BENDUKIDZE CAMPUS

18.11.2024 | 18:00

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Computer Modelling of Physical systems

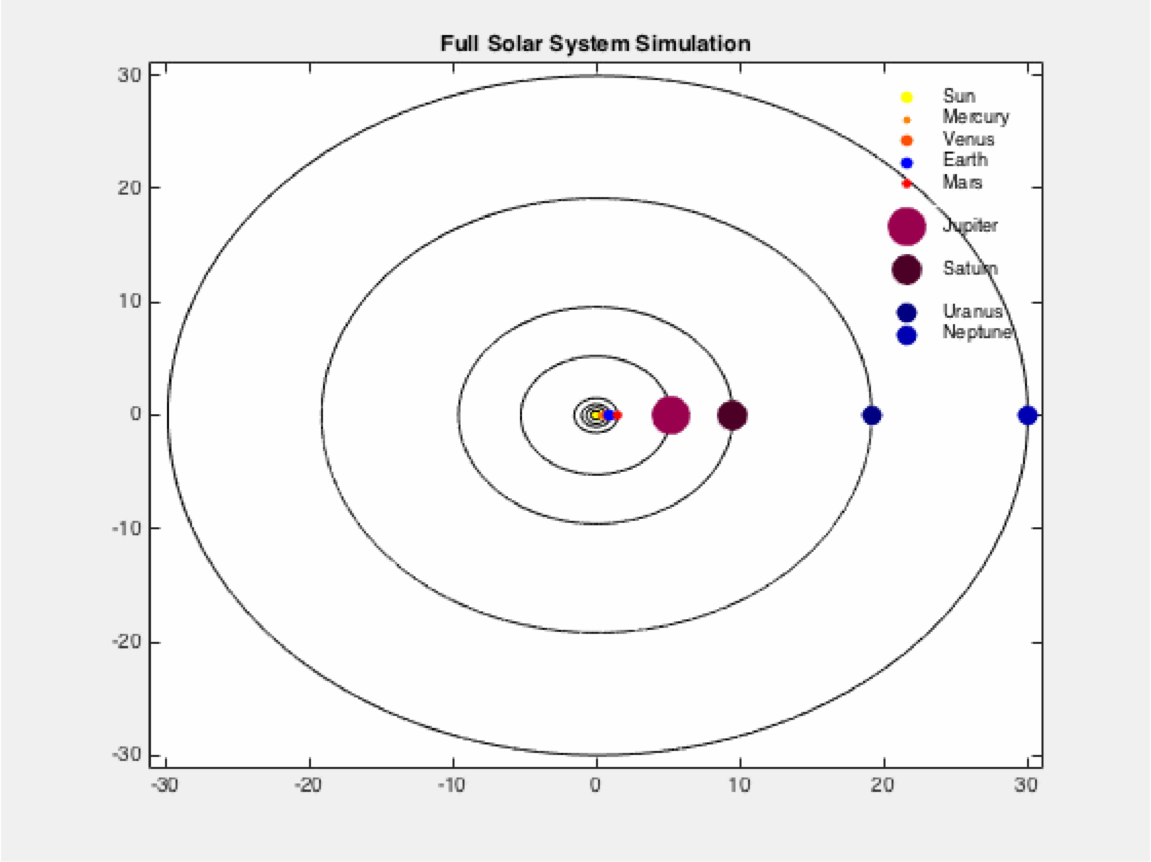
Computer Modelling of Physical systems

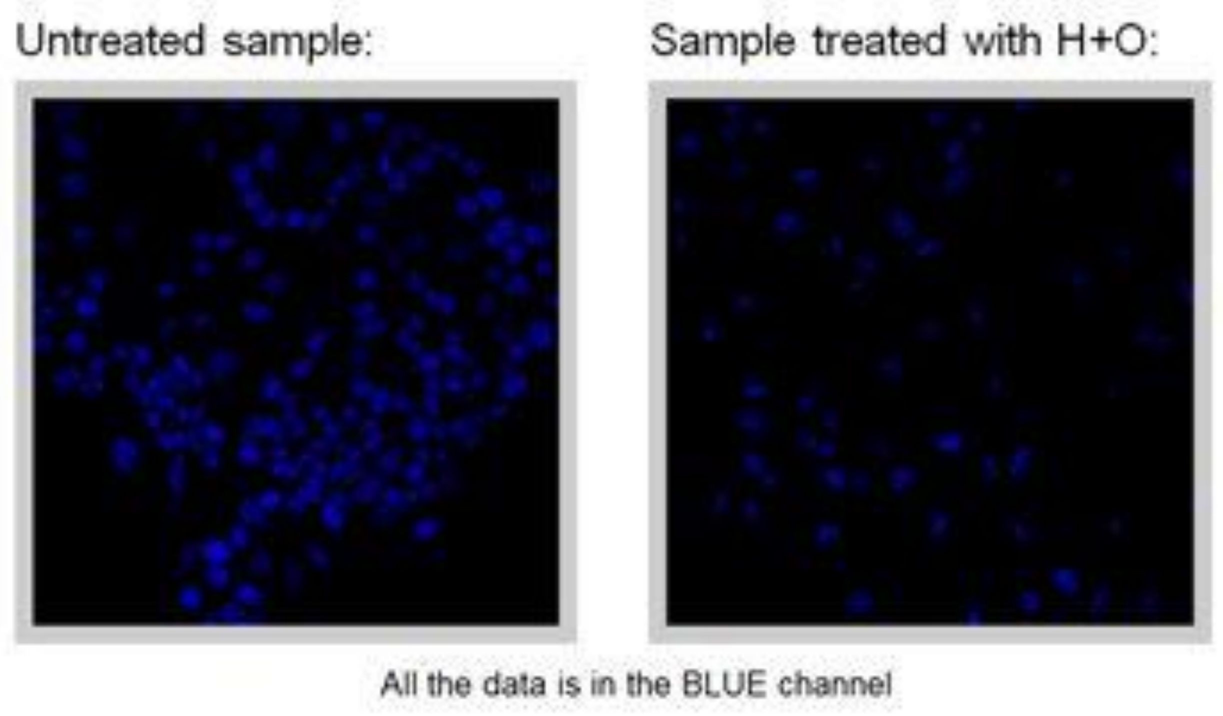
Seminar Series vol.1

Read and prepared by Zurabi Ugulava

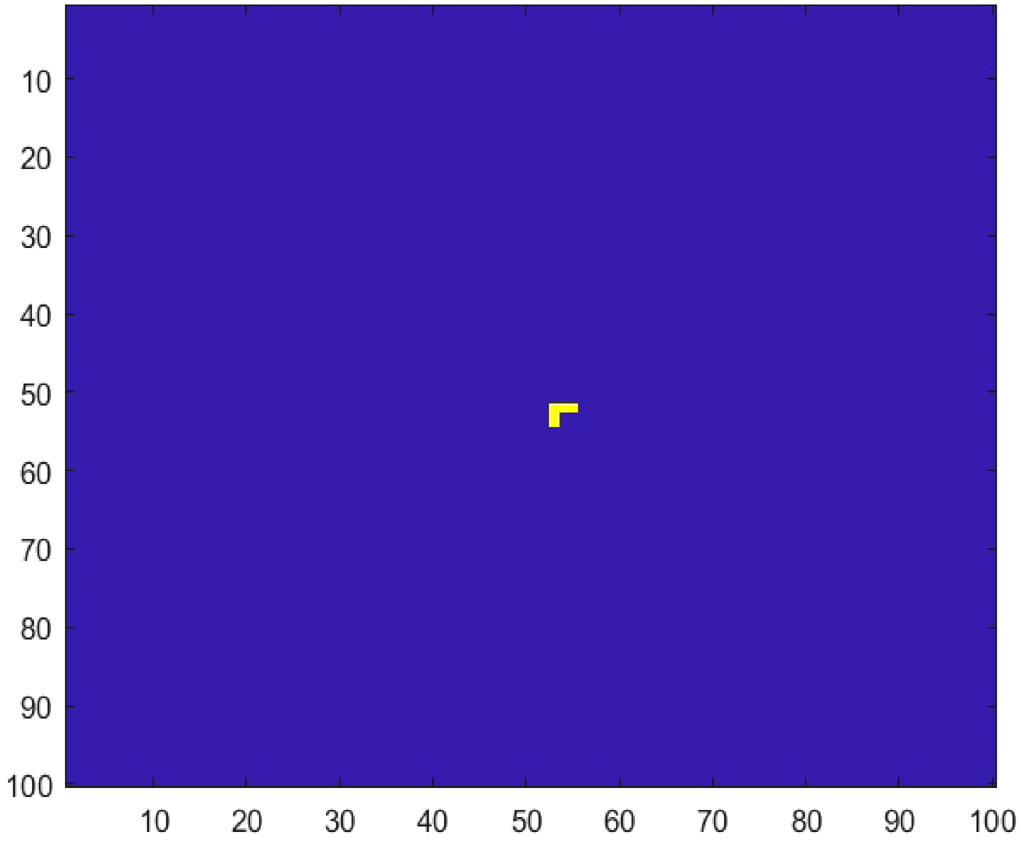
What to expect next?

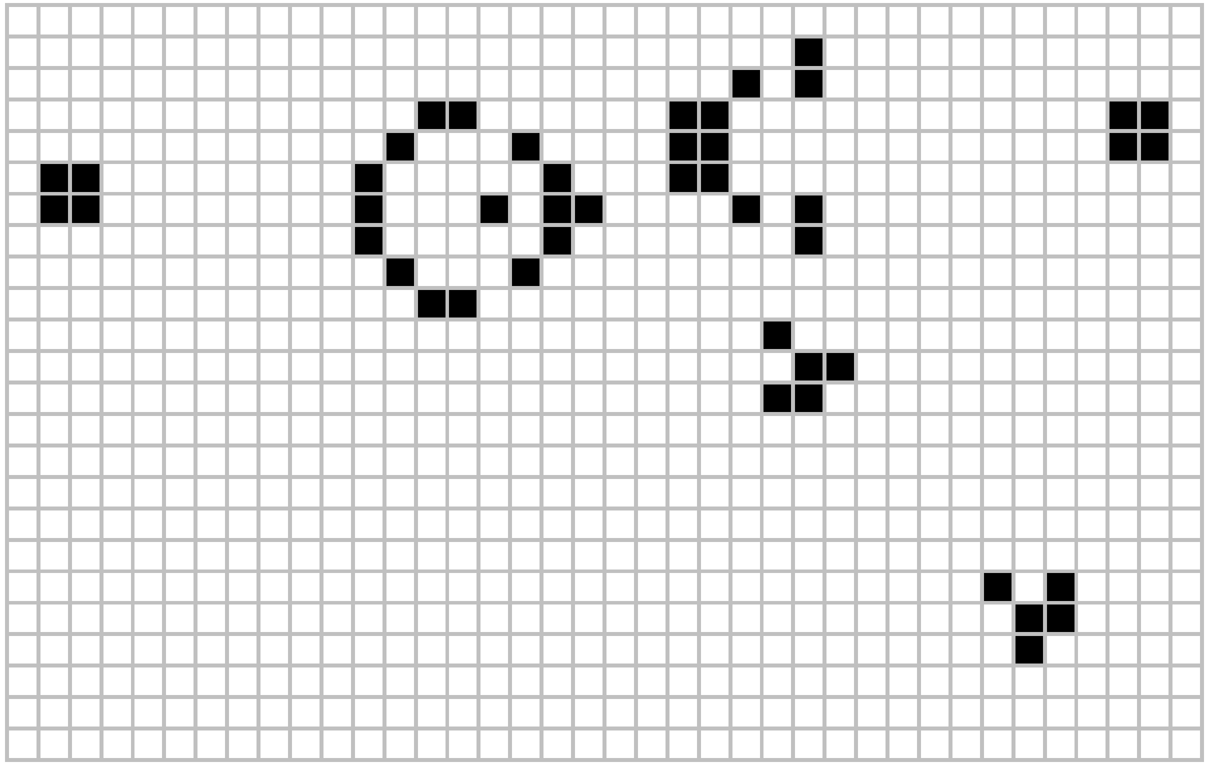
- Three Body problem/ Astrophysical insight
- Introduction to chaotic systems
- From Conwoy game to Ising 2D model MCS
- Data analysis module
- And many more…



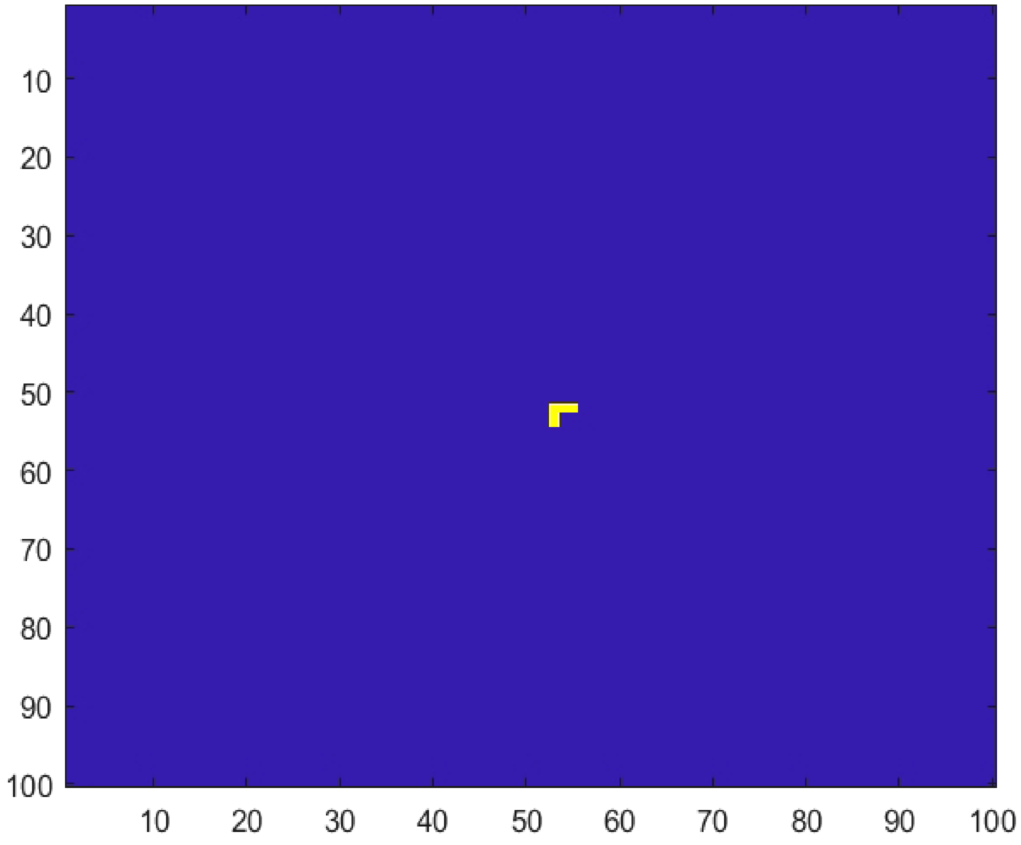


https://www.mathworks.com/company/technical-articles/using-image-processing-and-statistical-analysis-to-quantify-cell-scattering-for-cancer-drug-research.html





Bill Gosper's Glider Gun in action—a variation of Conway’s Game of Life. This image was made by using Life32 v2.15 beta, by Johan G. Bontes.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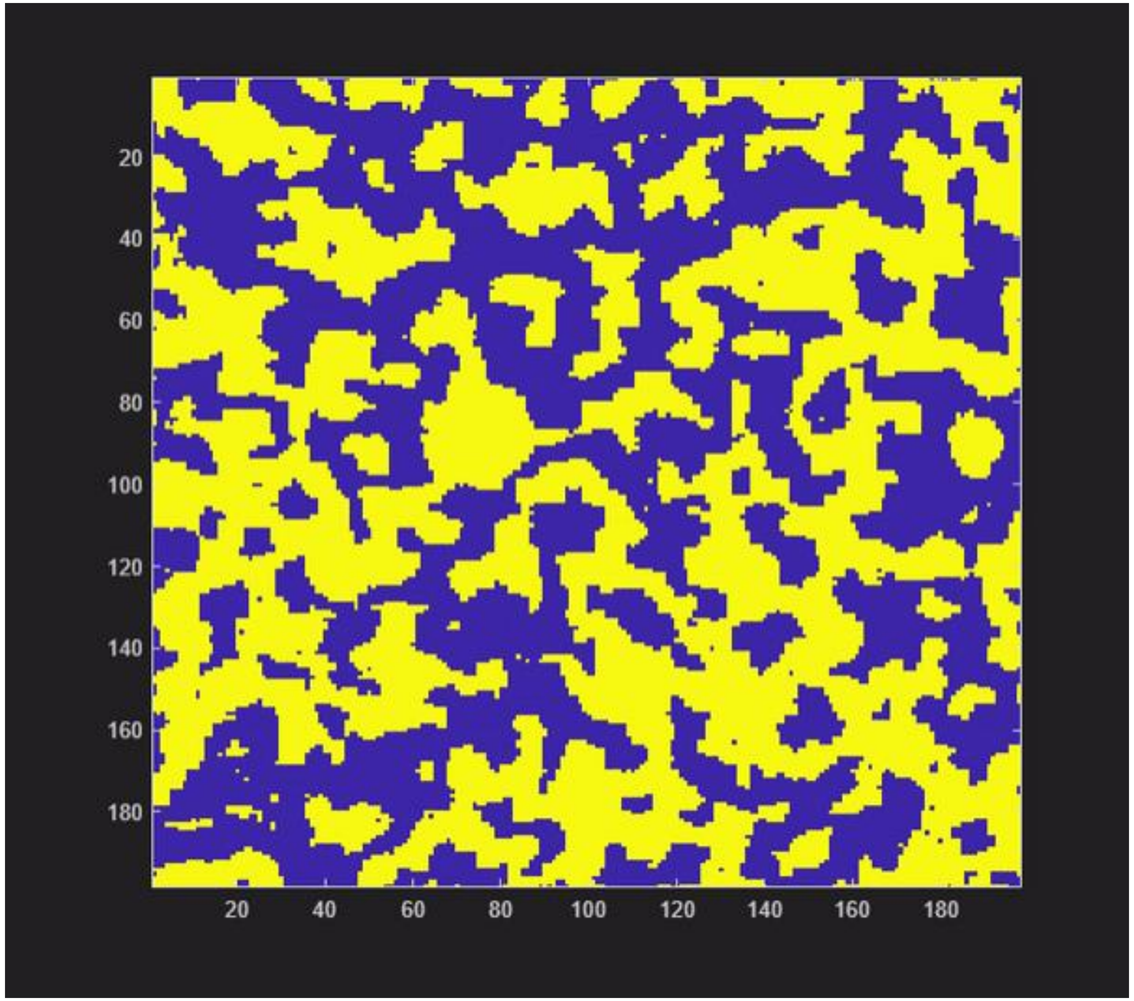
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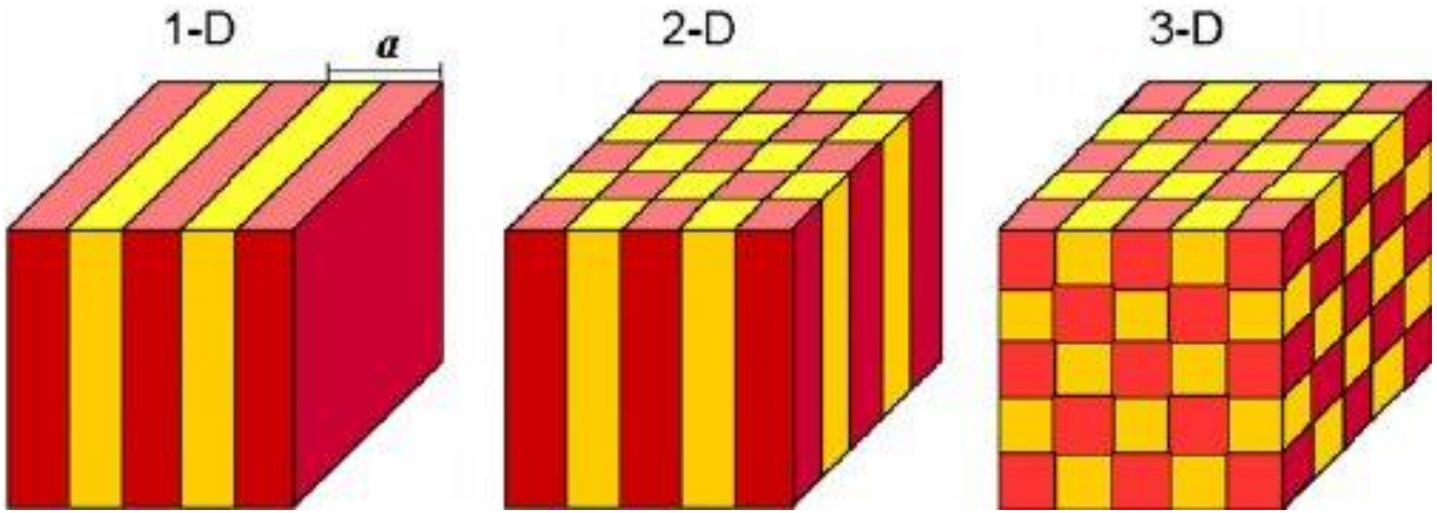
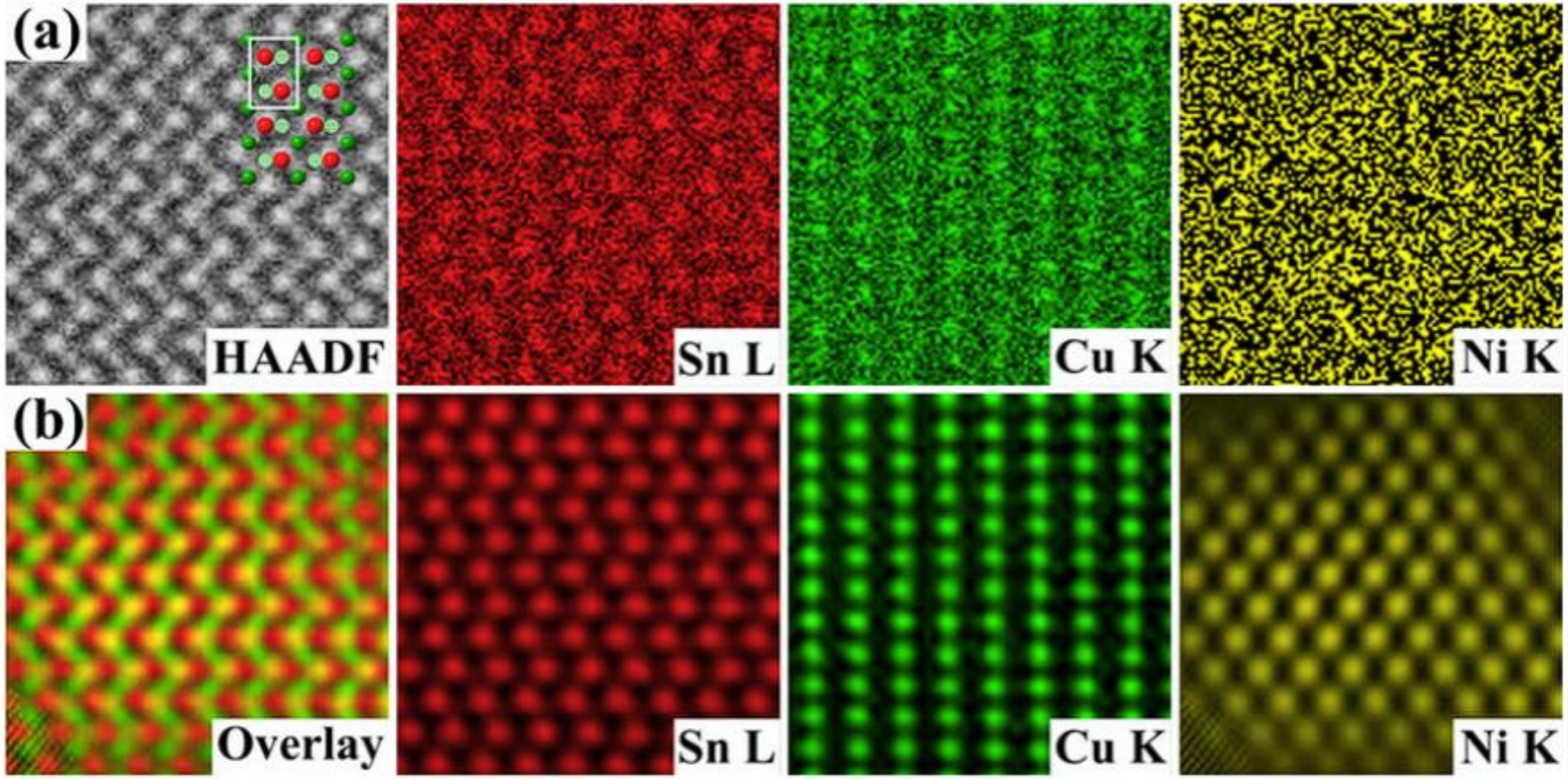


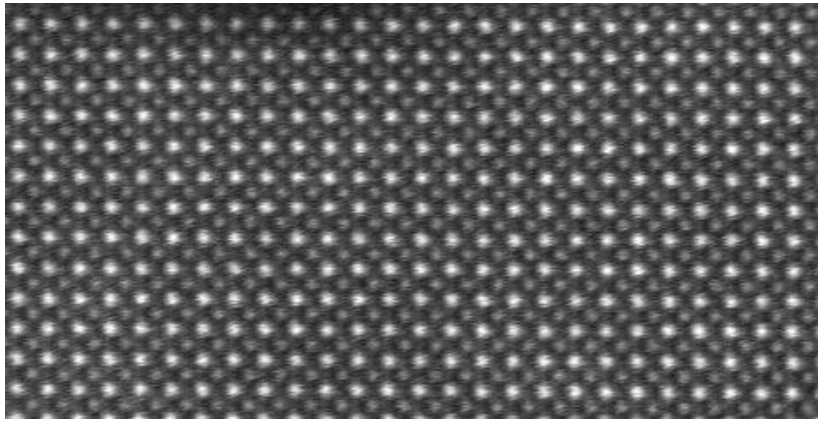
Intro to molecular dynamics

Physics of planar lattice

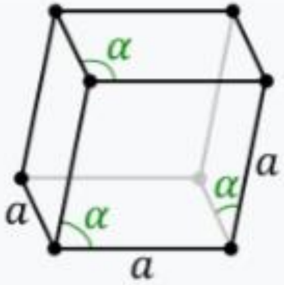
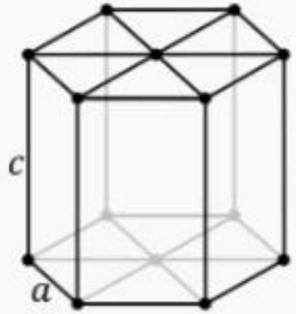


(a) The original atomic-resolution image and elemental mapping: Sn (red), Cu (green), Ni (yellow); (b) Noise reduction image of atomic-resolution elemental mapping: Overlay, Sn (red), Cu (green), Ni (yellow).

Matsumura, Syo. (2019). Atom locations in a Ni doped η-$(Cu,Ni)_6Sn_5$ intermetallic compound. Scripta Materialia. 158. 1-5. 10.1016/j.scriptamat.2018.08.020.



Strontium Titanate

Crystal system	Trigonal		Hexagonal
Lattice system	 Rhombohedral	 Hexagonal	
Example	 Dolomite (white)	 α-Quartz	 Beryl

Physical description

$$M\frac{dv}{dt} = \sum F_i$$

$$E = \frac{1}{2}mv^2 + \frac{1}{2}kx^2$$

$$p = \sum m_i v_i$$

Translate physics into code

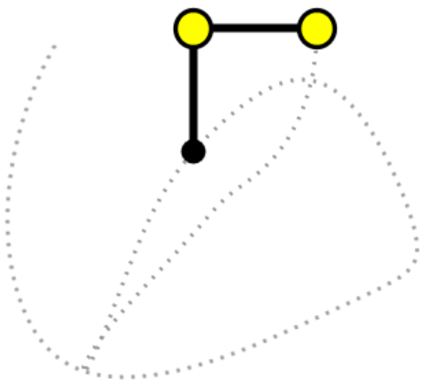
springmasssystem.m

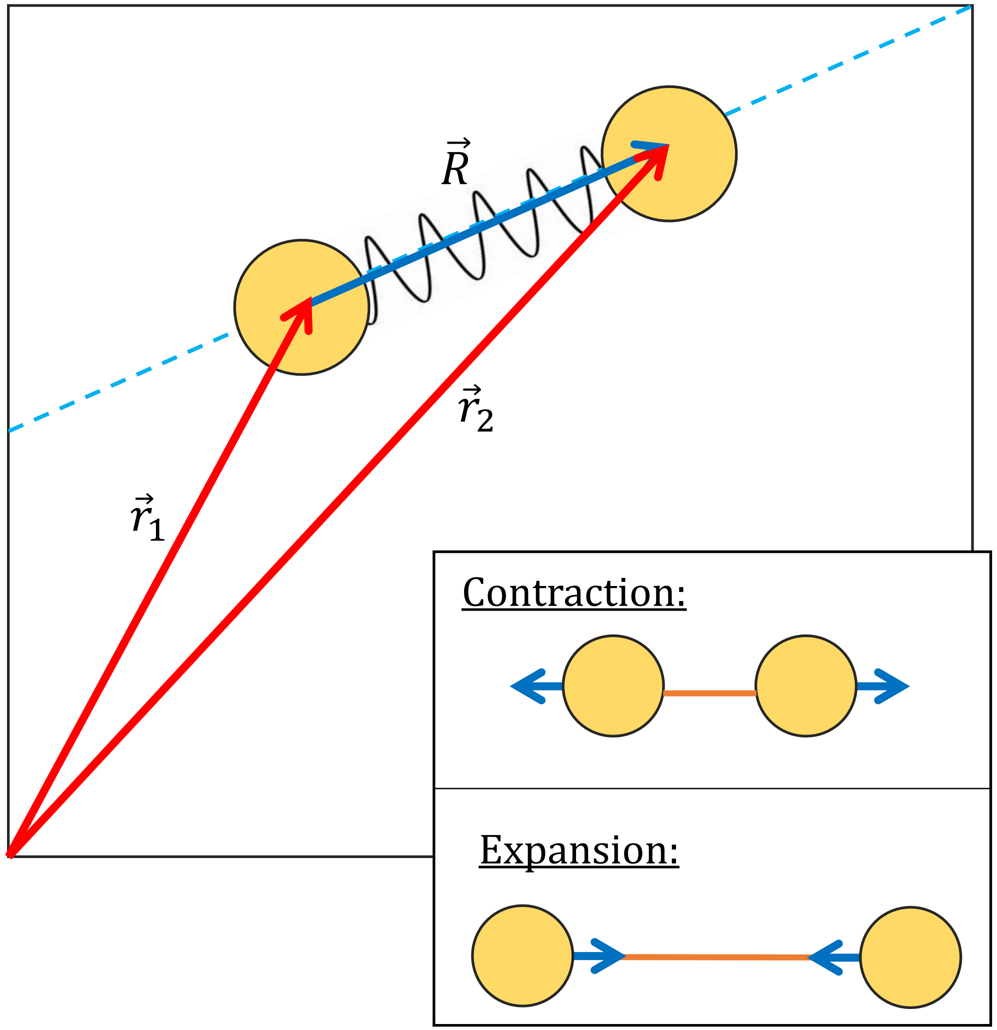
```
obj=VideoWriter('animation.avi');
obj.Quality=100;
obj.FrameRate=60;
open(obj);

for i=1:N

    %Acceleration increment
    if abs(y(i)-x(i))>l0
        x2(i)=k/m*abs(y(i)-x(i)-l0);
        y2(i)=-k/M*abs(y(i)-x(i)-l0);
    else
        x2(i)=-k/m*abs(y(i)-x(i)-l0);
        y2(i)=k/M*abs(y(i)-x(i)-l0);
```

Extract data in the desired form





Establishing the system in space:

$$\vec{r}_1 = (x_1, y_1, z_1)$$

$$\vec{r}_2 = (x_2, y_2, z_2)$$

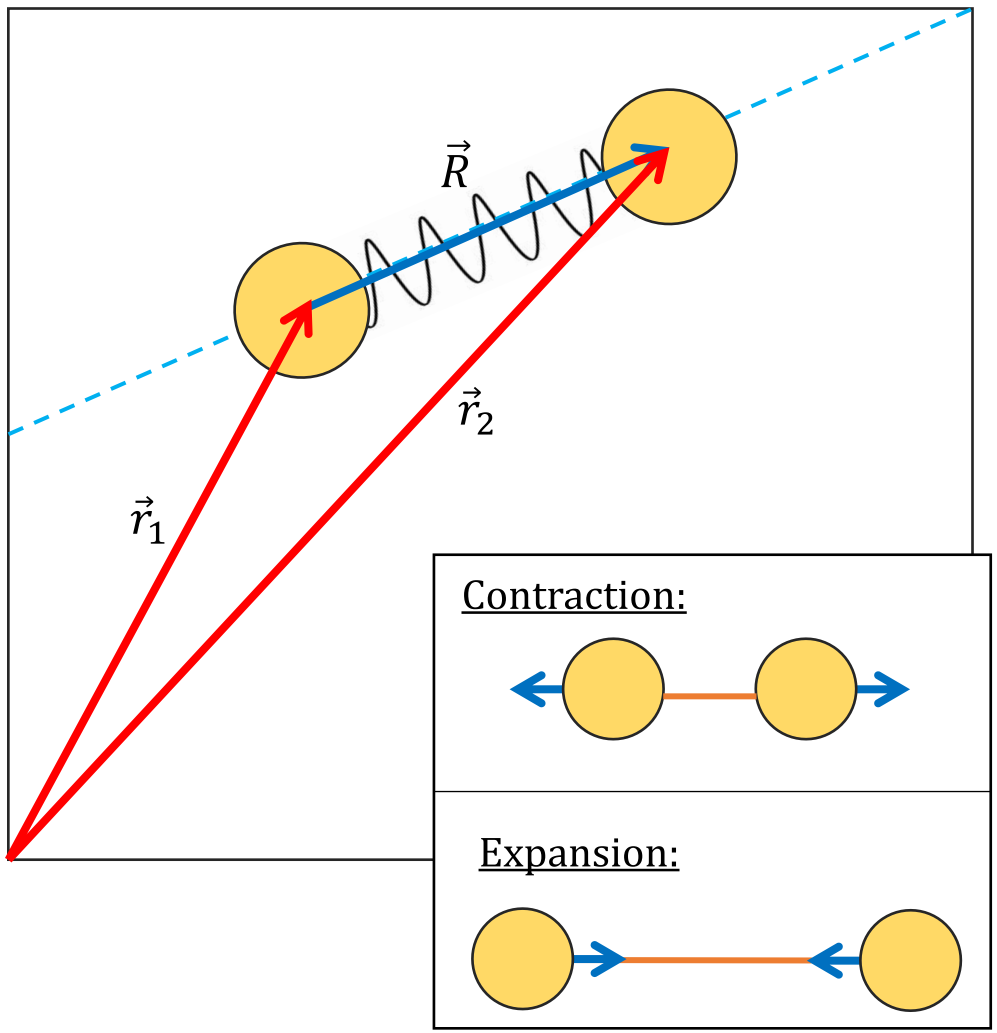
$$\vec{R} \equiv \vec{r}_{12} = \vec{r}_2 - \vec{r}_1$$

Ordinary Hook's Law:

$$x = |\vec{R}| - L_0$$

Force ~ displacement

$$\vec{F} = k\vec{x} = k\left(1 - \frac{|\vec{R}|}{L_0}\right)\hat{R}$$



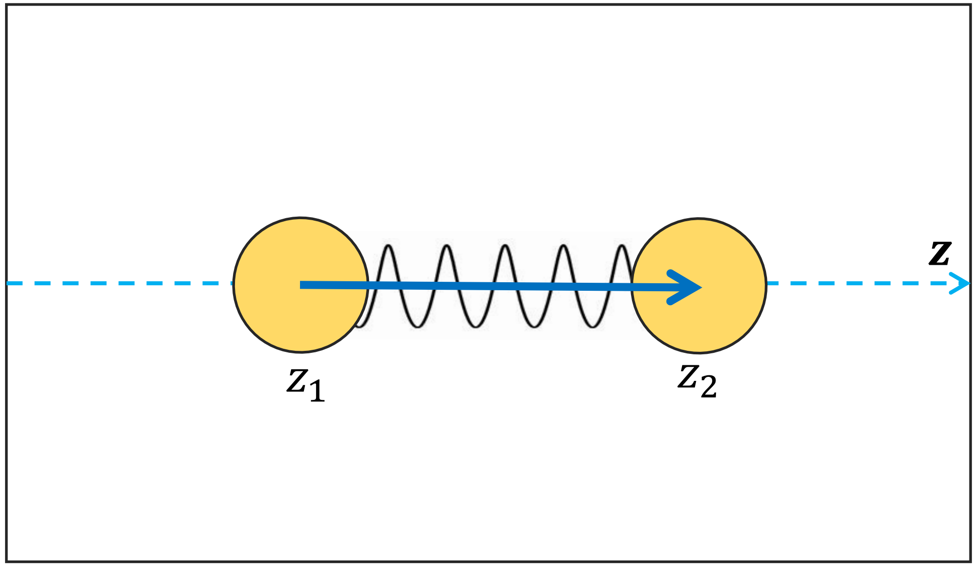
Ordinary Hook's Law:

$x = \lvert\vec{R}\rvert - L_0$	Force ~ displacement
$\vec{F} = k\vec{x} = kL_0\left(1 - \frac{\lvert\vec{R}\rvert}{L_0}\right)\hat{R}$	

Equations of motion:

$$m_1 \frac{d^2\vec{r}_1}{dt^2} = \vec{F} = kL_0\left(1 - \frac{|\vec{R}|}{L_0}\right)\hat{R}$$

$$m_2 \frac{d^2\vec{r}_2}{dt^2} = -\vec{F} = -kL_0\left(1 - \frac{|\vec{R}|}{L_0}\right)\hat{R}$$



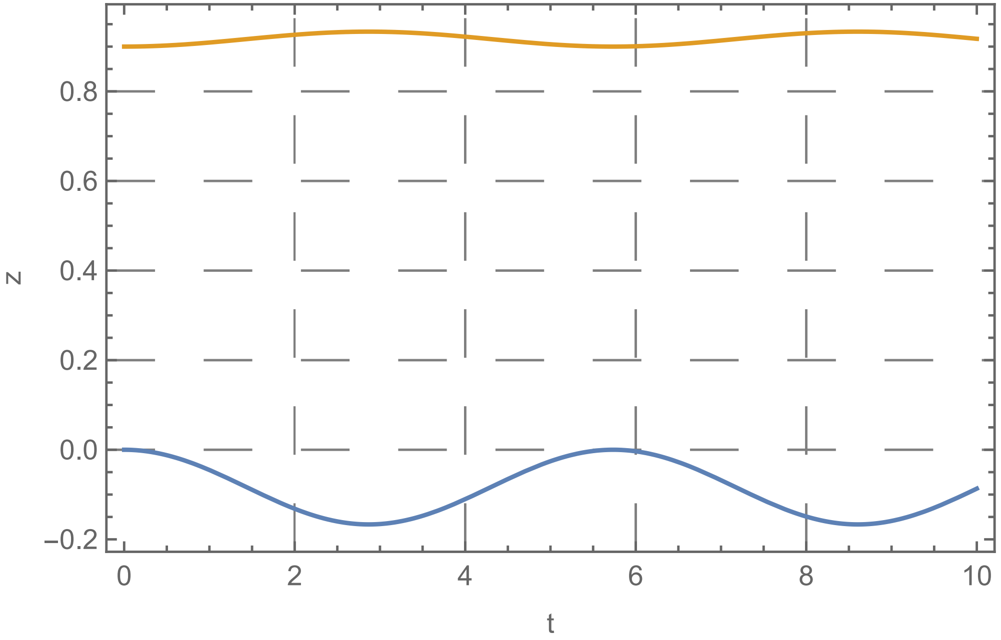
Equations of motion:

$$
\begin{cases}
m_1 \dfrac{d^2\vec{z}_1}{dt^2} = k(z_2 - z_1 - L_0)\hat{R} \\
m_2 \dfrac{d^2\vec{z}_2}{dt^2} = -k(z_2 - z_1 - L_0)\hat{R}
\end{cases}
$$

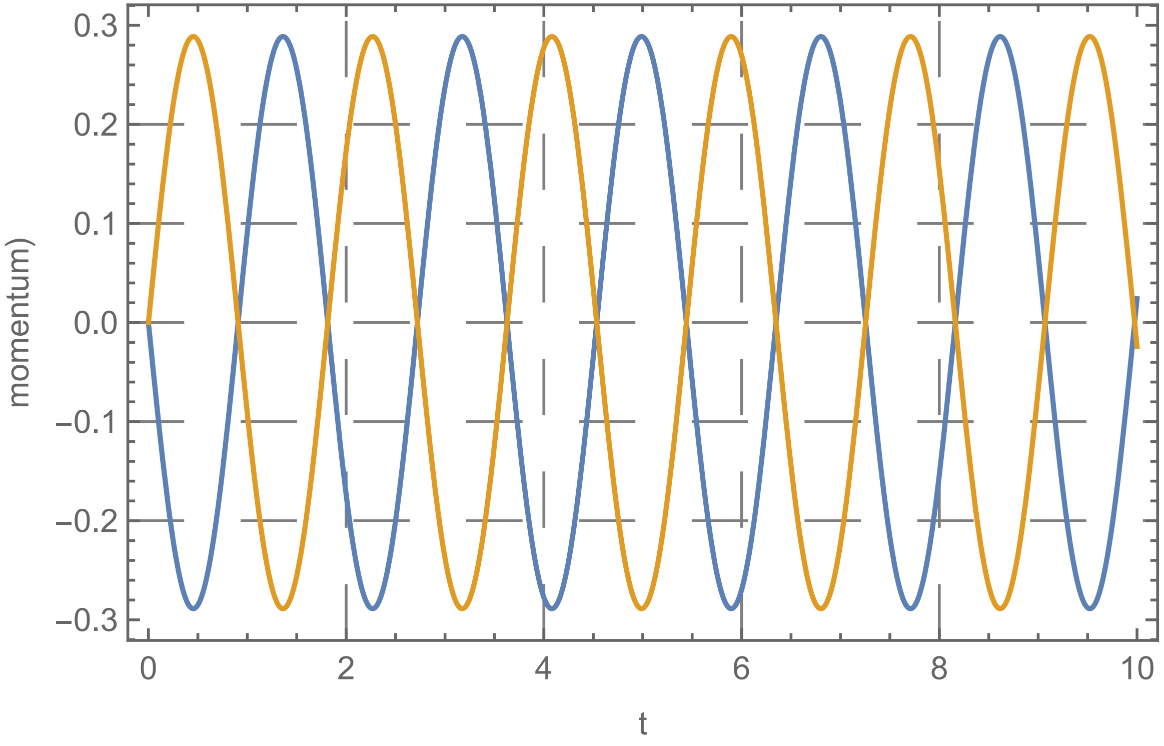
$$z_1(t) = A_1 \sin(\omega t + \varphi_1)$$

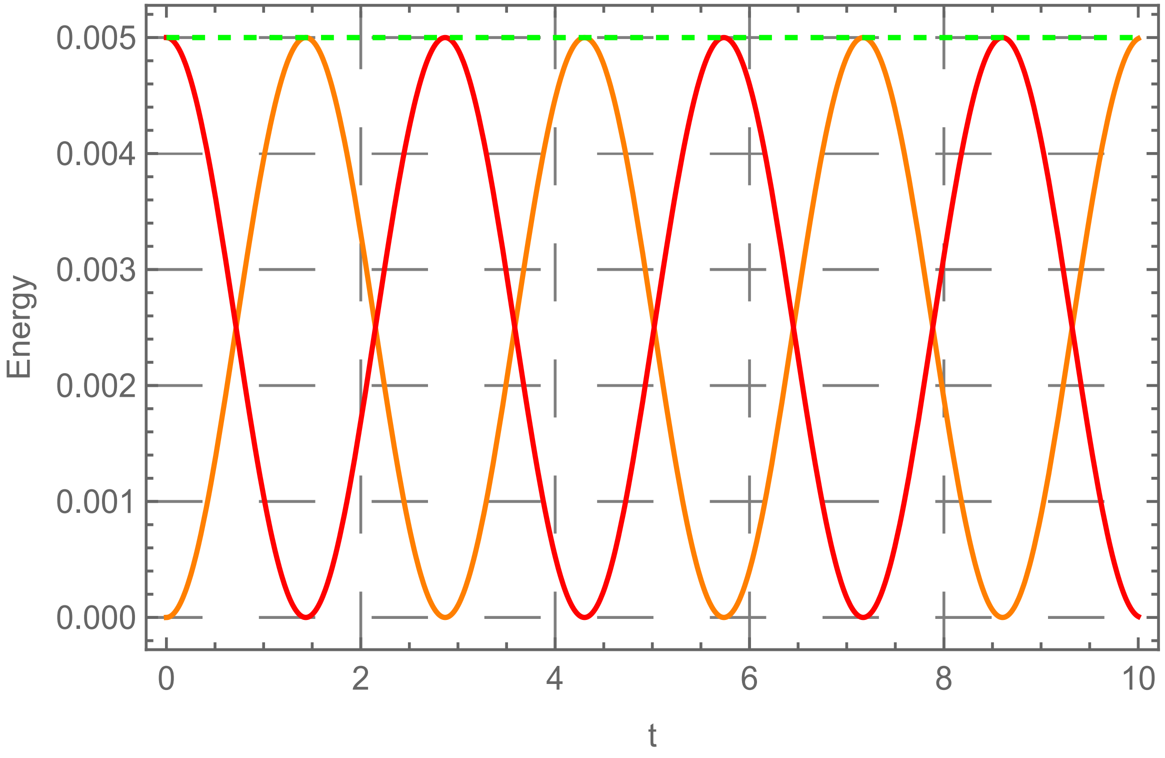
$$z_2(t) = A_2 \sin(\omega t + \varphi_2)$$

$$\omega^2 = \frac{\mu}{k} = \frac{1}{k} \cdot \frac{m_1 m_2}{m_1 + m_2}$$

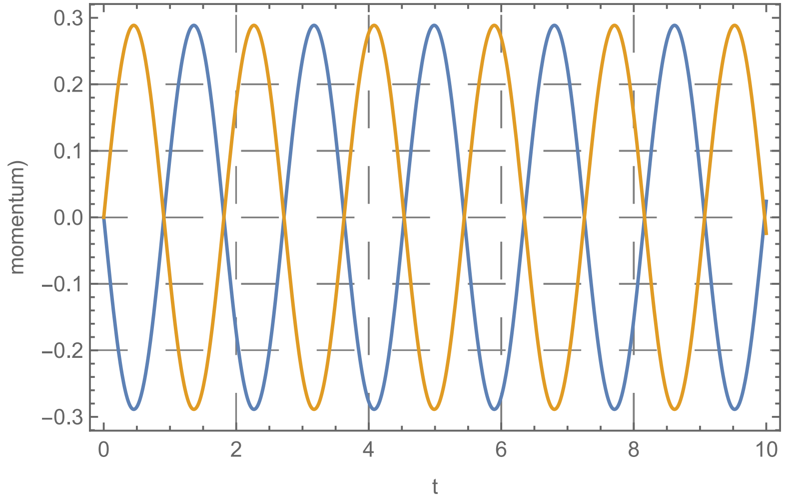


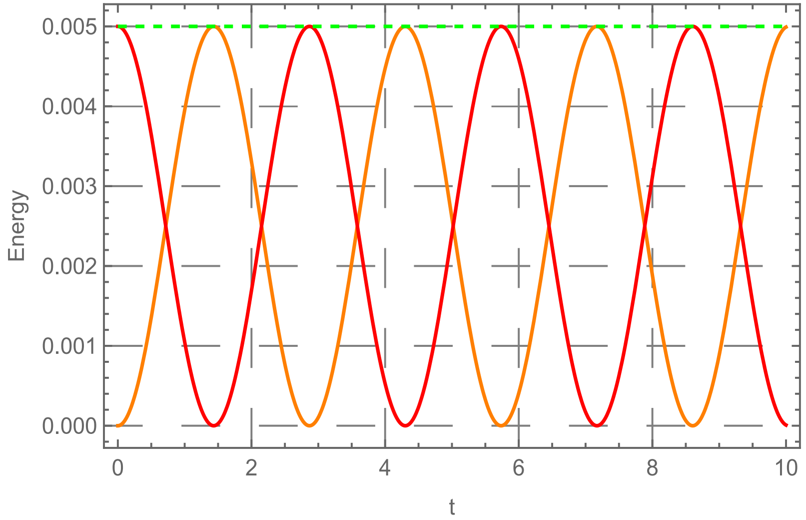
What to observe in periodic system:

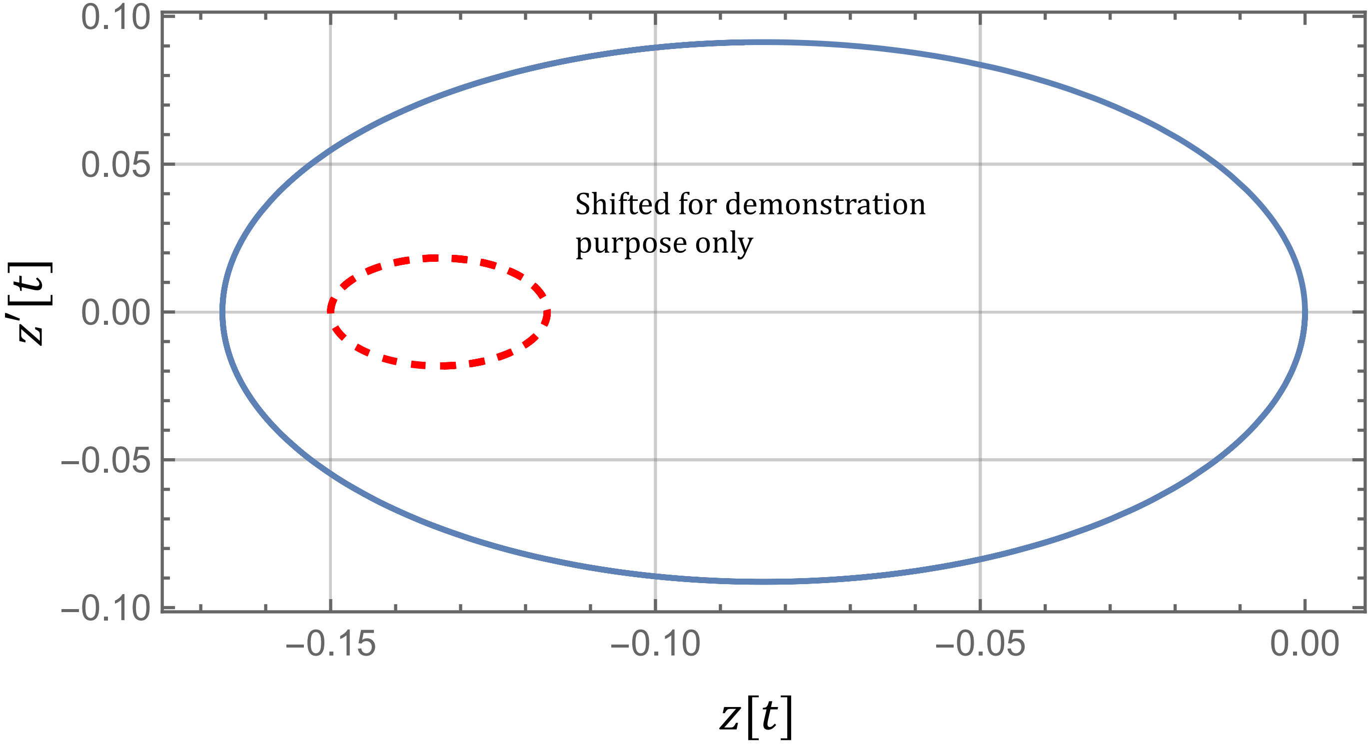




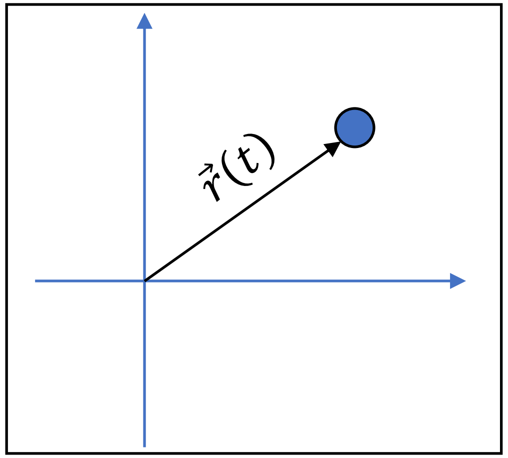
What to observe in periodic system:







Physical description:



Governing physics described by Differential equations!

But how do we handle differential equations?

Manual Integration/

$$f'(x) - \frac{1}{x} = 0 \qquad f(x) = \ln(x) + \mathcal{C}$$

$$f''(x) - x = 0 \qquad f(x) = \frac{1}{6}x^3 + \frac{1}{2}\mathcal{C}_1 x^2 + \mathcal{C}_2$$

Another way to handle them ?

Let's remember Taylor series:

$$f(\vec{r}, t + \delta t) = f(\vec{r}, t) + \frac{1}{1!}\left(\frac{df}{dt}\right)\delta t + \frac{1}{2!}\left(\frac{d^2 f}{dt^2}\right)\delta t^2 + \cdots$$

$$\underset{t_0}{\boxed{f(\vec{r}_t, t)}} \to \underset{t_1}{\boxed{f(\vec{r}_{t+\delta t}, t + \delta t)}} \to \underset{t_2}{\boxed{f\left(\vec{r}_{t_1+\delta t}, t_1 + \delta t\right)}} \to \cdots$$

Let's remember Taylor series:

$$\boxed{f(\vec{r}, t+\delta t) = f(\vec{r}, t) + \frac{1}{1!}\left(\frac{df}{dt}\right)\delta t} + \frac{1}{2!}\left(\frac{d^2 f}{dt^2}\right)\delta t^2 + \cdots$$

1^{st} order approximation

Euler Algorithm:	RK-4 Algorithm:
$f(\vec{r}, t+\delta t) = f(\vec{r}, t) + f'(\vec{r}, t)\,\delta t$	$f(\vec{r}, t+\delta t) = f(\vec{r}, t) + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)\,\delta t$
$f'(\vec{r}, t+\delta t) = f'(\vec{r}, t) + f''(\vec{r}, t)\,\delta t$	$k_1 = f'(\vec{r}, t)$
○ ○ ○	$k_2 = f'\left(\vec{r} + \frac{1}{2}k_1\delta t, t + \frac{1}{2}\delta t\right)$
$f^{n-2}(\vec{r}, t+\delta t) = f^{n-2}(\vec{r}, t) + f^{n-1}(\vec{r}, t)\,\delta t$	$k_3 = f'\left(\vec{r} + \frac{1}{2}k_2\delta t, t + \frac{1}{2}\delta t\right)$
$f^{n-1}(\vec{r}, t+\delta t) = f^{n-1}(\vec{r}, t) + f^{n}(\vec{r}, t)\,\delta t$	$k_4 = f'(\vec{r} + k_3\delta t, t + \delta t)$

What is required to run a Simulation?

Main physical quantities

```
m1 = 10; m2 = 1; k = 10; l = 1;
```

```
le = Sqrt[(x2[t] - x1[t])^2 + (y2[t] - y1[t])^2 + (z2[t] - z1[t])^2];
```

Governing Equations

```
eqs = {
   m1 * x1''[t] - k * (1 - l / le) * (x2[t] - x1[t]) == 0, m1 * y1''[t] - k * (1 - l / le) * (y2[t] - y1[t]) == 0,
   m1 * z1''[t] - k * (1 - l / le) * (z2[t] - z1[t]) == 0, m2 * y2''[t] + k * (1 - l / le) * (x2[t] - x1[t]) == 0,
   m2 * x2''[t] + k * (1 - l / le) * (y2[t] - y1[t]) == 0, m2 * z2''[t] + k * (1 - l / le) * (z2[t] - z1[t]) == 0};
```

Initial Conditions

```
init = {
   x1[0] == 2, y1[0] == 0, z1[0] == 0,
   x2[0] == 1.1, y2[0] == 0, z2[0] == 0,
   x1'[0] == 0, y1'[0] == 0, z1'[0] == 0,
   x2'[0] == 0, y2'[0] == 0, z2'[0] == 0};
```

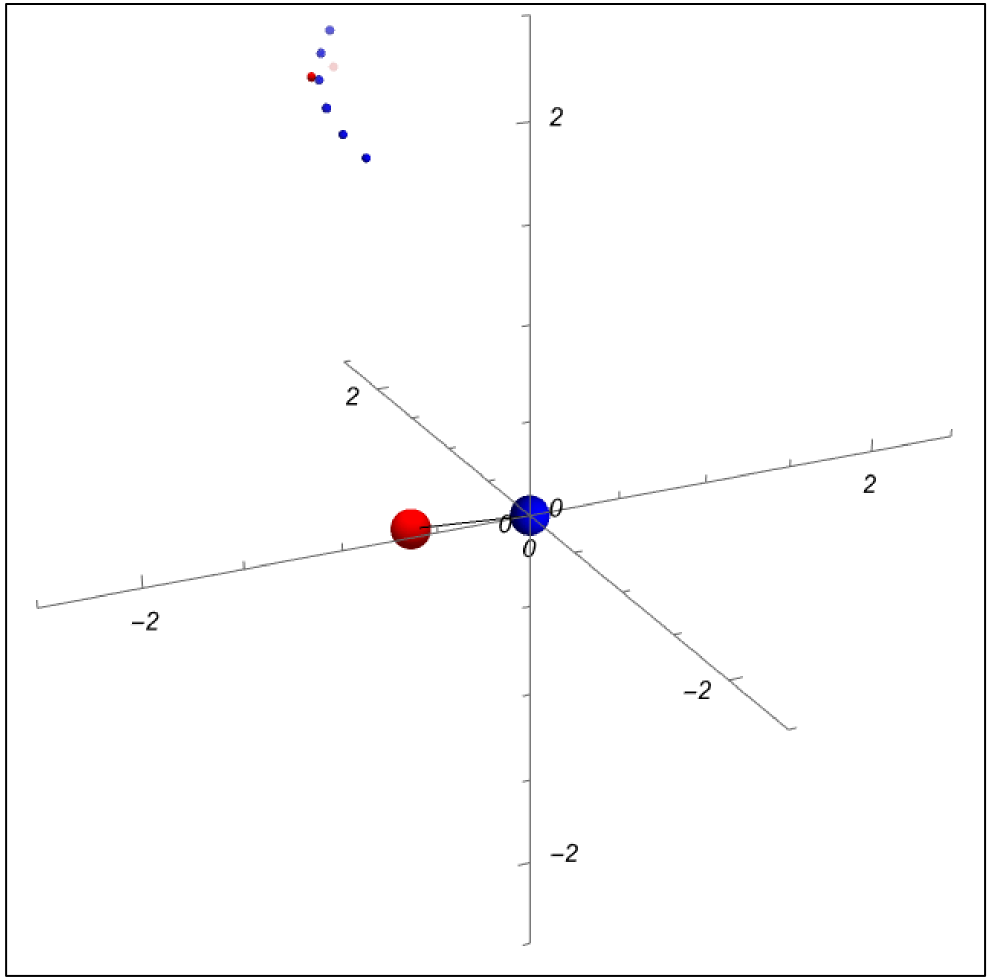
Solver Algorithm

```
sol = NDSolve[Join[eqs, init], {x1, y1, z1, x2, y2, z2}, {t, 0, 100}];
```

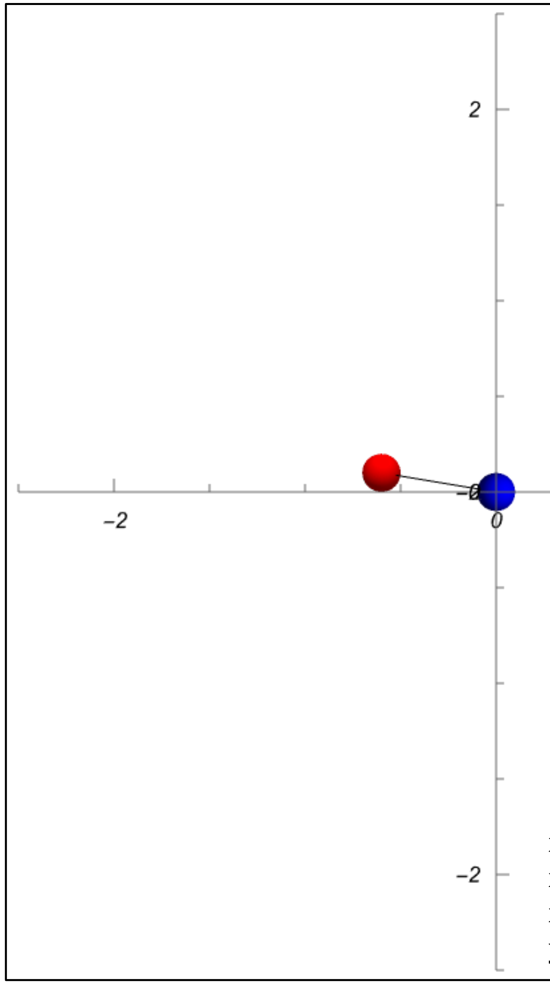
Visualization

```
Plot[Evaluate[{x1[t]}] /. sol, {t, 0, 10}]
```

Trajectory in 3D Space:

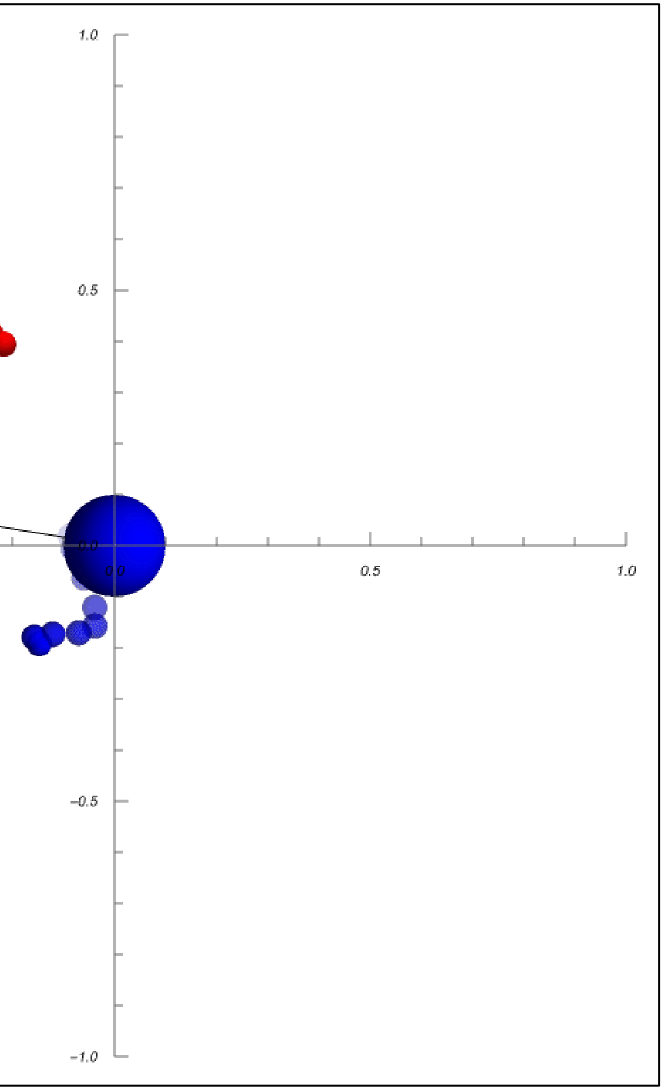


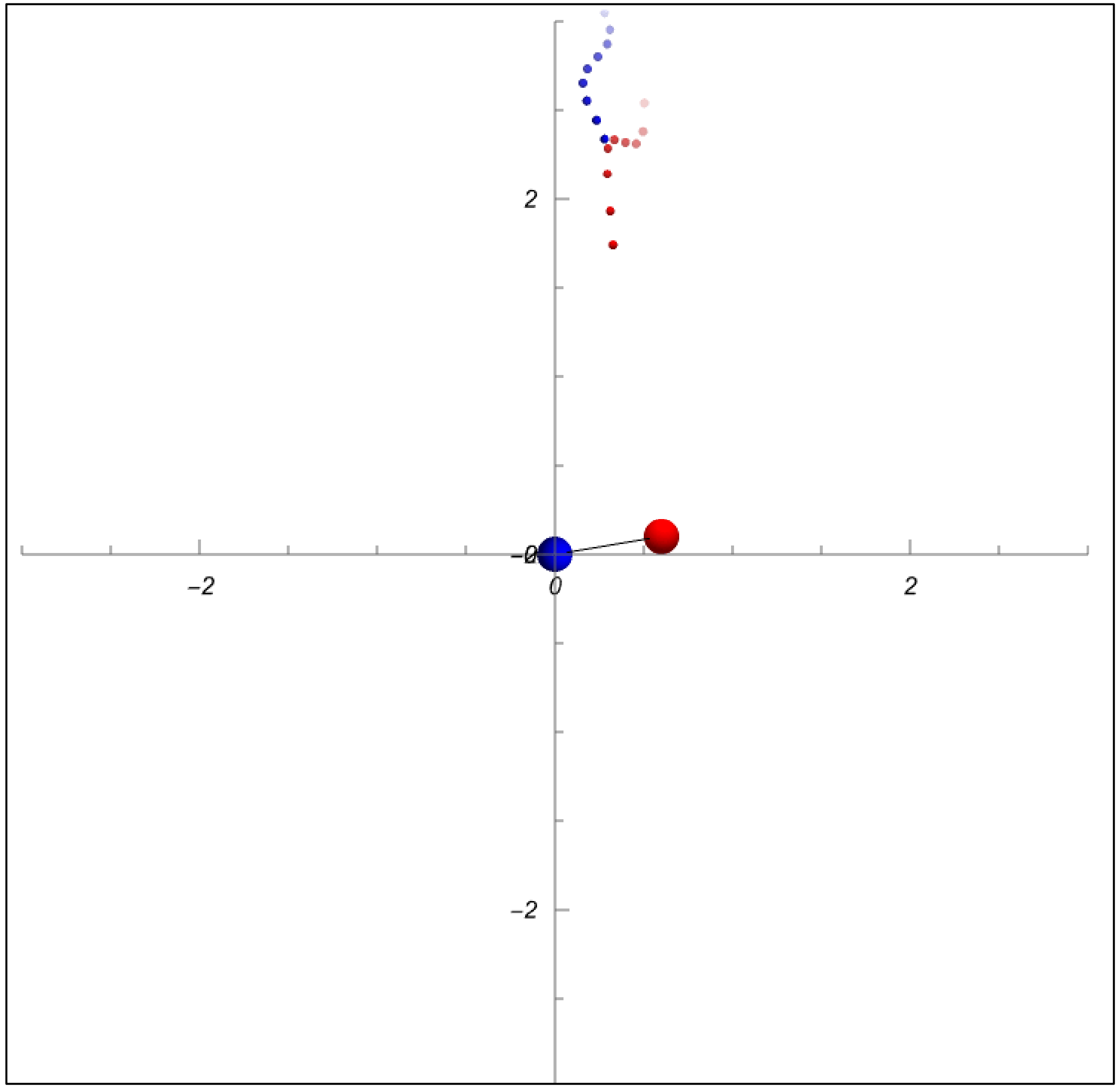
2D Projection



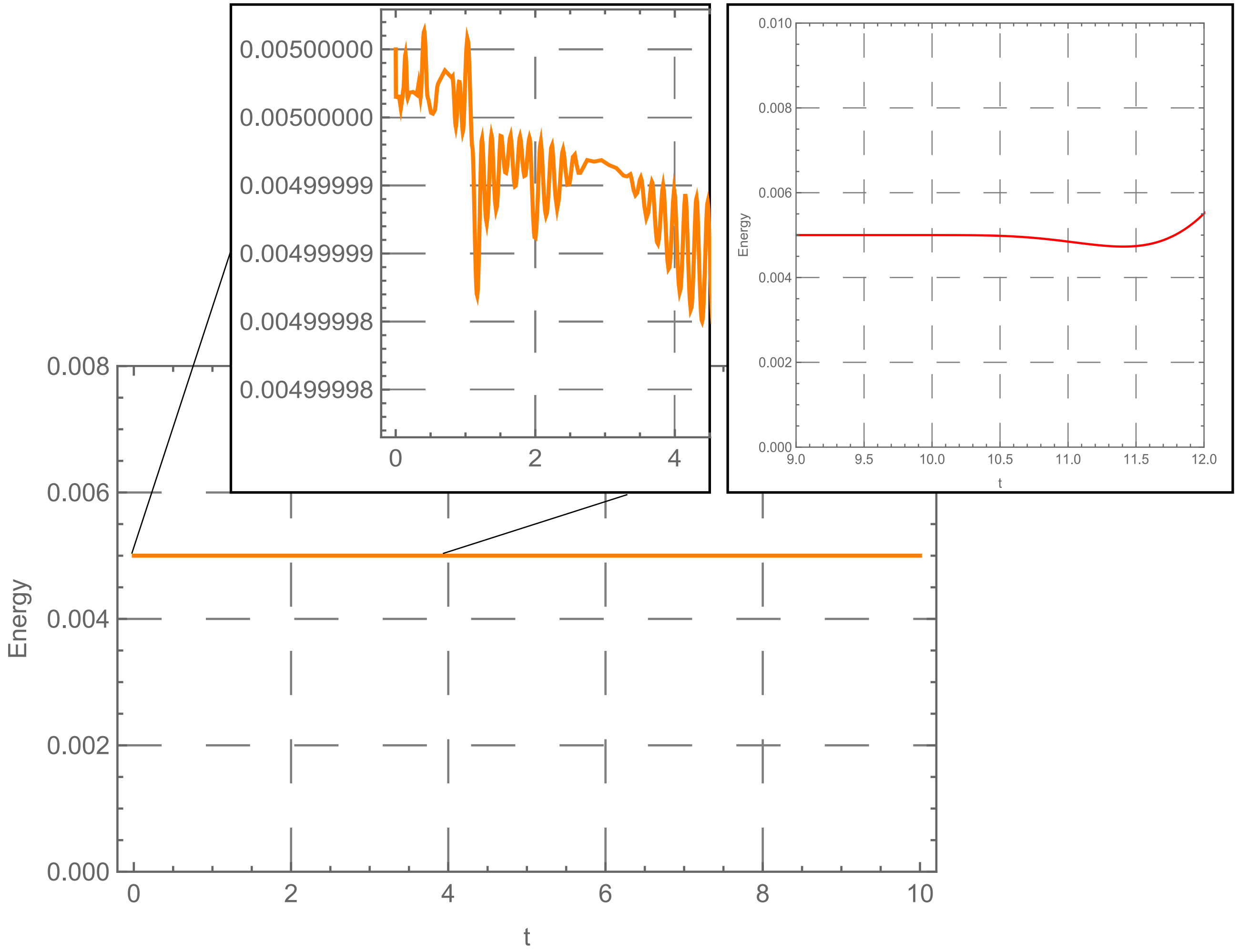
x1[0] = -0.6, y1[0] = 0.1,
x2[0] = y2[0] = z1[0]= z2[0] = 0
x1'[0] = x2'[0]= z2'[0] = 0
y1'[0] = y2'[0]= 0.1, z1'[0] = 0.2

Parametric plots





What could possibly go wrong?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0.00500000
0.00499999
0.00499999
0.00499998
0.00499998
0
2
4
0.010
0.008
0.006
0.004
0.002
0.000
9.0
9.5
10.0
10.5
11.0
11.5
12.0
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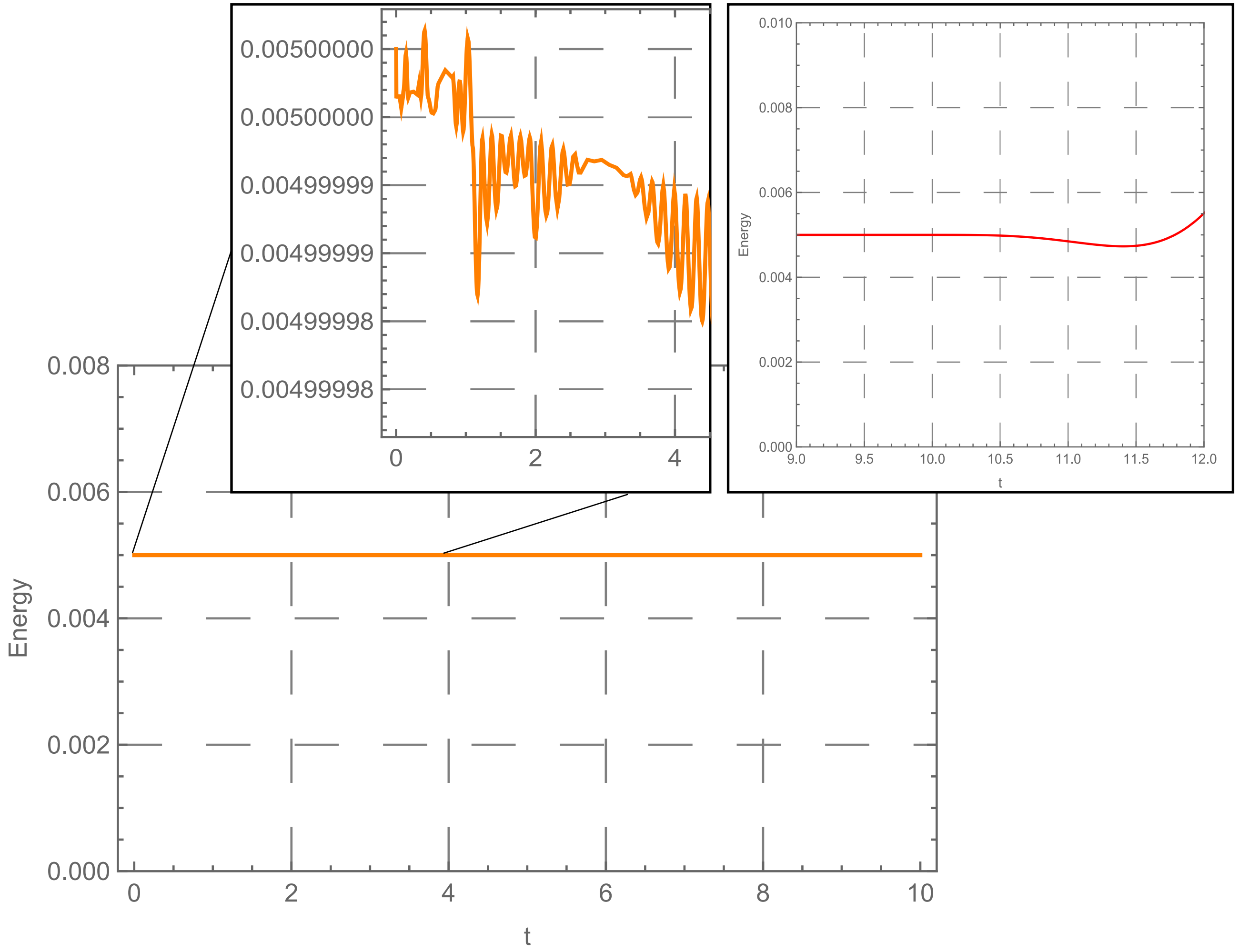
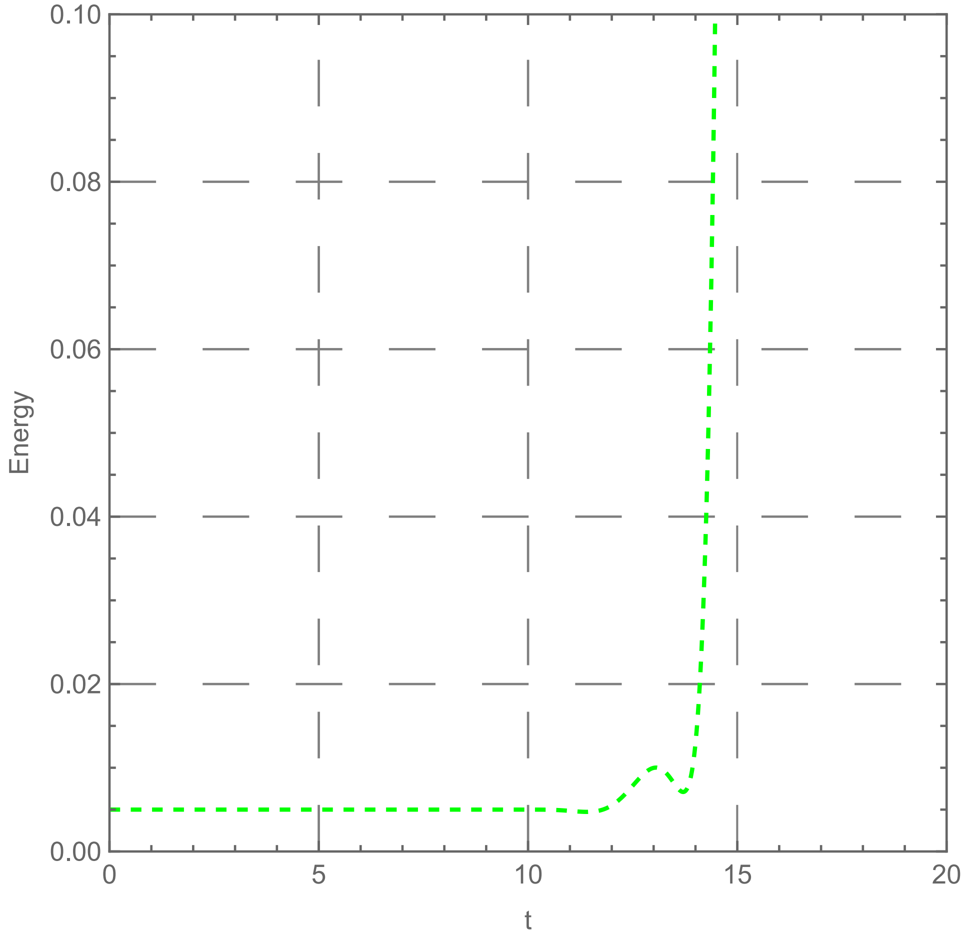
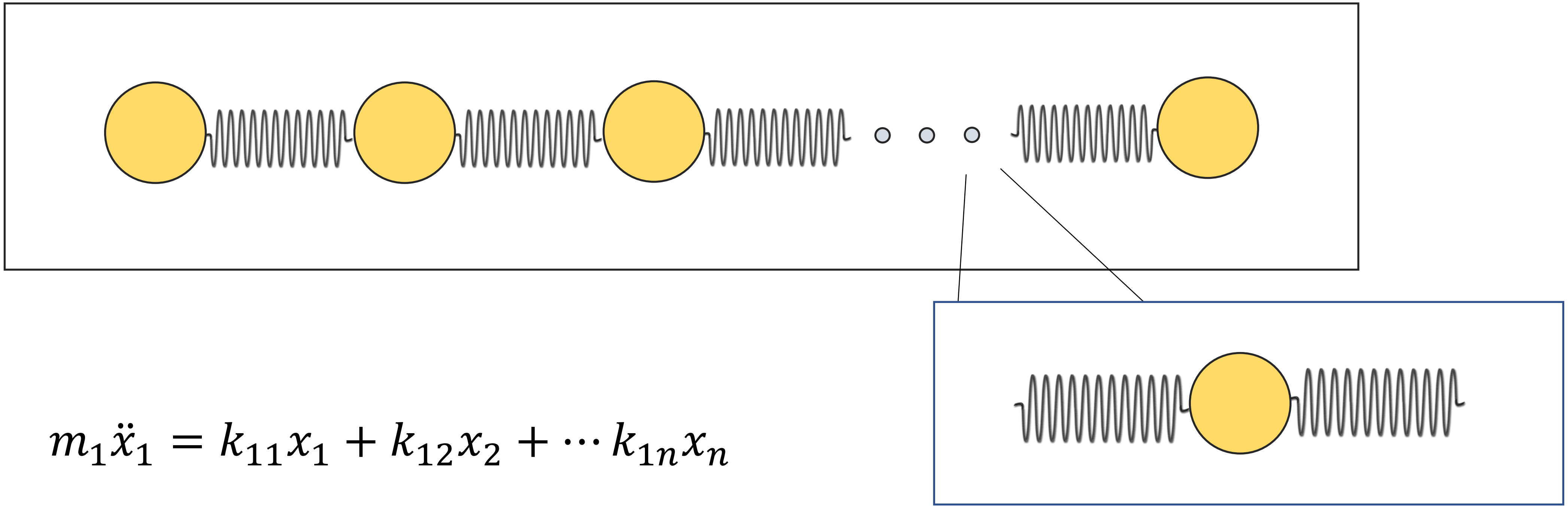
Energy
0.008
0.006
0.004
0.002
0.000
0
2
4
6
8
10
t
Energy





Truncation error always will be exposed after sufficient iterations

Moving onto the spring chain

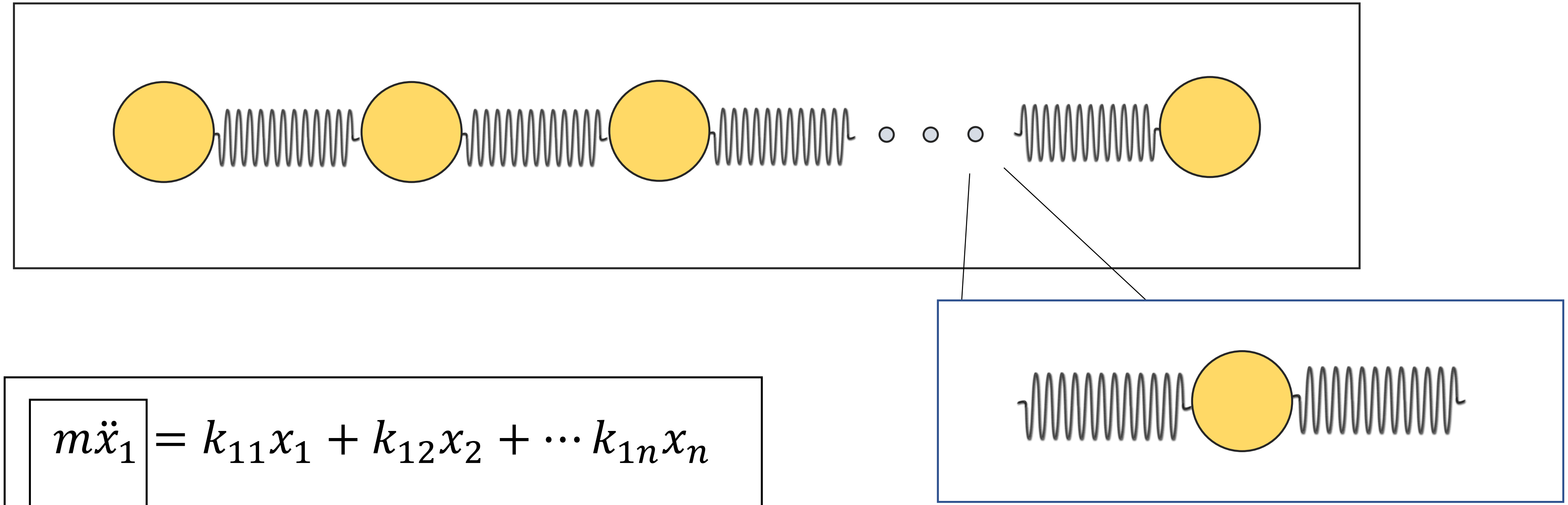


$$m_1\ddot{x}_1 = k_{11}x_1 + k_{12}x_2 + \cdots k_{1n}x_n$$

$$m_2\ddot{x}_2 = k_{21}x_1 + k_{22}x_2 + \cdots k_{2n}x_n$$

∘ ∘ ∘

$$m_n\ddot{x}_n = k_{n1}x_1 + k_{n2}x_2 + \cdots k_{nn}x_n$$



$$m\ddot{x}_1 = k_{11}x_1 + k_{12}x_2 + \cdots k_{1n}x_n$$

$$m\ddot{x}_2 = k_{21}x_1 + k_{22}x_2 + \cdots k_{2n}x_n$$

$$\circ \quad \circ \quad \circ$$

$$m\ddot{x}_n = k_{n1}x_1 + k_{n2}x_2 + \cdots k_{nn}x_n$$

Matrix form

$$m\begin{pmatrix} \ddot{x}_1 \\ \ddot{x}_2 \\ \ddot{x}_3 \\ \cdots \\ \ddot{x}_n \end{pmatrix} = \begin{pmatrix} k_{11} & \cdots & k_{n1} \\ \vdots & \ddots & \vdots \\ k_{1n} & \cdots & k_{nn} \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \cdots \\ x_n \end{pmatrix}$$

Small aid from Linear Algebra:

Matrix form

$$
m\begin{pmatrix} \ddot{x}_1 \\ \ddot{x}_2 \\ \ddot{x}_3 \\ \cdots \\ \ddot{x}_n \end{pmatrix} = \begin{pmatrix} k_{11} & \cdots & k_{n1} \\ \vdots & \ddots & \vdots \\ k_{1n} & \cdots & k_{nn} \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \cdots \\ x_n \end{pmatrix}
$$

$$
m\,\ddot{X} = K\,X
$$

Let's search solution in form of:

$$
X(t) = X_0 e^{i\omega t}
$$

Characteristic equation:

$$
-\omega^2 m\, X_0 e^{i\omega t} = K X_0 e^{i\omega t}
$$

Or simply we have eigenvalue problem:

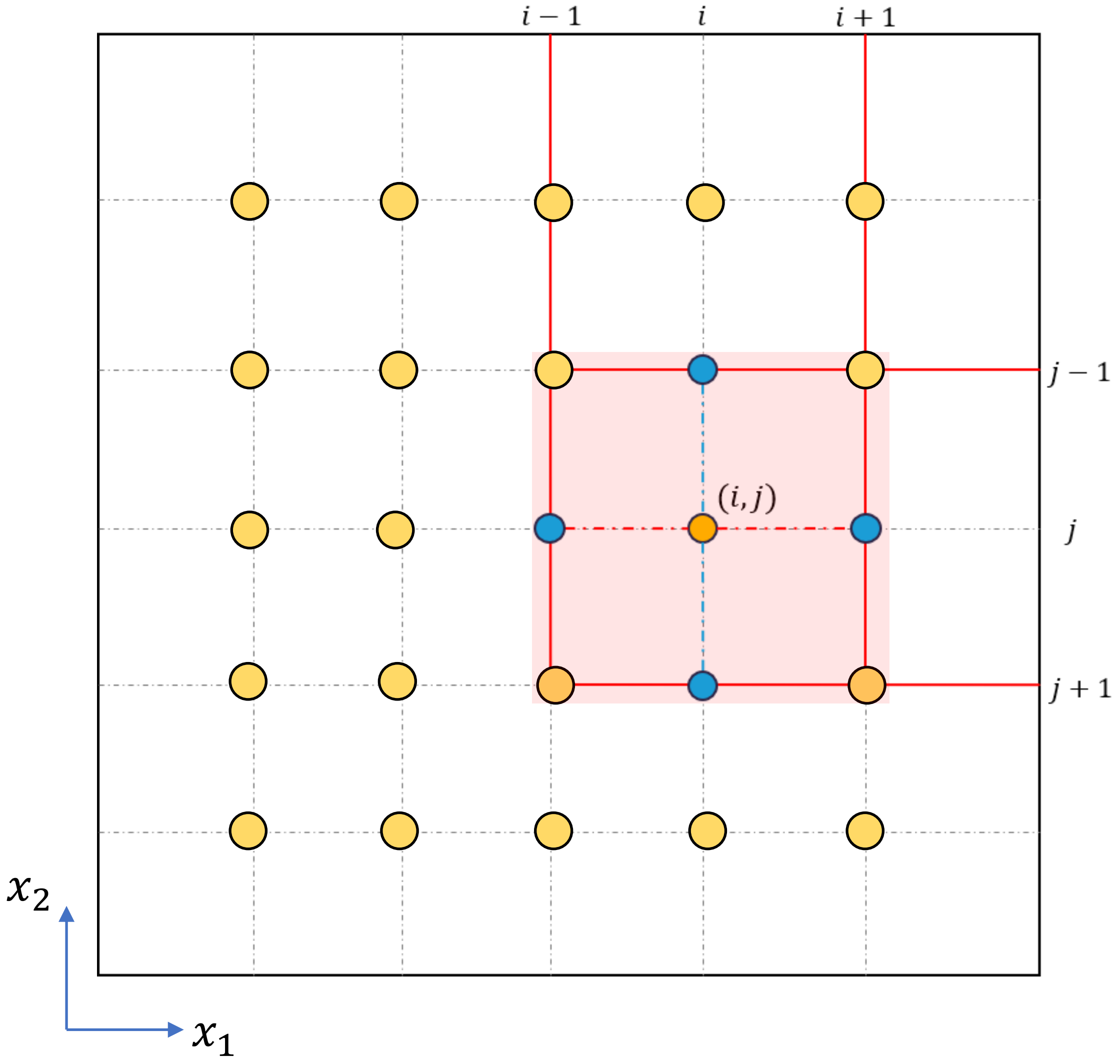
$$
(K + \omega^2 m I)X = 0
$$

$$
\boxed{\det(K + \omega^2 m I) = 0}
$$

$$
\det(K + \omega^2 m I) = 0
$$

I dare you to solve this set manually

2D Square lattice



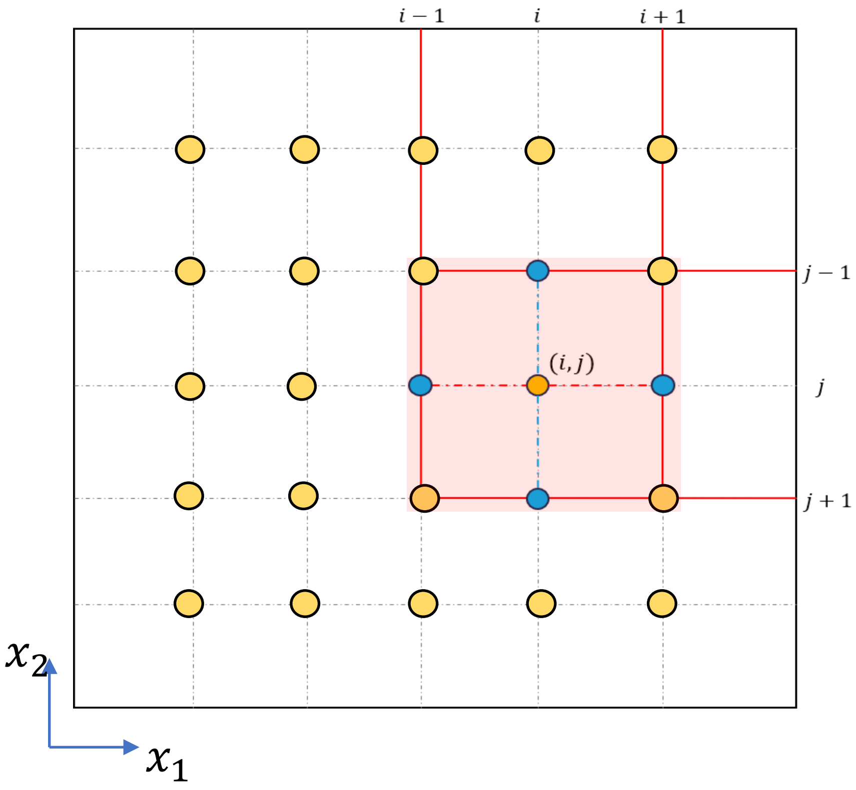
Discretization saves the day:

For (i,j) particle:

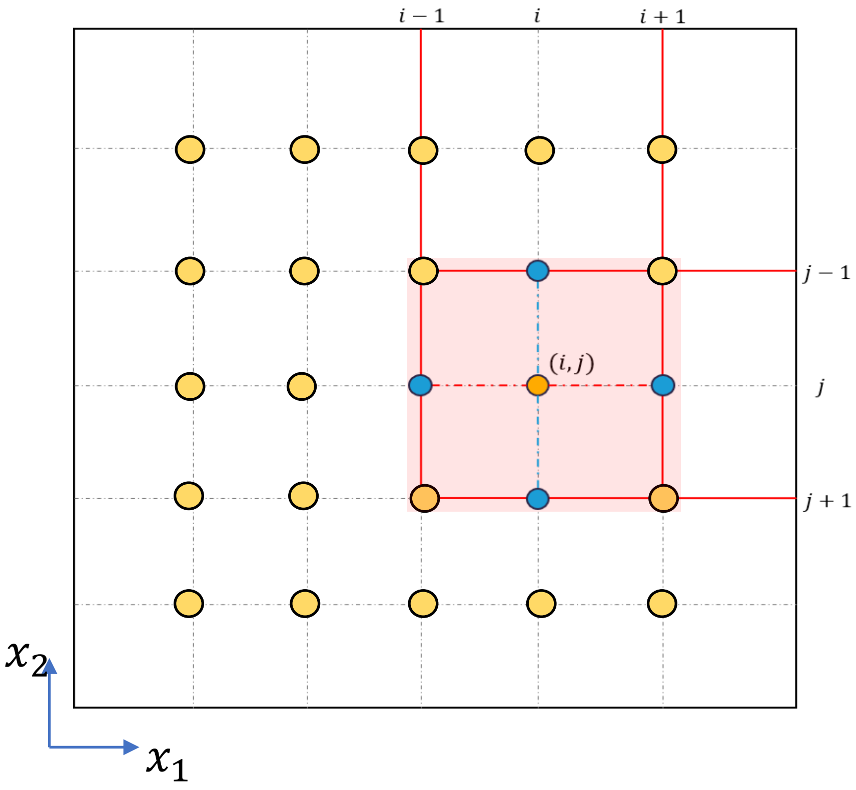
$$m\ddot{x}_{ij} = -k(x_{ij+1} - x_{ij}) + k(x_{ij} - x_{i-1j})$$
$$= k(x_{ij+1} + x_{ij-1} - 2x_{ij})$$

$$m\ddot{x}_{ij} = k(x_{ij+1} + x_{ij-1} - 2x_{ij})$$

But in our case we can always simulate piecewise way!!

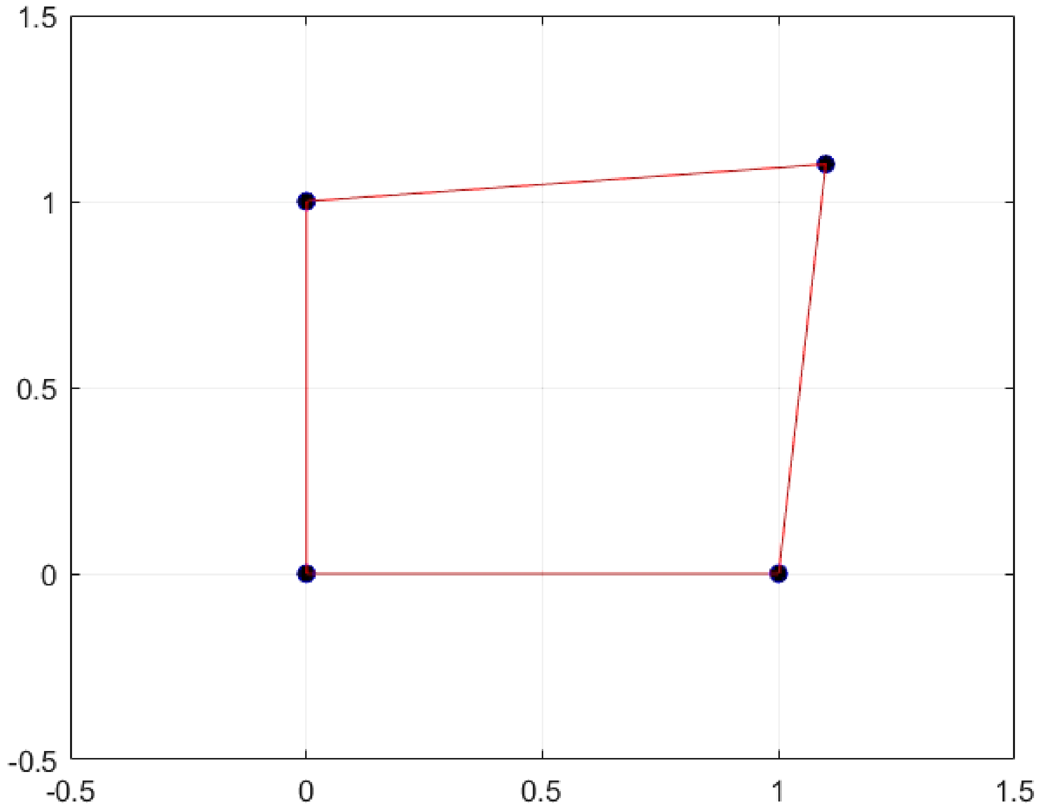


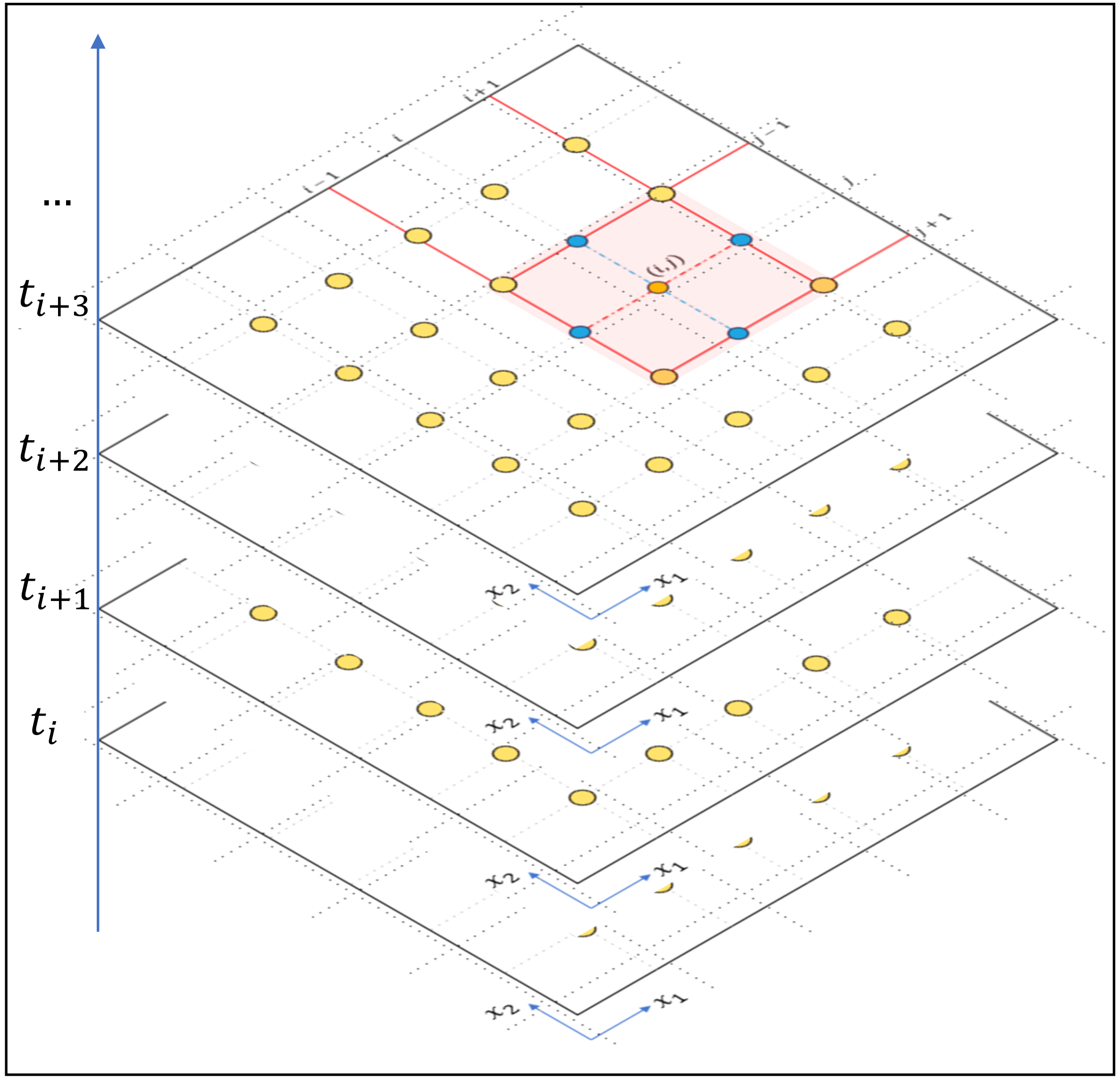

```
% lattice constants:
M=1;
k=100;
% distance and size:
lattice_width=5;
lattice_height=5;
l0=1;
xdis=1;
ydis=1;

%initial Coordinates
x_matrix=zeros(lattice_height,lattice_width);
y_matrix=zeros(lattice_height,lattice_width);

%initial velocities
vx_matrix=zeros(lattice_height,lattice_width);
vy_matrix=zeros(lattice_height,lattice_width);

%masses on the lattice
mass_matrix=zeros(lattice_height,lattice_width);
```




```matlab
% Horizontal springs (Runge-Kutta 4th order)
for a = 1:lattice_height
    for b = 1:lattice_width - 1
        % Calculate forces using RK4 for horizontal springs
        % Initial orientation and displacement vector
        orient = [x_matrix(a, b+1) - x_matrix(a, b), y_matrix(a, b+1) - y_matrix(a, b)];
        norm_orient = norm(orient);

        % Calculate intermediate forces for RK4
        ac1_k1 = (1 - l0 / norm_orient) * orient * k / mass_matrix(a, b);
        ac2_k1 = -(1 - l0 / norm_orient) * orient * k / mass_matrix(a, b+1);

        % Half step for k2
        orient_k2 = orient + 0.5 * dt * ac1_k1;
        norm_orient_k2 = norm(orient_k2);
        ac1_k2 = (1 - l0 / norm_orient_k2) * orient_k2 * k / mass_matrix(a, b);
        ac2_k2 = -(1 - l0 / norm_orient_k2) * orient_k2 * k / mass_matrix(a, b+1);

        % Half step for k3
        orient_k3 = orient + 0.5 * dt * ac1_k2;
        norm_orient_k3 = norm(orient_k3);
        ac1_k3 = (1 - l0 / norm_orient_k3) * orient_k3 * k / mass_matrix(a, b);
        ac2_k3 = -(1 - l0 / norm_orient_k3) * orient_k3 * k / mass_matrix(a, b+1);

        % Full step for k4
        orient_k4 = orient + dt * ac1_k3;
        norm_orient_k4 = norm(orient_k4);
        ac1_k4 = (1 - l0 / norm_orient_k4) * orient_k4 * k / mass_matrix(a, b);
        ac2_k4 = -(1 - l0 / norm_orient_k4) * orient_k4 * k / mass_matrix(a, b+1);

        % Update velocities using RK4 weighted sum
        vx_matrix(a, b) = vx_matrix(a, b) + dt * (ac1_k1(1) + 2*ac1_k2(1) + 2*ac1_k3(1) + ac1_k4(1)) / 6;
        vy_matrix(a, b) = vy_matrix(a, b) + dt * (ac1_k1(2) + 2*ac1_k2(2) + 2*ac1_k3(2) + ac1_k4(2)) / 6;

        vx_matrix(a, b+1) = vx_matrix(a, b+1) + dt * (ac2_k1(1) + 2*ac2_k2(1) + 2*ac2_k3(1) + ac2_k4(1)) / 6;
        vy_matrix(a, b+1) = vy_matrix(a, b+1) + dt * (ac2_k1(2) + 2*ac2_k2(2) + 2*ac2_k3(2) + ac2_k4(2)) / 6;
    end
end
```

Single cell simulation





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- **Lipson, R. & Lu, C. (2009). Photonic crystals: A unique partnership between light and matter. EUROPEAN JOURNAL OF PHYSICS Eur. J. Phys. 30. 33-48. 10.1088/0143-0807/30/4/S04.**

Suggested material to check out:

https://lampz.tugraz.at/~hadley/ss1/phonons/1d/1dphonons.php

Until we meet again?

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Appendix