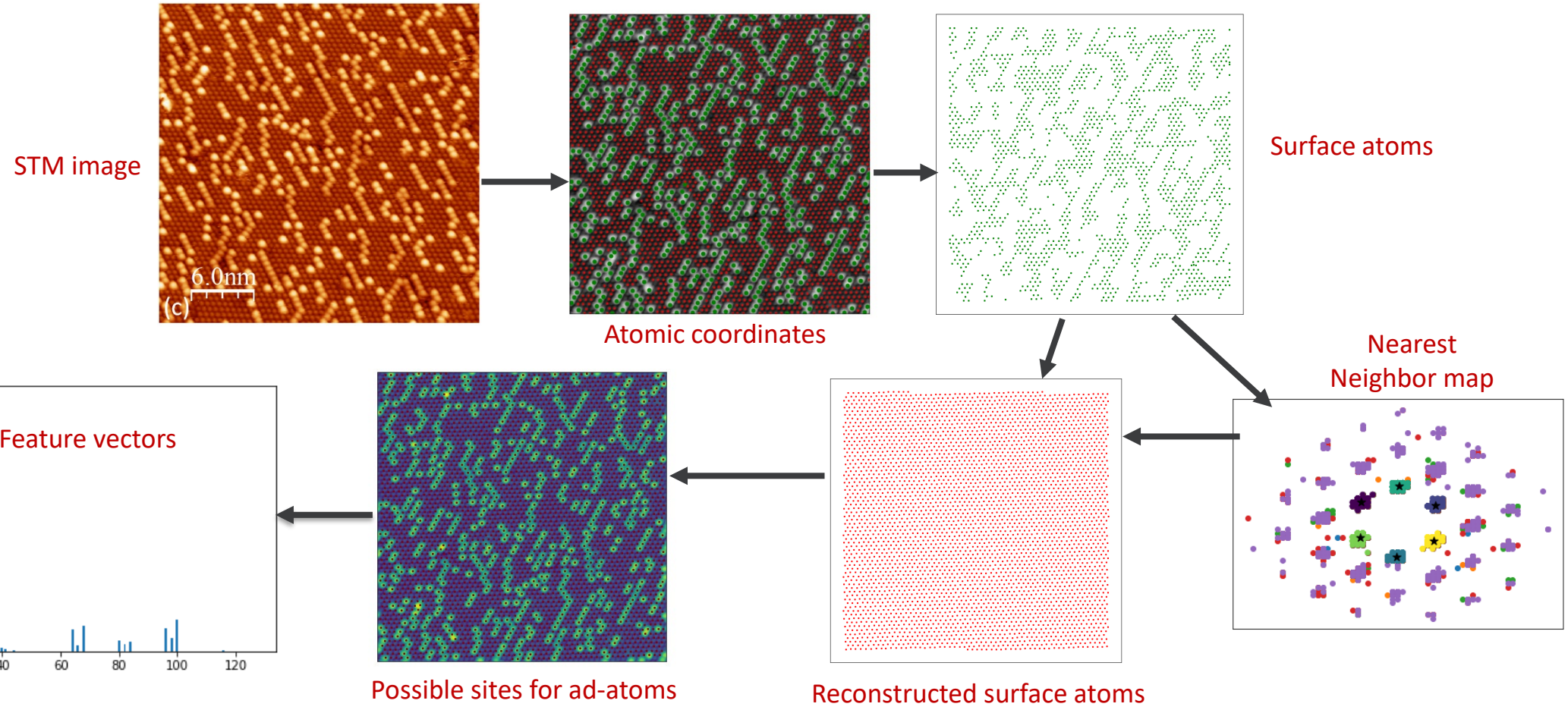
Ball and stick model of S adatoms on top of a CoSn subsurface of a $Co_3Sn_2S_2$ crystal



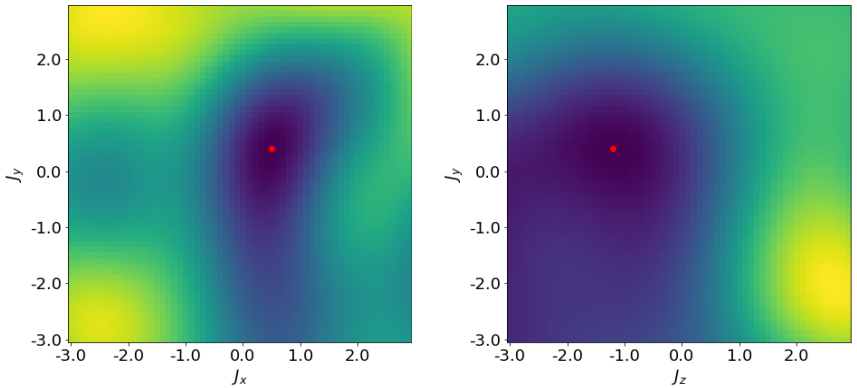


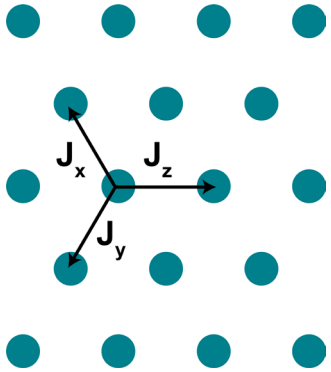
STM images that shows S-adatoms as bright spots and the hexagonal-subsurface lattice

Quantify STM Image



Reconstruct and Validate

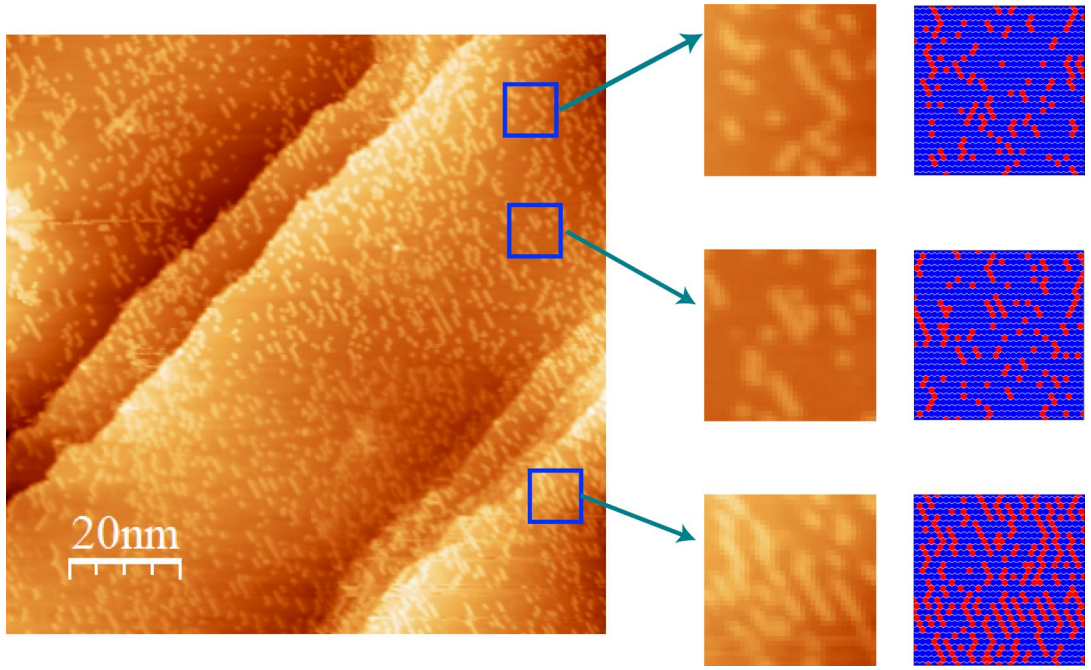




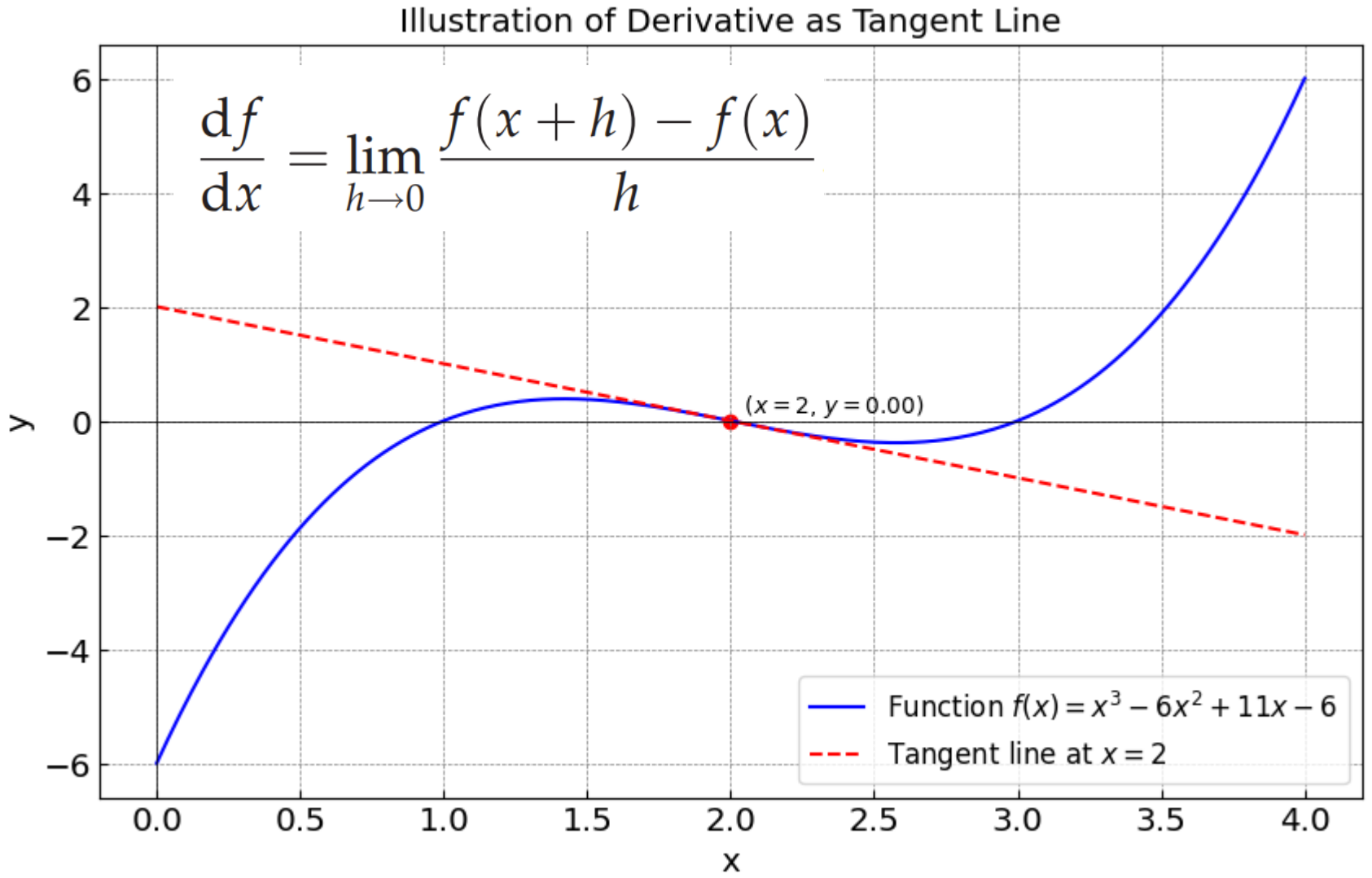
Optimal parameters:

- 2D: $J_x = J_y = 0.6$, $J_z = -1.5$
- 3D: $J_x = 0.5$, $J_y = 0.4$, $J_z = -1.2$

Evaluation

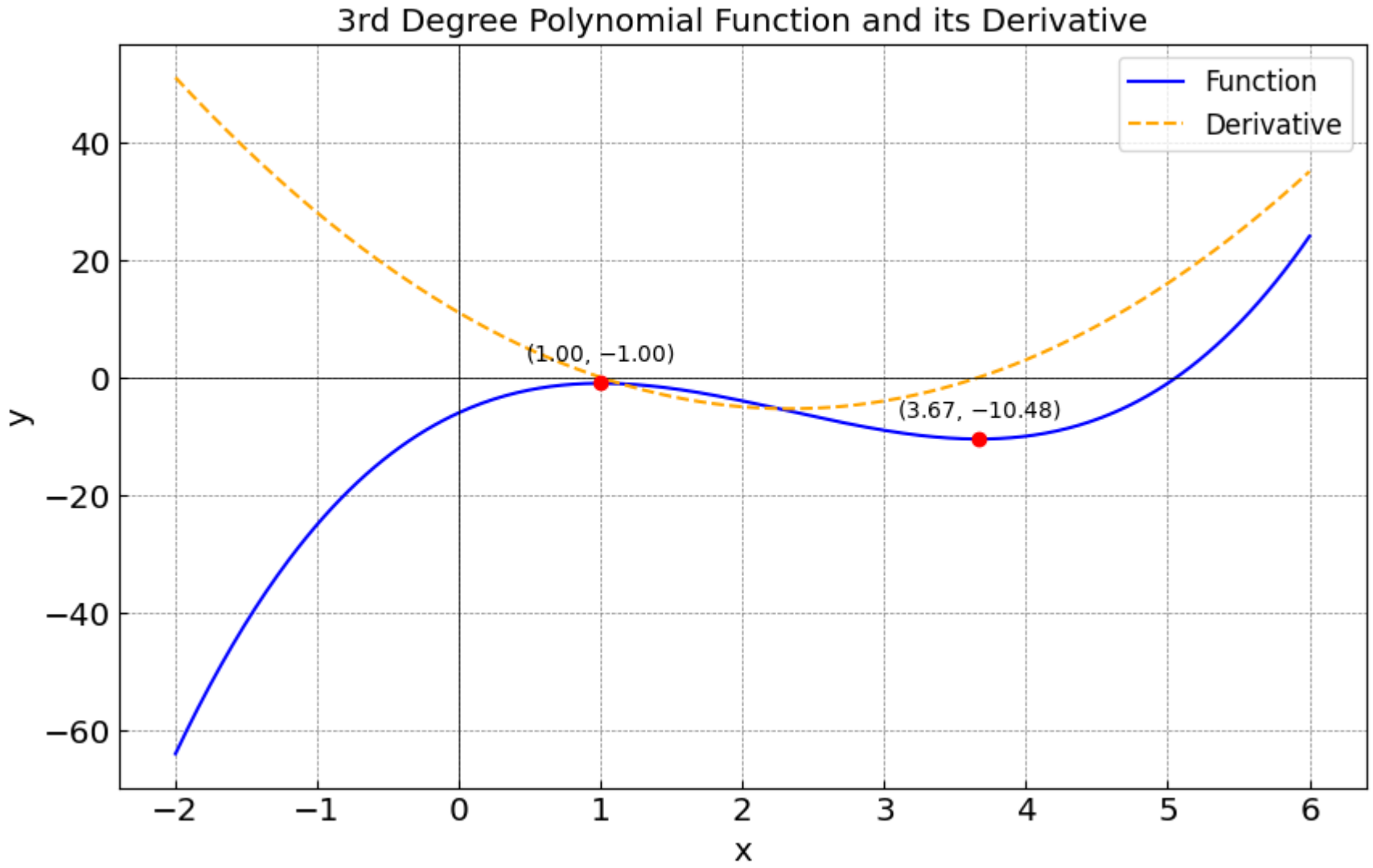


Derivative at a single point



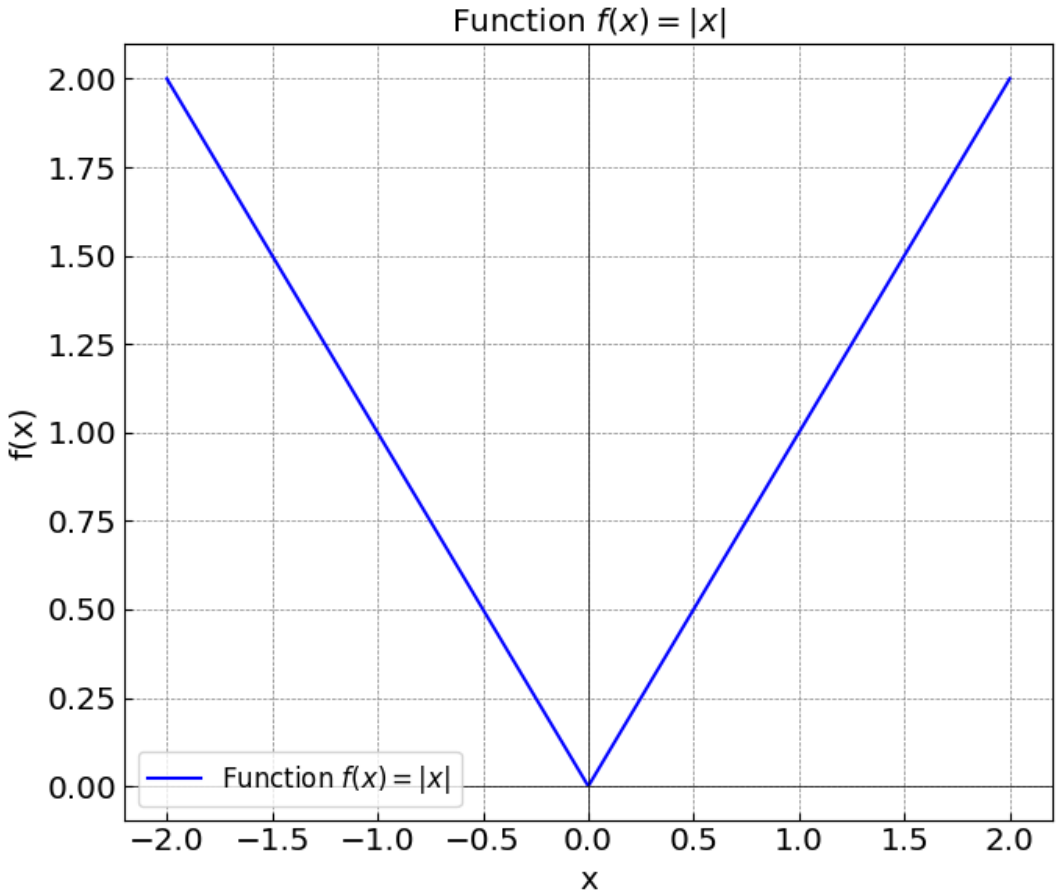
We need to define an arbitrary small step in space to define derivative

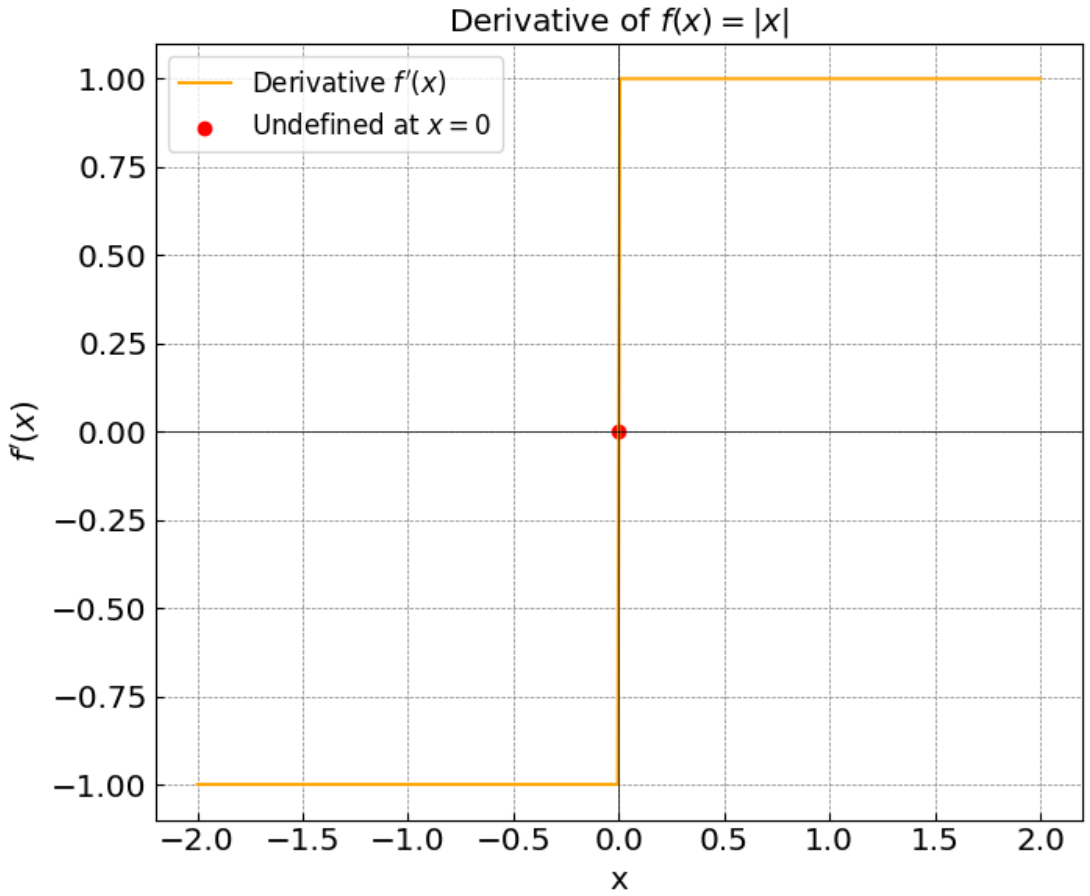
Derivative of a function



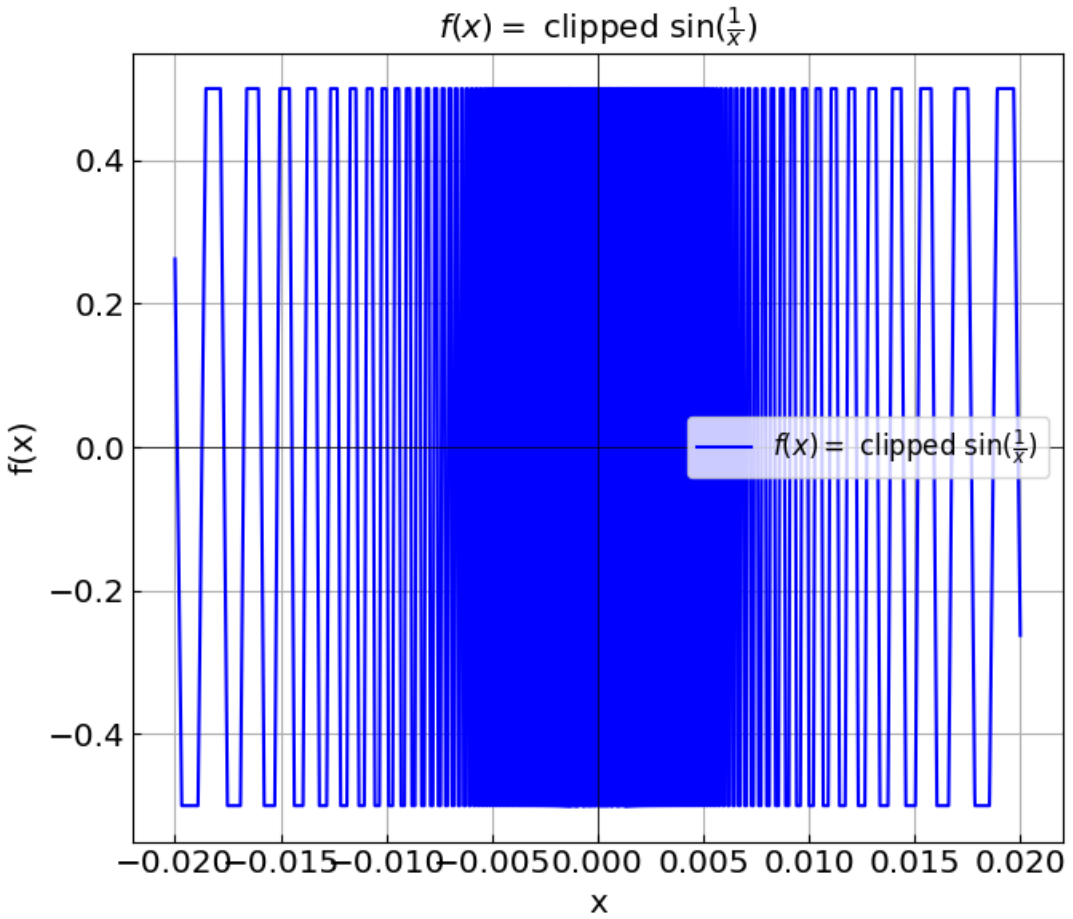
Zeroes of derivative are the extrema of the function

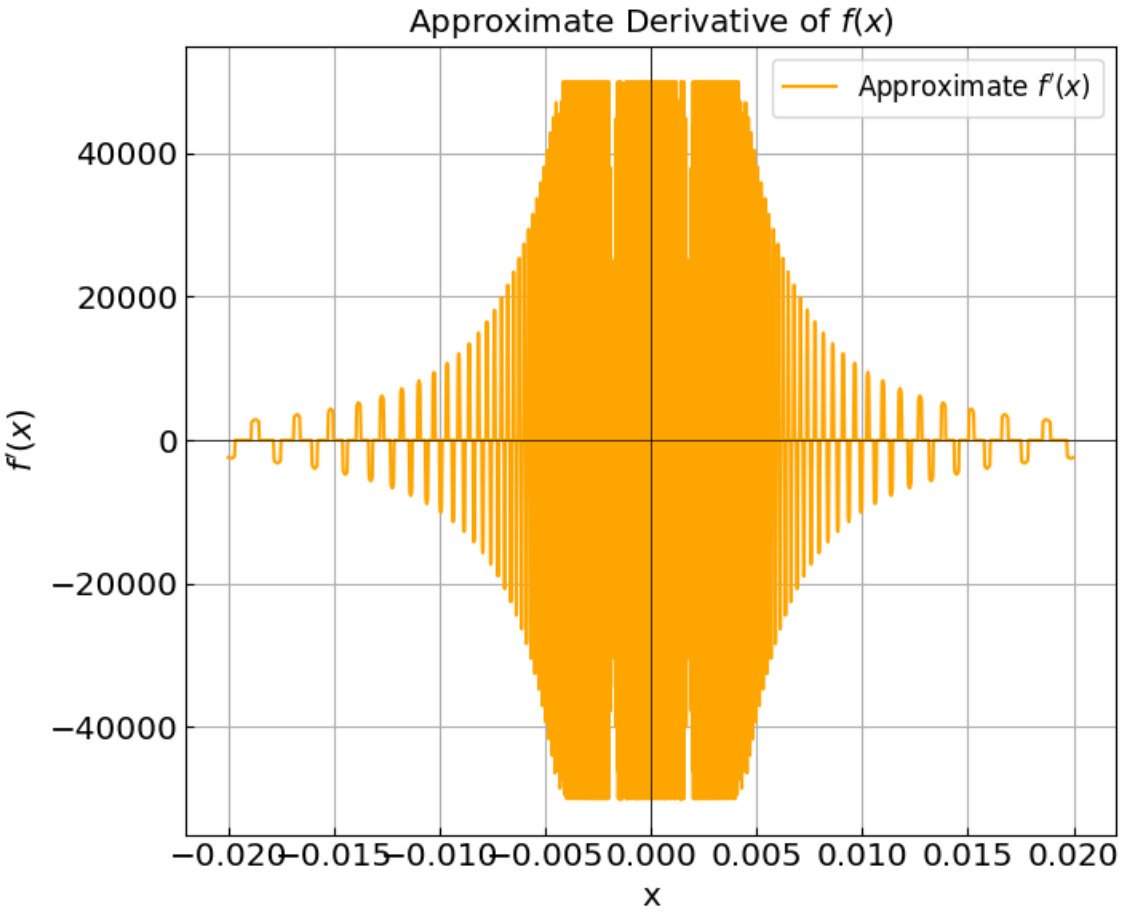
Not all functions are differentiable





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)

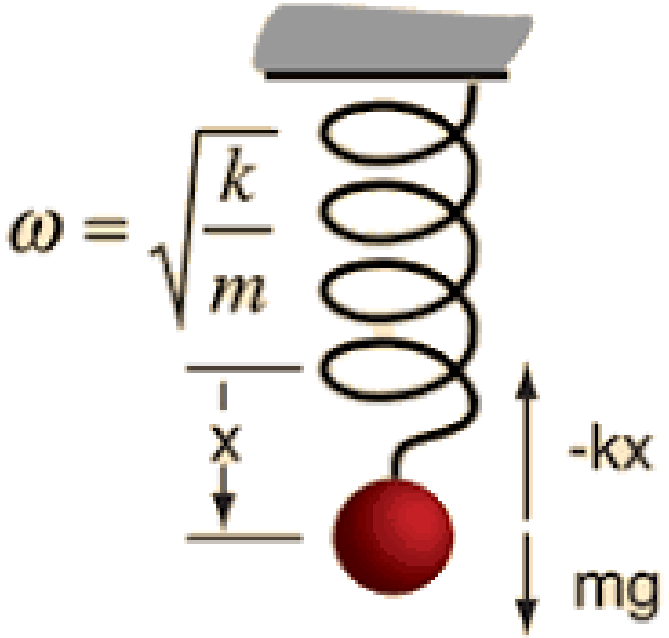
3.Equation of motion: $F= m\ dt^2/d^2x$.

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.



Hooke's Law:

$$F_{spring} = -kx$$

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

Initial and boundary value problems

Find: $\mathbf{z}(t) = [x(t), y(t), \dot{x}(t), \dot{y}(t)]$

Boundry Conditions:

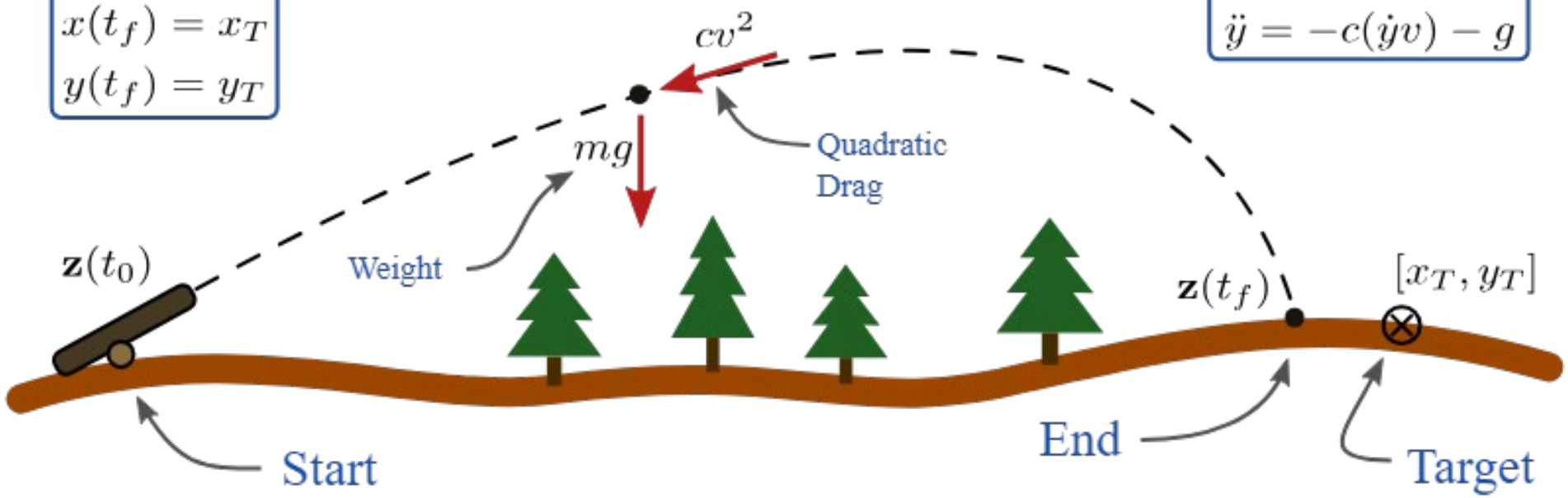
$$x(t_0) = 0$$
$$y(t_0) = 0$$
$$x(t_f) = x_T$$
$$y(t_f) = y_T$$

Cost Function:

$$J = \dot{x}(t_0)^2 + \dot{y}(t_0)^2$$

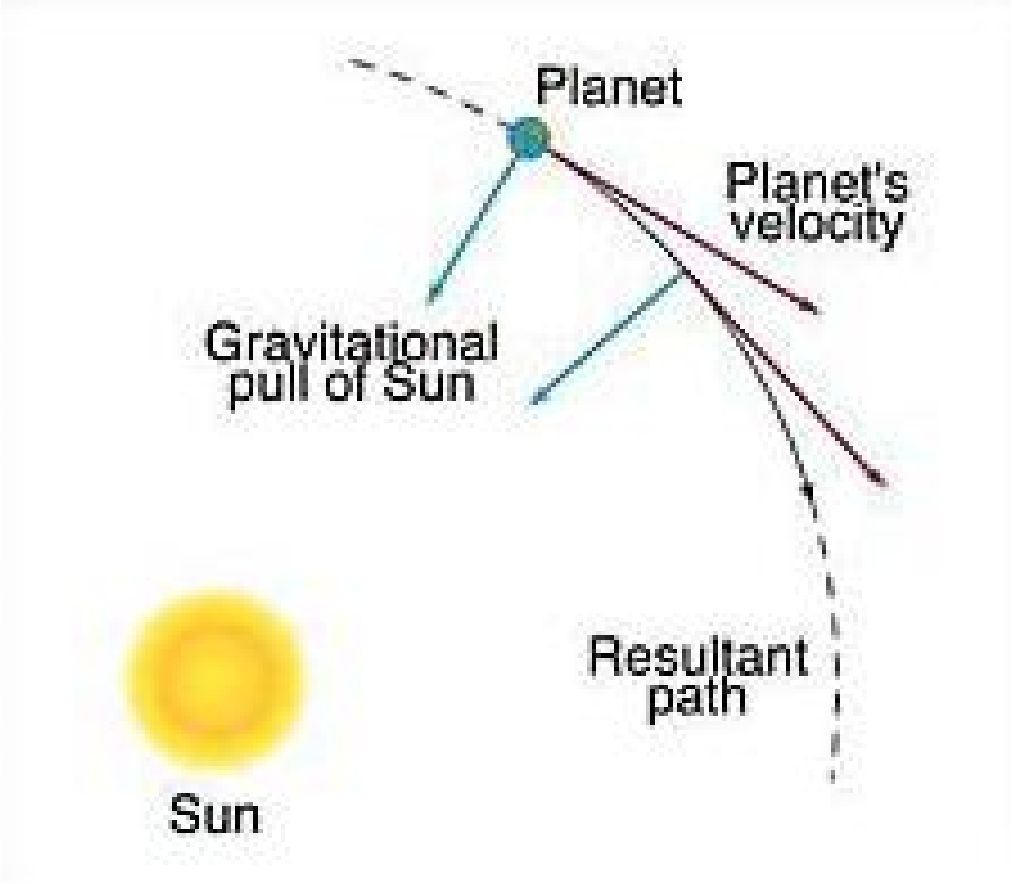
Dynamics:

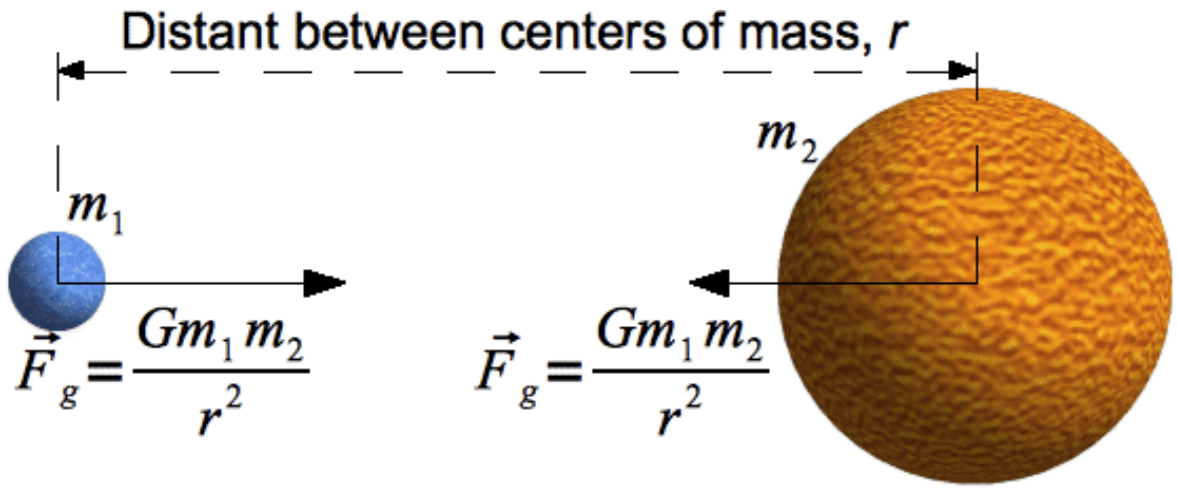
$$v = \sqrt{\dot{x}^2 + \dot{y}^2}$$
$$\ddot{x} = -c(\dot{x}v)$$
$$\ddot{y} = -c(\dot{y}v) - g$$



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

Stationary solutions





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

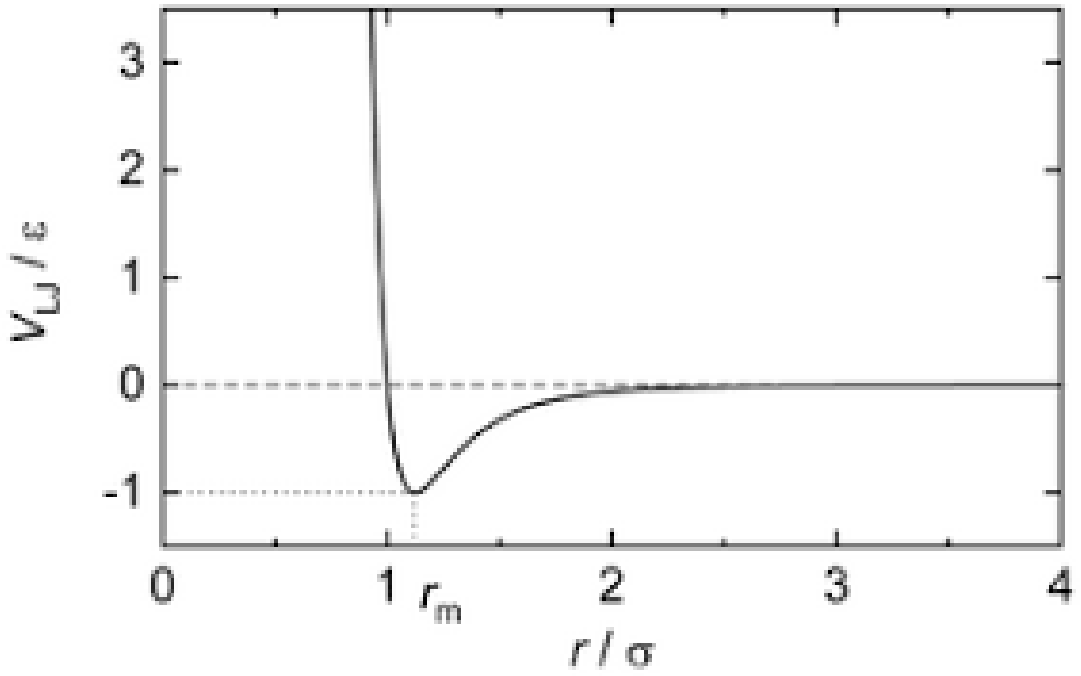
https://erikajanesite.wordpress.com/2017/09/24/225/

Molecular dynamics

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

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

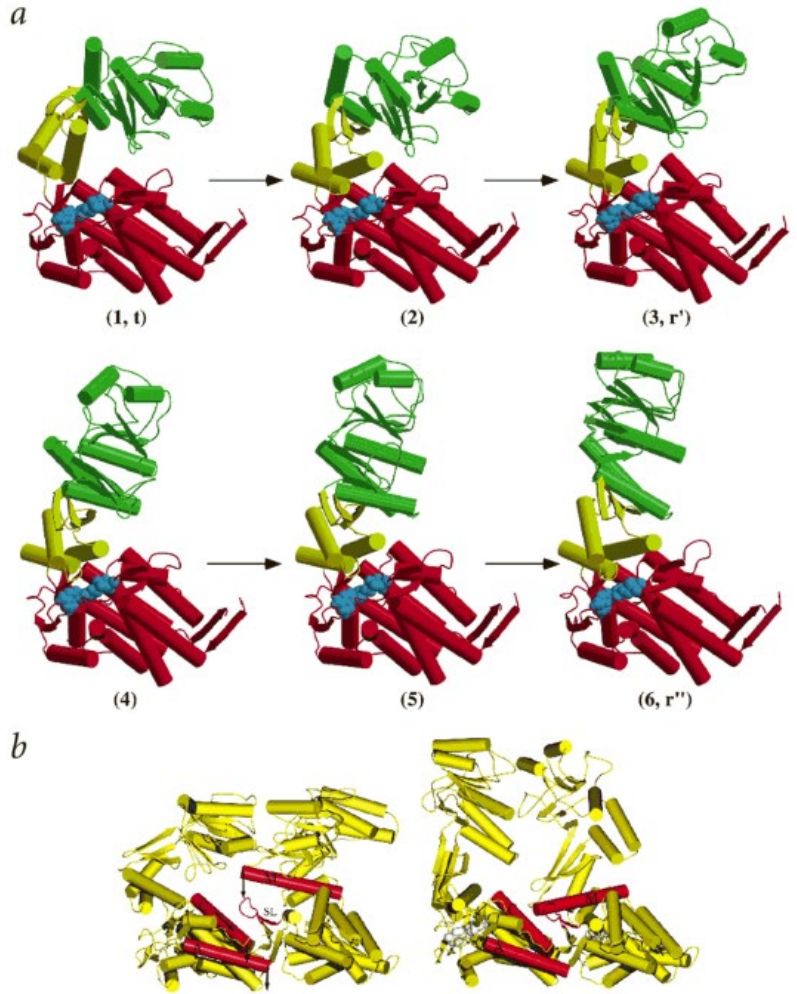
- Box simulation
  - Periodic boundary conditions
  - Minimum-image convention



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

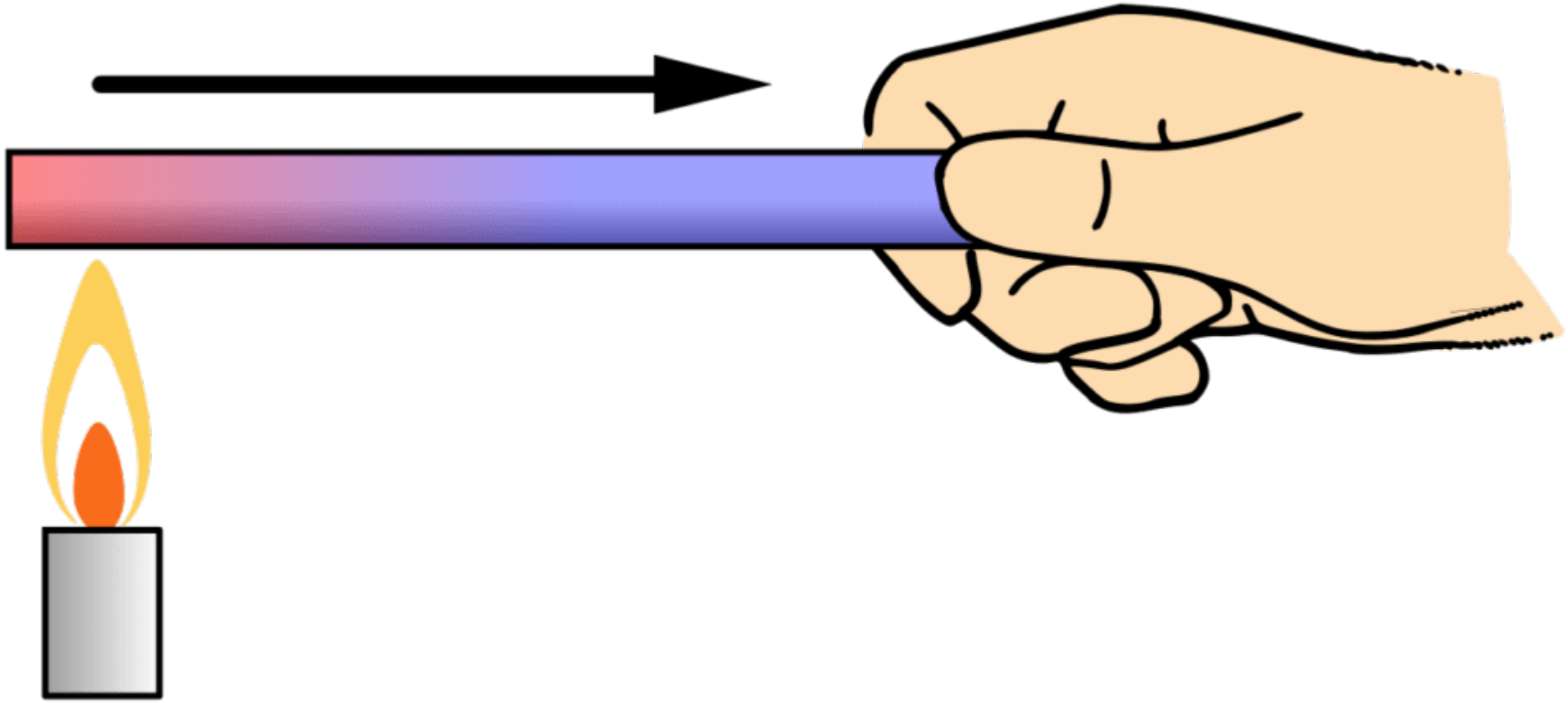
- MD simulations give access to the **equation of state**

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:

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

where $\dot{q}$ 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:

$$U = \rho c_p T$$

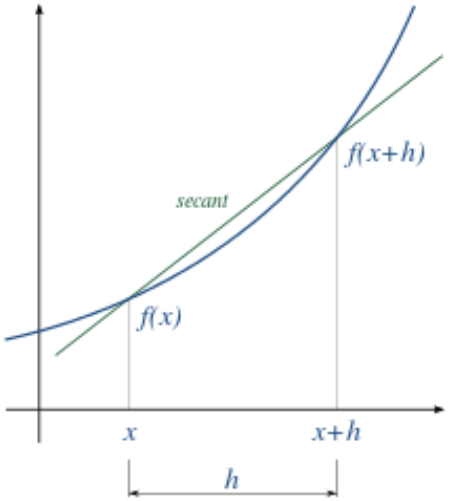
1.Substituting this into the conservation of energy equation and using Fourier's law, we get the heat equation for a homogeneous, isotropic material without internal heat generation as:

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

Numerical differentiation

Generic problem: evaluate

$$\frac{\mathrm{d}f}{\mathrm{d}x} = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$



We need numerical differentiation when

- Function f is known at a discrete set of points
- Too expensive/cumbersome to do directly
  - E.g. when f(x) itself is a solution to a complex web of non-linear equations, calculating f'(x) explicitly will require rewriting all the equations

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Forward difference

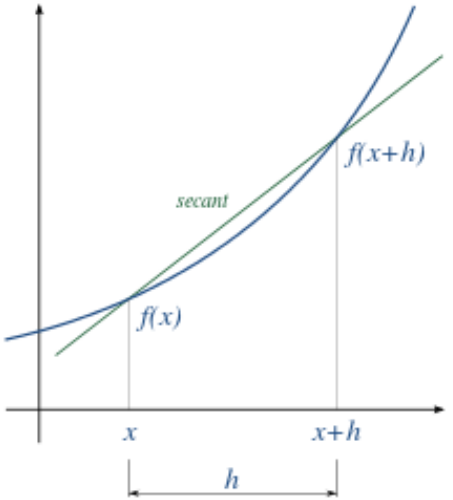
Simply approximate

$$\frac{\mathrm{d}f}{\mathrm{d}x} = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

by

$$\frac{\mathrm{d}f}{\mathrm{d}x} \simeq \frac{f(x+h) - f(x)}{h}$$

where *h* is finite



Taylor theorem:

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \dots$$

gives the approximation error estimate of

$$R_{\text{forw}} = -\frac{1}{2}hf''(x) + \mathcal{O}(h^2)$$

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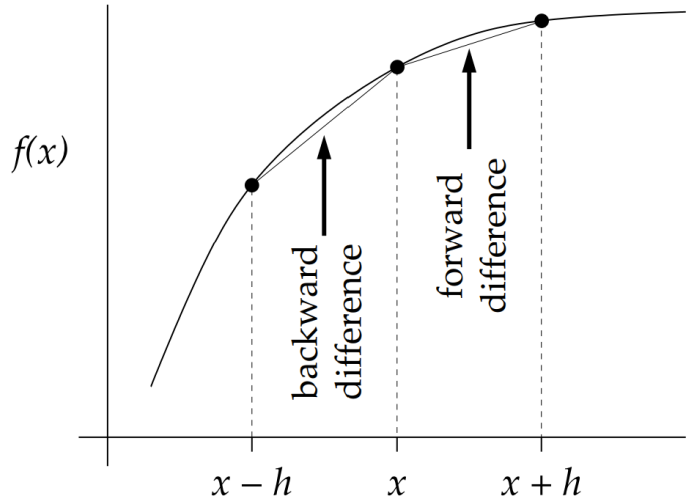
Backward difference

Backward difference

$$\frac{\mathrm{d}f}{\mathrm{d}x} \simeq \frac{f(x) - f(x-h)}{h}$$



Taylor theorem:

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2}f''(x) + \ldots$$

gives the approximation error estimate of

$$R_{\text{back}} = \frac{1}{2}hf''(x) + \mathcal{O}(h^2)$$

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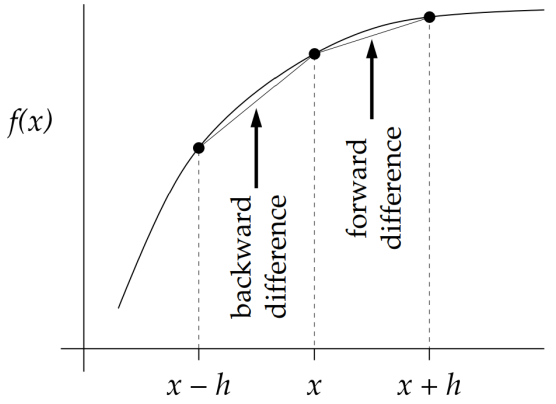
Central difference

Recall the forward and backward difference and their errors

$$\frac{\mathrm{d}f}{\mathrm{d}x} \simeq \frac{f(x+h)-f(x)}{h} \qquad \frac{\mathrm{d}f}{\mathrm{d}x} \simeq \frac{f(x)-f(x-h)}{h}$$

$$R_{\mathrm{forw}} = -\frac{1}{2}hf''(x) + \mathcal{O}(h^2) \qquad R_{\mathrm{back}} = \frac{1}{2}hf''(x) + \mathcal{O}(h^2)$$



Taking the average of the two cancels out the *O(h)* error term

central difference $$\frac{df}{dx} \simeq \frac{f(x+h)-f(x-h)}{2h}$$

Error estimate:

$$R_{\mathrm{cent}} = -\frac{f'''(x)}{6}h^2 + \mathcal{O}(h^3)$$

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High-order central difference

To improve the approximation error use more than two function evaluations, e.g.

$$\frac{df}{dx} \simeq \frac{Af(x+2h) + Bf(x+h) + Cf(x) + Df(x-h) + Ef(x-2h)}{h} + O(h^4)$$

Determine *A,B,C,D,E* using Taylor expansion to cancel all terms up to h^4

$$\frac{df}{dx} \simeq \frac{-f(x+2h) + 8f(x+h) - 8f(x-h) + f(x-2h)}{12h} + \frac{h^4}{30} f^{(5)}(x)$$

High-order terms:

Derivative	Accuracy	−5	−4	−3	−2	−1	0	1	2	3	4	5
1	2					−1/2	0	1/2				
	4				1/12	−2/3	0	2/3	−1/12			
	6			−1/60	3/20	−3/4	0	3/4	−3/20	1/60		
	8		1/280	−4/105	1/5	−4/5	0	4/5	−1/5	4/105	−1/280	

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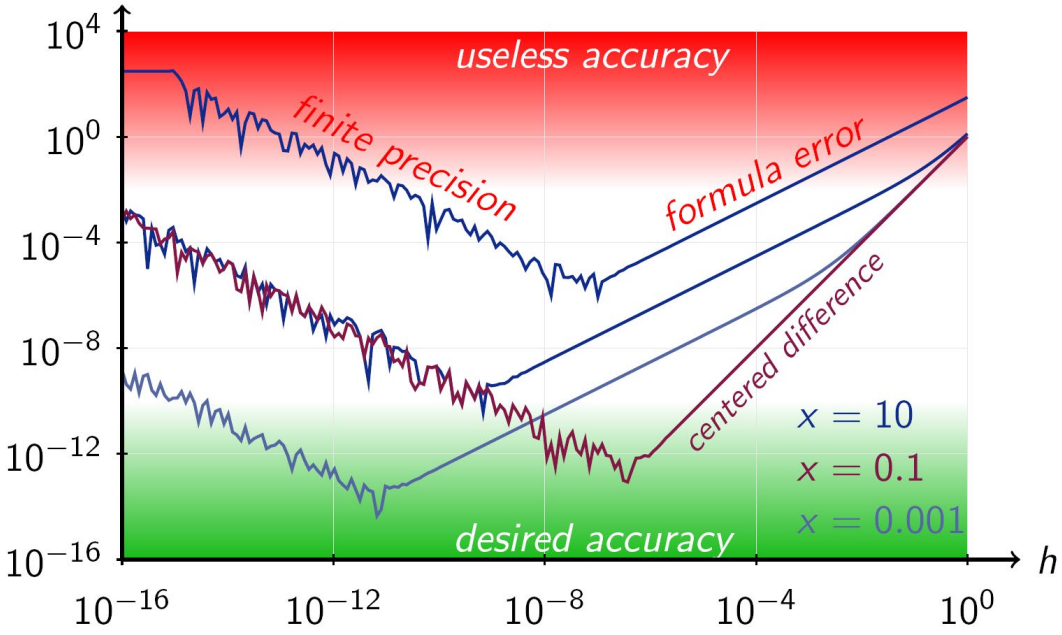
Balancing truncation and round-off errors

If *h* is too small, round-off errors become important

- cannot distinguish *x* and *x+h* and/or *f(x+h)* and *f(x)* with enough accuracy



Credit: Wikipedia

As a rule of thumb, if ε is machine precision and the truncation error is of order $O(h^n)$, then *h* should not be much smaller than $h \sim \sqrt[n+1]{\varepsilon}$

The higher the finite difference order is, the larger *h* should be

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Balancing truncation and round-off errors

Let f(x) = exp(x)

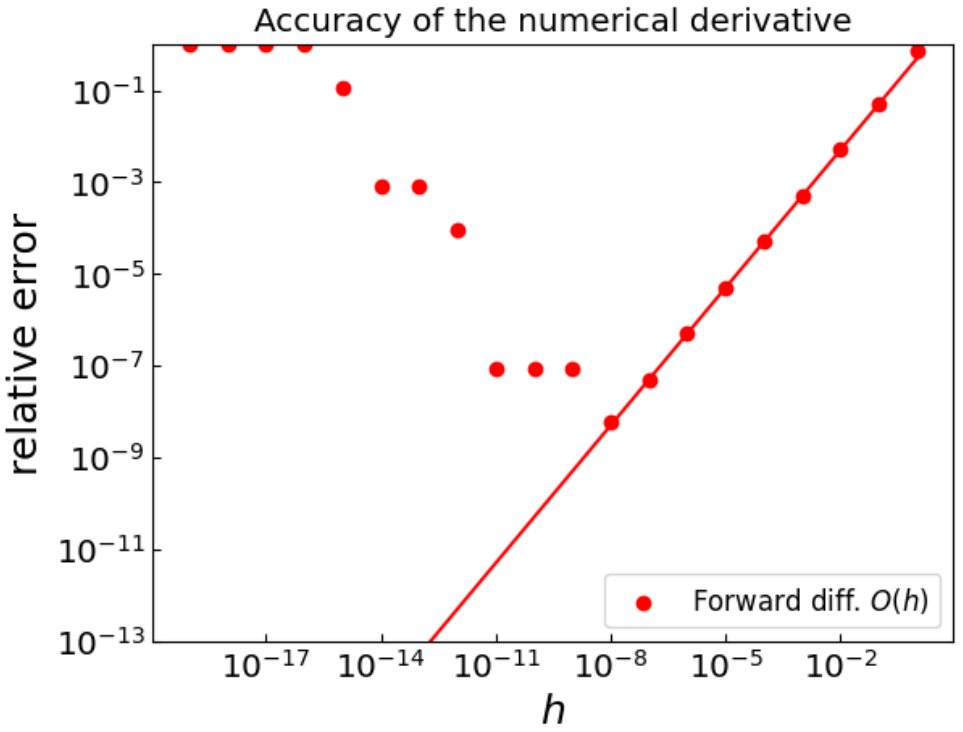
Calculate the derivatives at x = 0

```
def f(x):
    return np.exp(x)

def df(x):
    return np.exp(x)
```

Forward difference O(h):

Optimal $h \sim \sqrt[2]{10^{-16}} \sim 10^{-8}$



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Balancing truncation and round-off errors

Let f(x) = exp(x)

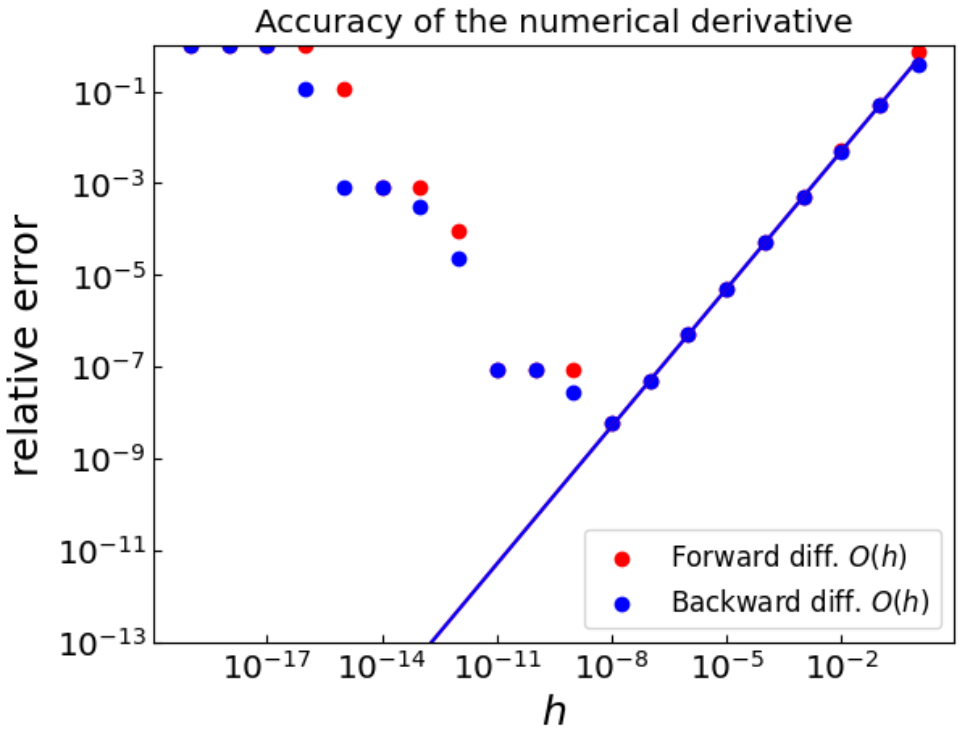
Calculate the derivatives at x = 0

```
def f(x):
    return np.exp(x)

def df(x):
    return np.exp(x)
```

Backward difference O(h):

Optimal $h \sim \sqrt[2]{10^{-16}} \sim 10^{-8}$



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Balancing truncation and round-off errors

Let f(x) = exp(x)

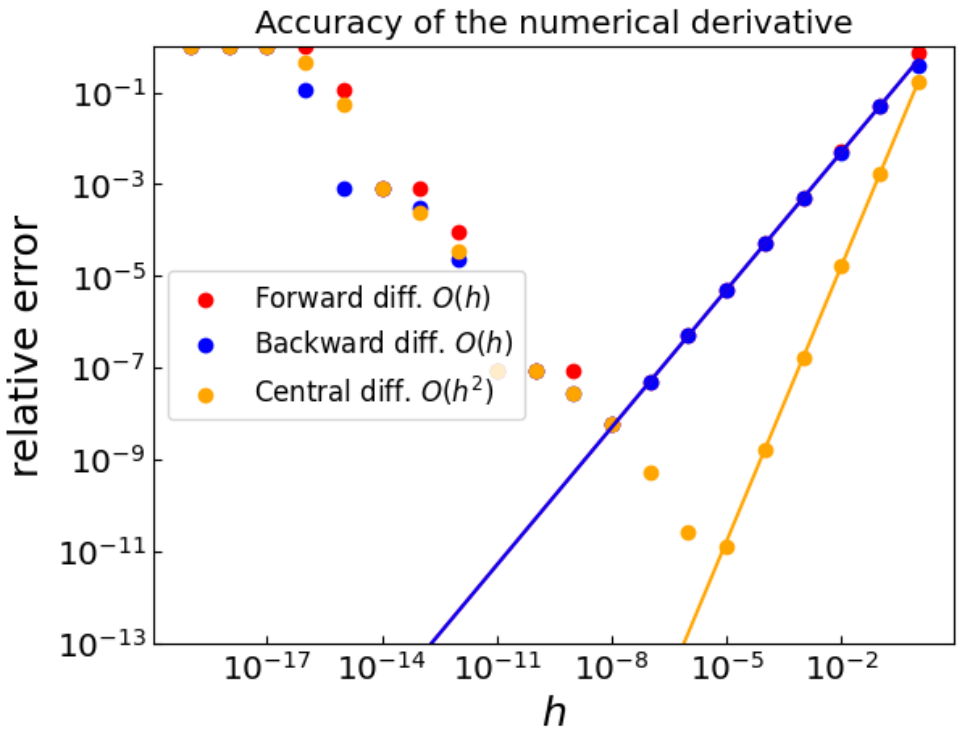
Calculate the derivatives at x = 0

```
def f(x):
    return np.exp(x)

def df(x):
    return np.exp(x)
```

Central difference $O(h^2)$:

Optimal $h \sim \sqrt[3]{10^{-16}} \sim 10^{-5}$



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Balancing truncation and round-off errors

Let f(x) = exp(x)

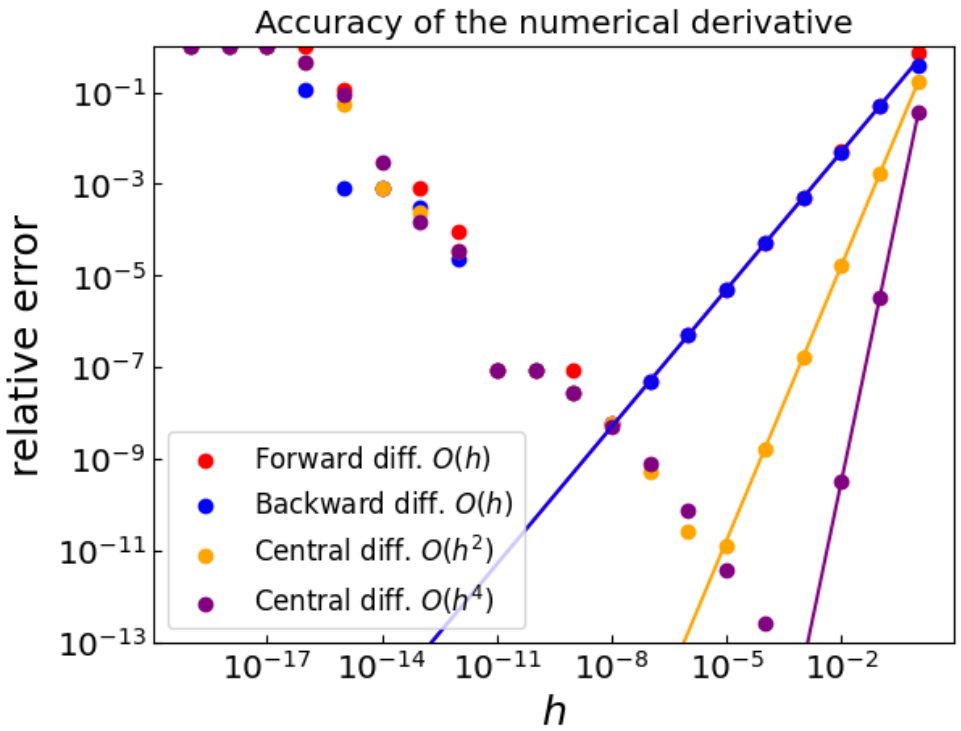
Calculate the derivatives at x = 0

```
def f(x):
    return np.exp(x)

def df(x):
    return np.exp(x)
```

Central difference O(h⁴):

Optimal $h \sim \sqrt[5]{10^{-16}} \sim 10^{-3}$



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High-order derivatives

Central difference

$$\frac{df}{dx}(x) \simeq \frac{f(x+h/2) - f(x-h/2)}{h}$$

Now apply the central difference again to *f'(x+h/2)* and *f'(x-h/2)*

$$\begin{aligned} f''(x) &\simeq \frac{f'(x+h/2) - f'(x-h/2)}{h} \\ &= \frac{[f(x+h) - f(x)]/h - [f(x) - f(x-h)]/h}{h} \\ &= \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}. \end{aligned}$$

General formula (to order *h*)

$$f^{(n)}(x) = \frac{1}{h^n} \sum_{k=0}^{n} (-1)^k \binom{n}{k} f\left[x + (n/2 - k)h\right] + O(h^2)$$

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Second derivative

```python
def d2f_central(f,x,h):
    return (f(x+h) - 2*f(x) + f(x-h)) / (h**2)
```

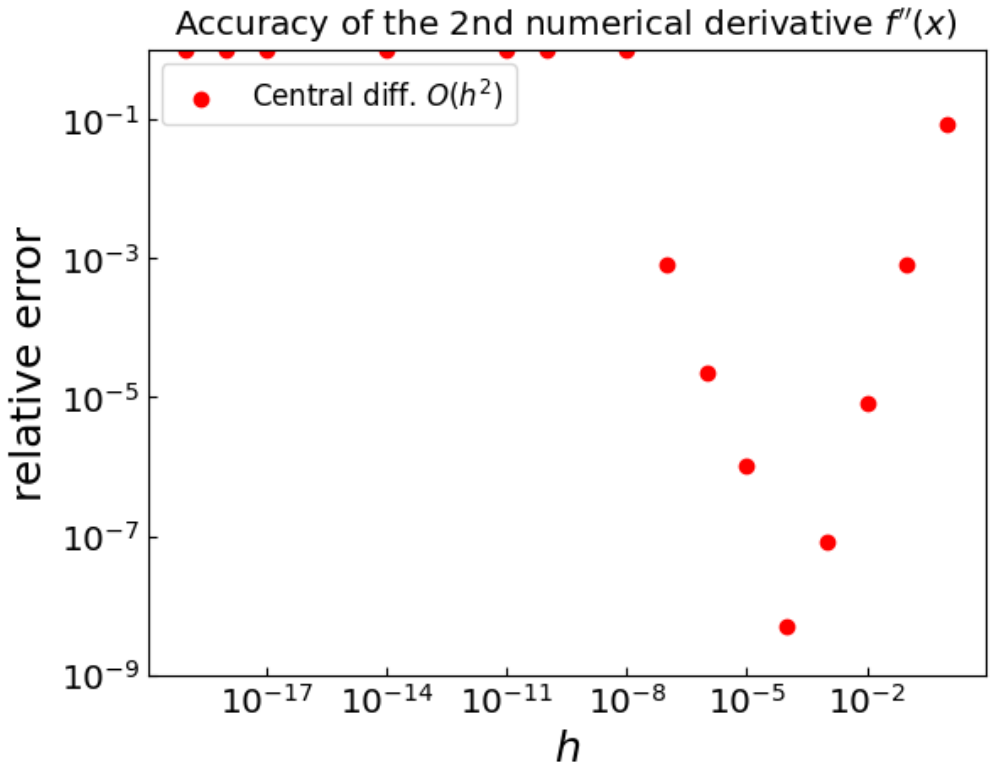
f(x) = exp(x)

```python
def f(x):
    return np.exp(x)

def df(x):
    return np.exp(x)

def d2f(x):
    return np.exp(x)
```

Optimal $h \sim \sqrt[4]{10^{-16}} \sim 10^{-4}$



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Partial derivatives

Let us have *f(x,y)*
Use central difference to calculate first-order derivatives

$$\frac{\partial f}{\partial x} = \frac{f(x+h/2,y) - f(x-h/2,y)}{h}$$
$$\frac{\partial f}{\partial y} = \frac{f(x,y+h/2) - f(x,y-h/2)}{h}$$

Reapply the central difference to calculate $\partial^2 f(x,y)/\partial x \partial y$

$$\frac{\partial^2 f}{\partial x \partial y} = \frac{f(x+h/2,y+h/2) - f(x-h/2,y+h/2) - f(x+h/2,y-h/2) + f(x-h/2,y-h/2)}{h^2}$$

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Summary: Numerical differentiation

- Forward/backward differences
  - Useful when we are given a grid of function values
  - Have limited accuracy (linear in *h*)

- Central difference
  - More precise than forward/backward differences (quadratic in *h*)
  - Gives f'(x) estimate at the midpoint of function evaluation points

- Higher-order formulas are obtained by using more than two function evaluations
  - Can be used when limited number of function evaluations available

- Straightforwardly extendable to high-order and partial derivatives

- Balance between truncation and round-off error must be respected
  - *h* should not be taken too small

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Numerical derivative and ordinary differential equations

Ordinary differential equation

$$\frac{dx}{dt} = f(x, t),$$

with initial condition

$$f(x, t_0) = f_0$$

Use the forward difference to approximate dx/dt

$$\frac{dx}{dt} \approx \frac{x(t+h) - x(t)}{h}$$

gives the **Euler method** of solving the equation for x(t)

$$x(t+h) = x(t) + h\, f[x(t), t]$$

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Ordinary Differential Equations (ODE)

First-order ordinary differential equation (ODE) is an equation of the form

$$\frac{dx}{dt} = f(x, t),$$

with initial condition

$$x(t = 0) = x_0$$

This determines the x(t) dependence at t>0.

In many physical applications *t* plays the role of the time variable (classical mechanics problems), although this is not always the case.

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When we need numerical methods for ODEs

The solution to an ODE

$$\frac{dx}{dt} = f(x, t), \qquad x(t = 0) = x_0$$

can formally be written as

$$x(t) = x_0 + \int_0^t f[x(t'), t'])dt'$$

If f does not depend on x, the solution can be obtained through (numerical) integration

In some other cases the solution can be obtained through the separation of variables, e.g.

$$\frac{dx}{dt} = \frac{2x}{t}$$

In all other cases, the solution has to be obtained numerically.

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Numerical methods for ODEs

Typically obtain the solution by taking small steps from *x(t)* to *x(t+h)*

Characteristics:

- Explicit or implicit
  - Explicit methods: use *x(t)* to calculate *x(t+h)* directly
  - Implicit methods: have to solve a (non-linear) equation for *x(t+h)*

- Accuracy
  - Truncation error at each step is of order $O(h^n)$
  - Some schemes are explicitly time-reversal and/or conserve energy
  - Adaptive methods adjust the step size *h* to control the error to the desired accuracy

- Stability
  - Whether the accumulated error is bounded (that's where implicit methods shine)

- Consistency
  - Consistent methods reproduce the exact solution in the limit $h \to 0$

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Euler's method

$$\frac{dx}{dt} = f(x, t),$$

Let us apply the Taylor expansion to express *x(t+h)* in terms of *x(t)*:

$$x(t+h) = x(t) + h\frac{dx}{dt} + O(h^2)\ .$$

Given that dx/dt = f(x,t) and neglecting the high-order terms in *h* we have

$$x(t+h) \approx x(t) + h\,f[x(t), t] \qquad \textit{Euler method}$$

We can iteratively apply this relation starting from t = 0 to evaluate x(t) at t > 0.

This is the essence of the **Euler method** -- the simplest method for solving ODEs numerically.

Error:

- Local (per time step): $O(h^2)$
- Global (N=t_{end}/h time steps): O(h)

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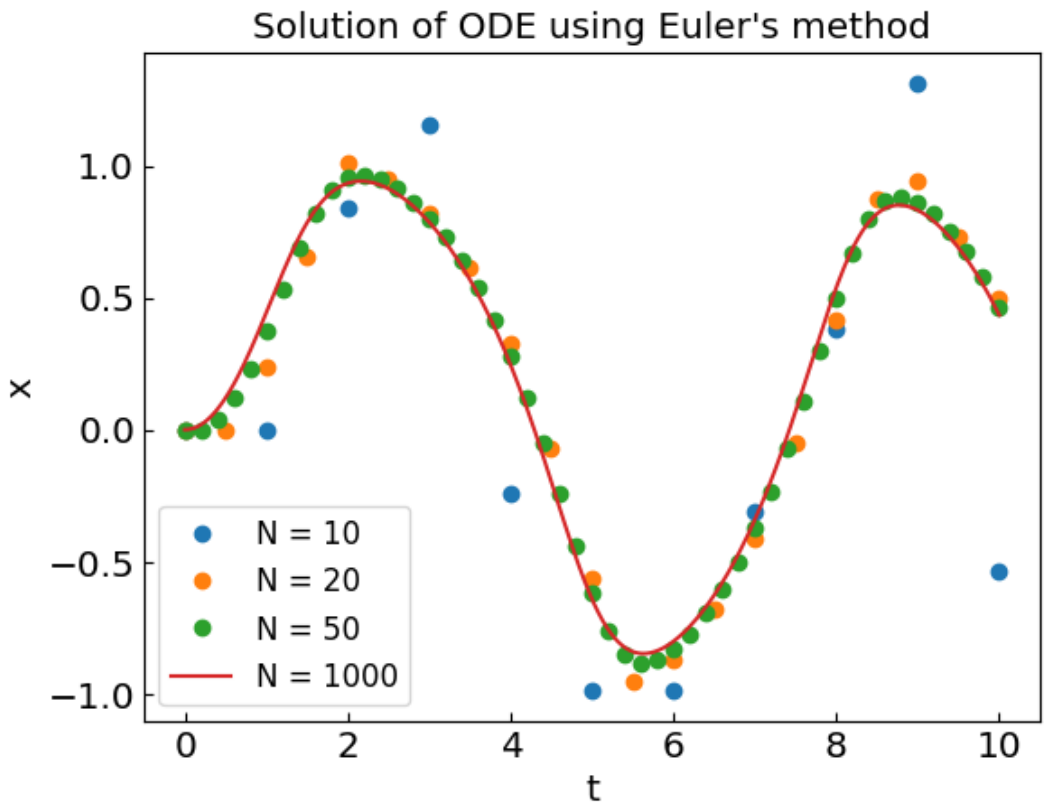
Euler's method

```python
import numpy as np

def ode_euler_step(f, x, t, h):
    """Perform a single step h using Euler's scheme.

    Args:
    f: the function that defines the ODE.
    x: the value of the dependent variable at the present step.
    t: the present value of the time variable.
    h: the time step

    Returns:
    xnew: the value of the dependent variable at the step t+h
    """
    return x + h * f(x,t)

def ode_euler(f, x0, t0, h, nsteps):
    """Solve an ODE dx/dt = f(x,t) from t = t0 to t = t0 + h*steps using Euler's method.

    Args:
          f: the function that defines the ODE.
         x0: the initial value of the dependent variable.
         t0: the initial value of the time variable.
          h: the time step
     nsteps: the total number of Euler steps

    Returns:
    t,x: the pair of arrays corresponding to the time and dependent variables
    """

    t = np.zeros(nsteps + 1)
    x = np.zeros(nsteps + 1)
    x[0] = x0
    t[0] = t0
    for i in range(0, nsteps):
        t[i + 1] = t[i] + h
        x[i + 1] = ode_euler_step(f, x[i], t[i], h)
    return t,x
```

$$\frac{dx}{dt} = -x^3 + \sin t, \qquad x(t=0) = 0.$$



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Midpoint method (2nd order Runge-Kutta)

Euler's method essentially corresponds to approximating the derivative dx/dt with a *forward difference*

$$\frac{dx}{dt} = f(x,t) \approx \frac{x(t+h) - x(t)}{h} + \mathcal{O}(h).$$

Recall that central (midpoint) difference gives better accuracy

$$f(x, t+h/2) \approx \frac{x(t+h) - x(t)}{h} + \mathcal{O}(h^2).$$

therefore

$$x(t+h) = x(t) + hf[x(t+h/2), t+h/2)] + \mathcal{O}(h^3)$$

How to calculate *x(t+h/2)* in r.h.s? Use Euler's method $x(t+h/2) = x(t) + \frac{1}{2}hf(x,t) + \mathcal{O}(h^2)$

Therefore, $x(t+h) = x(t) + hf\left[x(t) + \frac{1}{2}hf(x,t), t + \frac{1}{2}h\right] + \mathcal{O}(h^3)$, which can be written in two steps

$$\begin{aligned} k_1 &= h\,f(x,t), && \textit{trial step} \\ k_2 &= h\,f(x + k_1/2, t + h/2), && \textit{real step} \\ x(t+h) &= x(t) + k_2\ . \end{aligned}$$

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https://github.com/vlvovch/PHYS6350-ComputationalPhysics

Midpoint method (2nd order Runge-Kutta)

```python
def ode_rk2_step(f, x, t, h):
    """Perform a single step h using 2nd order Runge-Kutta scheme.

    Args:
    f: the function that defines the ODE.
    x: the value of the dependent variable at the present step.
    t: the present value of the time variable.
    h: the time step

    Returns:
    xnew: the value of the dependent variable at the step t+h
    """
    k1 = h * f(x,t)
    k2 = h * f(x + k1/2., t + h /2.)
    return x + k2

def ode_rk2(f, x0, t0, h, nsteps):
    """Solve an ODE dx/dt = f(x,t) from t = t0 to t = t0 + h*steps using Euler's method.

    Args:
          f: the function that defines the ODE.
         x0: the initial value of the dependent variable.
         t0: the initial value of the time variable.
          h: the time step
     nsteps: the total number of Euler steps

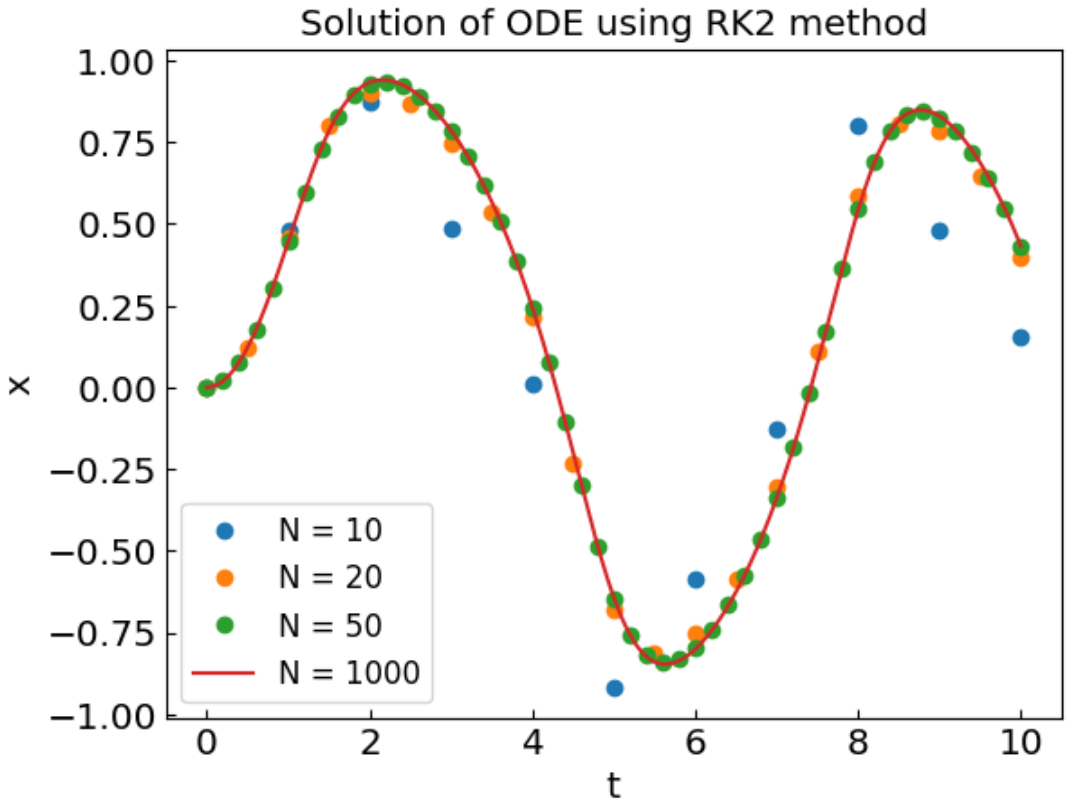
    Returns:
    t,x: the pair of arrays corresponding to the time and dependent variables
    """

    t = np.zeros(nsteps + 1)
    x = np.zeros(nsteps + 1)
    x[0] = x0
    t[0] = t0
    for i in range(0, nsteps):
        t[i + 1] = t[i] + h
        x[i + 1] = ode_rk2_step(f, x[i], t[i], h)
    return t,x
```

Error:

- Local (per time step): $O(h^3)$
- Global (N=t_{end}/h time steps): $O(h^2)$

$$\frac{dx}{dt} = -x^3 + \sin t, \qquad x(t=0) = 0.$$



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Midpoint method (2nd order Runge-Kutta)

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    Args:
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    h: the time step

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    """
    k1 = h * f(x,t)
    k2 = h * f(x + k1/2., t + h /2.)
    return x + k2

def ode_rk2(f, x0, t0, h, nsteps):
    """Solve an ODE dx/dt = f(x,t) from t = t0 to t = t0 + h*steps using Euler's method.

    Args:
          f: the function that defines the ODE.
         x0: the initial value of the dependent variable.
         t0: the initial value of the time variable.
          h: the time step
     nsteps: the total number of Euler steps

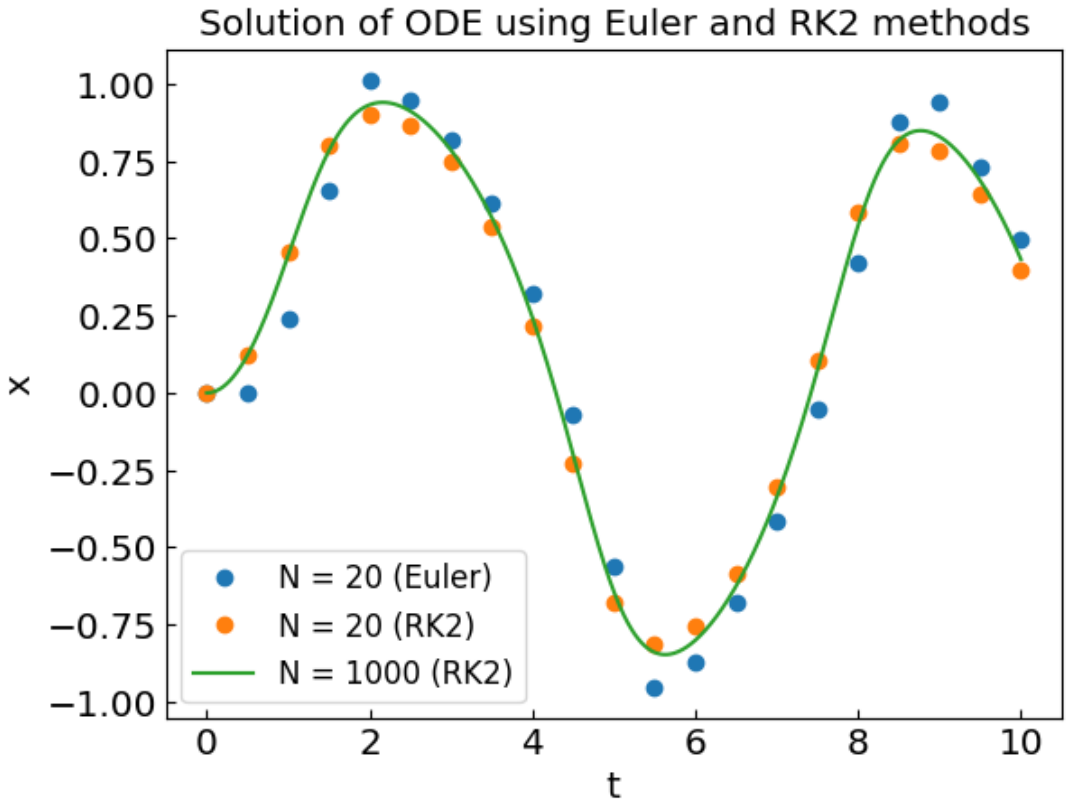
    Returns:
    t,x: the pair of arrays corresponding to the time and dependent variables
    """

    t = np.zeros(nsteps + 1)
    x = np.zeros(nsteps + 1)
    x[0] = x0
    t[0] = t0
    for i in range(0, nsteps):
        t[i + 1] = t[i] + h
        x[i + 1] = ode_rk2_step(f, x[i], t[i], h)
    return t,x
```

Error:

- Local (per time step): $O(h^3)$
- Global (N=t_{end}/h time step): $O(h^2)$

$$\frac{dx}{dt} = -x^3 + \sin t, \qquad x(t=0) = 0.$$



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Classical 4th order Runge-Kutta method

The above logic can be generalized to cancel high-order error terms in various powers in *h,* requiring more and more evaluations of function *f*(x,t) at intermediate steps.

The following classical 4th-order Runge-Kutta method is often considered a sweet spot.

It corresponds to the following scheme:

$$
\begin{aligned}
k_1 &= h\,f(x, t), \\
k_2 &= h\,f(x + k_1/2, t + h/2), \\
k_3 &= h\,f(x + k_2/2, t + h/2), \\
k_4 &= h\,f(x + k_3, t + h), \\
x(t + h) &= x(t) + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)\ .
\end{aligned}
$$

Error:

- Local (per time step): $O(h^5)$
- Global (N=t_{end}/h time steps): $O(h^4)$

The classical 4th-order Runge-Kutta method is a good first choice for solving physics ODEs.

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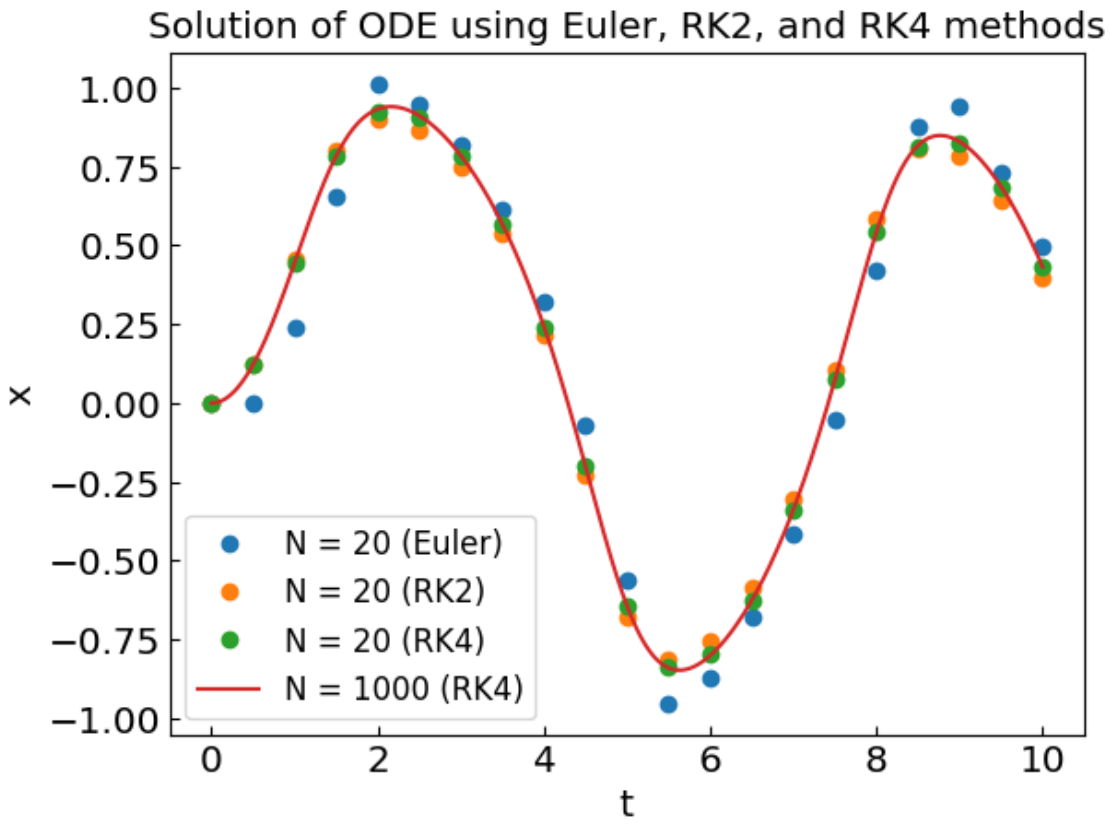
Classical 4th order Runge-Kutta method

```python
def ode_rk4_step(f, x, t, h):
    """Perform a single step h using 4th order Runge-Kutta method.

    Args:
    f: the function that defines the ODE.
    x: the value of the dependent variable at the present step.
    t: the present value of the time variable.
    h: the time step

    Returns:
    xnew: the value of the dependent variable at the step t+h
    """
    k1 = h * f(x,t)
    k2 = h * f(x + k1/2., t + h /2.)
    k3 = h * f(x + k2/2., t + h /2.)
    k4 = h * f(x + k3, t + h)
    return x + (k1 + 2. * k2 + 2. * k3 + k4) / 6.

def ode_rk4(f, x0, t0, h, nsteps):
    """Solve an ODE dx/dt = f(x,t) from t = t0 to t = t0 + h*steps using 4th order Runge-Kutta method.

    Args:
          f: the function that defines the ODE.
         x0: the initial value of the dependent variable.
         t0: the initial value of the time variable.
          h: the time step
     nsteps: the total number of Euler steps

    Returns:
    t,x: the pair of arrays corresponding to the time and dependent variables
    """

    t = np.zeros(nsteps + 1)
    x = np.zeros(nsteps + 1)
    x[0] = x0
    t[0] = t0
    for i in range(0, nsteps):
        t[i + 1] = t[i] + h
        x[i + 1] = ode_rk4_step(f, x[i], t[i], h)
    return t,x
```

$$\frac{dx}{dt} = -x^3 + \sin t, \qquad x(t=0) = 0.$$



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Adaptive time step

$$\frac{dx}{dt} = f(x, t)$$

The choice of the time step is important to reach the desired accuracy/performance.

- *h* too large: the desired accuracy not reached
- *h* too small: we waste computing resources on unnecessary iterations
- Local truncation error itself is a function of time depending on the behavior of f(x,t)

Adaptive time step: make a local error estimate and adjust *h* to correspond to the desired accuracy

Ways to estimate the error:

- Make two small steps (*h*) and compare x(t+2h) to the one from a single double step *2h*
- Use two methods of a different order and compare their results (e.g. Runge-Kutta-Fehlberg method RKF45)

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Adaptive time step in RK4 using double step

Recall that the error for one RK4 time step h is of order ch^5.
Let us take two RK4 steps h to approximate $x(t+2h) \approx x_1$. Then,

$$x(t+2h) \approx x_1 + 2ch^5$$

Now take single RK4 step $x(t+2h) \approx x_2$ of length $2h$

$$x(t+2h) \approx x_2 + 32ch^5$$

The local error estimate for a single RK4 time step h is then

$$\epsilon_{\text{RK4}} = |ch^5| = \frac{|x_1 - x_2|}{30}.$$

If the desired accuracy per unit time is δ, the desired accuracy per time step h' is

$$h'\delta = ch'^5$$

so the time step should be adjusted from h to h' as

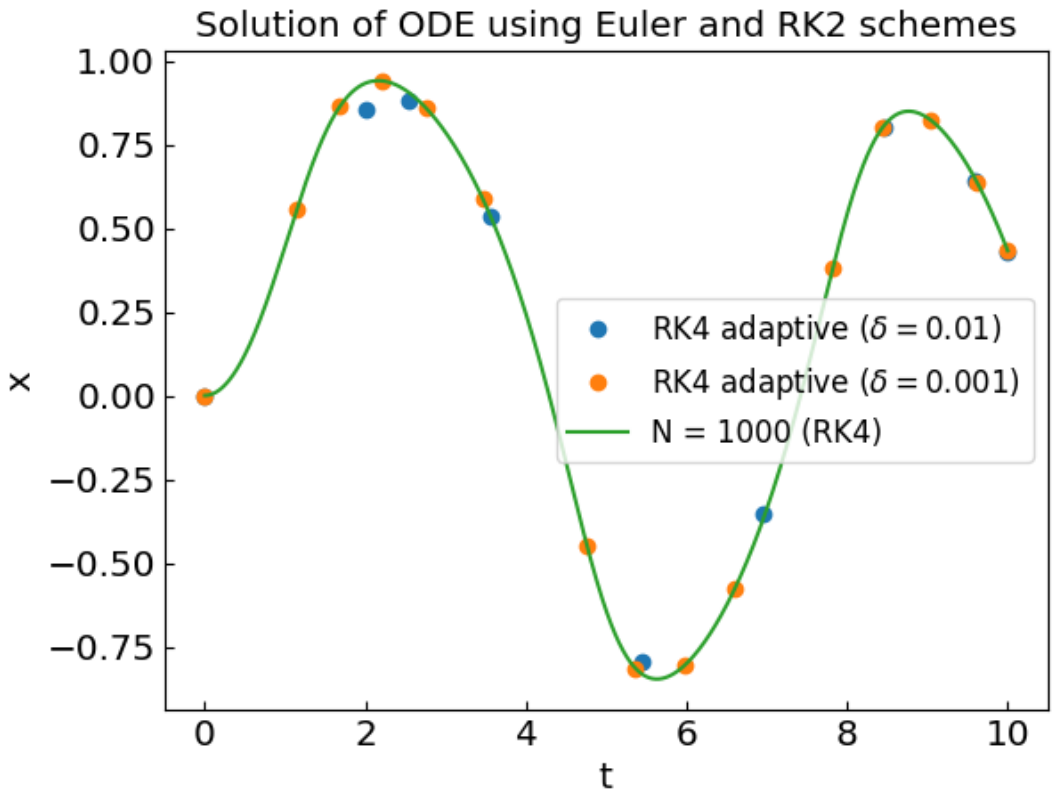
$$h' = h\left(\frac{30h\delta}{|x_1 - x_2|}\right)^{1/4}.$$

- $h'>h$: our step size is too small, move on to x(t+2h) and increase the step size to h'
- $h'<h$: our step size is too large, decrease step size to h' and try the current step again

RK4 method with adaptive step size

```python
def ode_rk4_adaptive(f, x0, t0, h0, tmax, delta = 1.e-6):

    ts = [t0]
    xs = [x0]
    h = h0
    t = t0
    i = 0
    while (t < tmax):
        if (t + h >= tmax):
            ts.append(tmax)
            h = tmax - t
            xs.append(ode_rk4_step(f, xs[i], ts[i], h))
            t = tmax
            break

        x1 = ode_rk4_step(f, xs[i], ts[i], h)
        x1 = ode_rk4_step(f, x1, ts[i] + h, h)
        x2 = ode_rk4_step(f, xs[i], ts[i], 2*h)

        rho = 30. * h * delta / np.abs(x1 - x2)
        if rho < 1.:
            h *= rho**(1/4.)
        else:
            if (t + 2.*h) < tmax:
                xs.append(x1)
                ts.append(t + 2*h)
                t += 2*h
            else:
                xs.append(ode_rk4_step(f, xs[i], ts[i], h))
                ts.append(t + h)
                t += h
            i += 1
            h = min(2.*h, h * rho**(1/4.))

    return ts,xs
```

$$\frac{dx}{dt} = -x^3 + \sin t, \qquad x(t=0) = 0.$$



Step size tends to decrease when dx/dt (the r.h.s) is large

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Stability, stiff equations, and implicit methods

Consider the following ODE

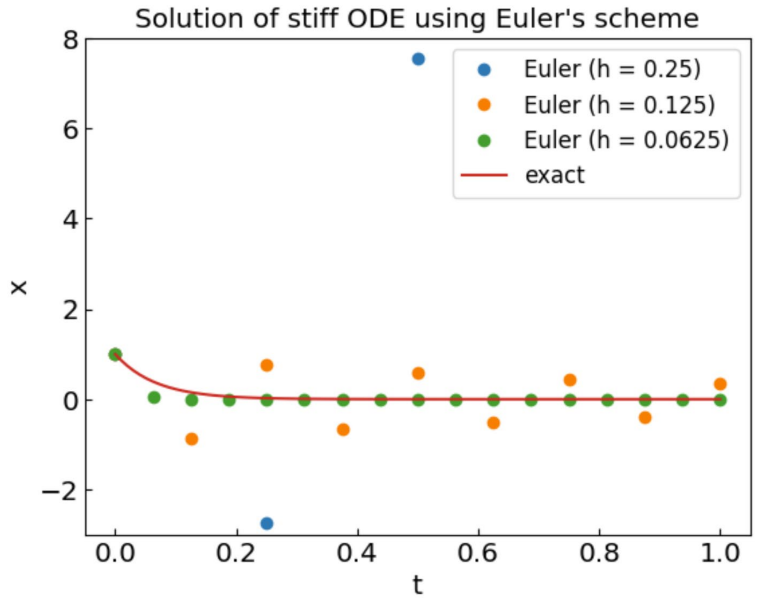
$$\frac{dx}{dt} = -15x, \qquad \textit{stiff equation}$$

with the initial condition *x(t=0)=1*.

The exact solution is of course $x(t) = e^{-15t}$ and goes to zero at large times.

Let us apply Euler's method with h=1/4, 1/8, 1/16

Divergence for h=1/4!



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Stability, stiff equations, and implicit methods

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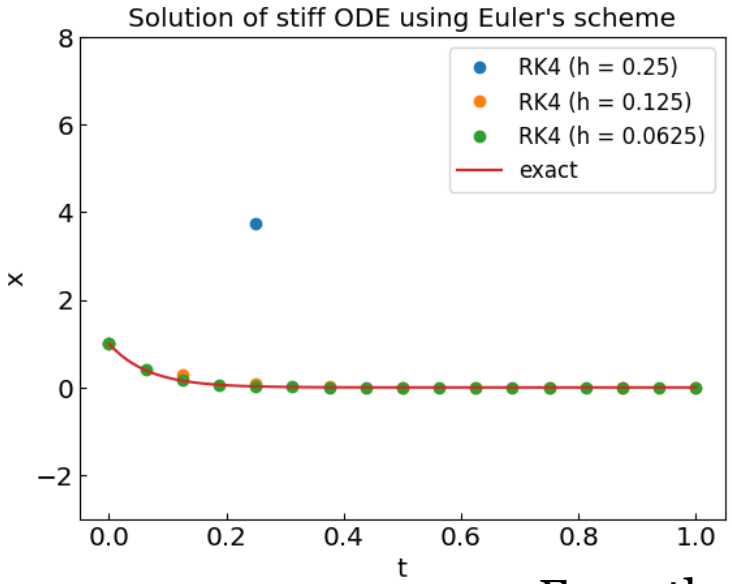
with x(t=0)=1.

The exact solution is of course $x(t) = e^{-15t}$ and goes to zero at large times.

Let us apply Euler's method with h=1/4, 1/8, 1/16

Divergence for h=1/4!

RK4: better but still diverges for h=1/4



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Euler methods and stiff equations

Recall that in Euler's method x(t+h) = x(t) + h f(x,t)

For $\frac{dx}{dt} = -15x,$ we have $x_{n+1} = x_n - 15hx_n = (1-15h)x_n = (1-15h)^n x_0, \qquad x_n \equiv x(t+nh)$

If |1-15h|>1, i.e. h>2/15, the Euler method diverges!

Solution: *implicit methods*

Implicit Euler method: $\mathbf{x}(\mathbf{t}+\mathbf{h}) = x(t) + hf[\mathbf{x}(\mathbf{t}+\mathbf{h}), t+h]$

Our stiff equation: $x_{n+1} = x_n - 15hx_{n+1}$ thus $x_{n+1} = \frac{x_n}{1+15h} = \frac{x_0}{(1+15h)^n} \overset{n\to\infty}{\to} 0$ for all $h > 0$.

- Implicit methods are *more stable* than explicit methods
- But require solving non-linear equation for *x(t+h)* at each step
- *Semi-implicit methods:* use one iteration of Newton's method to solve for *x(t+h)*

Other implicit methods: trapezoidal rule, family of implicit Runge-Kutta methods

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