Comprehensive Documentation: Modular Ion Simulation Codebase

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Contents

1 Introduction

Dear reader! This document was written in the summer of 2025 as part of a 10 week REU (Research Experience for Undergraduates) with the University of Washington in Boris Blinov's ion-trapping group. While participating in the REU, I worked with Boris Blinov ('big Boris')[1], Boris Pashinsky ('little Boris')[2], and various other students including Carl Thomas[3], Hunter Parker[4], Rebecca[5], Jane Gunn[6], and Simon. This project was based on the paper [1] where we wrote code to simulate the motion of trapped ions in two dimensions.

1.1 Github

The code for the project is hosted on github here: github.com/jfbeda/trapped_ion_simulation.

2 Units

We do not follow the conventions of [2] with respect to units. We take as unit of length the micrometer (µm), our unit of time the microsecond (µs), and our unit of mass the atomic mass unit (amu). We also fix the value of the electron charge (e) and the Boltzmann constant (k_B). This allows us to define a unit of energy, κ, which is defined as

$$\kappa \overset{\text{def}}{=} (\text{amu})(\mu\text{m}^2)(\mu\text{s}^{-2}) \approx 1.660\,54 \times 10^{-27}\,\text{J} \approx 10.364\,253\,704\,3\,\text{neV}. \tag{1}$$

In these natural units the vacuum permittivity is given by:

$$\begin{aligned} \epsilon_0 &= 8.854\,18 \times 10^{-12}\,\text{C}^2\,\text{kg}^{-1}\,\text{m}^{-3}\,\text{s}^2 \qquad (2) \\ &= 8.854\,18 \times 10^{-12} \left(\frac{1}{1.602\,18 \times 10^{-19}\,\text{e}} \right)^2 \left(\frac{1}{1.660\,54 \times 10^{-27}\,\text{amu}} \right)^{-1} (10^6\,\mu\text{m})^{-3} (10^6\,\mu\text{s})^2 \qquad (3) \\ \epsilon_0 &= 5.727\,660\,742\,3 \times 10^{-7}\,\text{e}^{-2} \mu\text{m}^{-3}\,\mu\text{s}^2 \text{amu} \qquad (4) \end{aligned}$$

We shall call our natural units of temperature θ defined as

$$\theta \overset{\text{def}}{=} \frac{\kappa}{k_B} \approx 0.120\,272\,422\,607\,\text{mK} \tag{5}$$

In summary, below we present all the units. Those in bold are fixed by assumption. The others are calculated

- **length**: µm
- **time**: µs
- **mass**: amu
- **charge**: $e = 1e$
- **Boltzmann constant**: $k_B = 1k_B$

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- energy: $\kappa = (\text{amu})(\mu\text{m}^2)(\mu\text{s}^{-2}) \approx 10.364\,253\,704\,3\,\text{neV}$
- frequency: MHz
- vacuum permittivity: $\epsilon_0 \approx 5.727\,660\,742\,3 \times 10^{-7}\, e^{-2}\mu\text{m}^{-3}\,\mu\text{s}^2\text{amu}$
- Coulomb constant: $k = \frac{1}{4\pi\epsilon_0} \approx 1.389\,353\,789\,02 \times 10^5\, e^2\mu\text{m}^3\,\mu\text{s}^{-2}\text{amu}^{-1}$
- temperature: $\theta = \kappa/k_B \approx 0.120\,272\,422\,607\,\text{mK}$
- force: $(\text{amu})(\mu\text{m})(\mu\text{s}^{-2}) \approx 1.660\,54 \times 10^{-21}\,\text{N}$
- damping parameter: $(\text{amu})(\mu\text{s}^{-1})$
- reduced plank constant: $\hbar \approx 0.063\,507\,799\,295\,889\,\kappa\,\mu\text{s}$

Generally, in our simulations we take $m = 137.327\,\text{amu}$ is the mass of a Barium ion. We take $\omega = 1\,\text{MHz}$.

Note: All physical quantities in the code are in terms of these natural units except where otherwise specified. For example, a variable called `temperature` will be measured in units of θ, whereas `tempeature_mK` would be in units of mK.

3 Theoretical Background

Note that this section is long, and the majority is *not* required for a deep and complete understanding of the code.

3.1 The problem

Consider a set of N charged particles of mass m in a potential $V(x,y) = \frac{1}{2}m\omega_x^2x^2 + \frac{1}{2}m\omega_y^2y^2$. Suppose without loss of generality that $\omega_x \geq \omega_y$. Define the *isotropy parameter* $\gamma = \frac{\omega_y}{\omega_x}$. As a result of the convention that $\omega_x \geq \omega_y$, we observe that $0 < \gamma \leq 1$. The *anisotropy parameter*, $\alpha \overset{\text{def}}{=} \frac{1}{\gamma}$ we will not use[7]. Note that $1 \leq \alpha < \infty$. For ease of notation, let us fix $\omega_x \overset{\text{def}}{=} \omega$ such that $\omega_y = \gamma\omega$. Thus the new potential is given by

$$V(x,y) = \frac{1}{2}m\omega^2x^2 + \frac{1}{2}m\omega^2\gamma^2y^2 = \frac{1}{2}m\omega^2(x^2 + (\gamma y)^2). \tag{6}$$

This can be written in terms of the position vector $\vec{r} = (x,y)^T$ by defining the matrix $\Gamma = \begin{bmatrix} 1 & 0 \\ 0 & \gamma^2 \end{bmatrix}$. This allows us to write

$$V(\vec{r}) = \frac{1}{2}m\omega^2(\vec{r}^T\Gamma\vec{r}). \tag{7}$$

The potential resulting from the Coulomb interaction between the charged particles is

$$V_c = \sum_{i>j}\sum_{j} \frac{k}{|\vec{r_i} - \vec{r_j}|} = \sum_{i>j}\sum_{j} \frac{k}{\sqrt{(x_i - x_j)^2 + (y_i - y_j)^2}} \tag{8}$$

[7] In other texts and in the literature γ is called the anisotropy parameter, and is still fixed to lie between zero and 1. I prefer calling γ the isotropy parameter, because the larger γ is (the closer it is to 1) the more isotropic the potential

for some constant $k = \frac{q^2}{4\pi\epsilon_0}$. Thus the Lagrangian of the system is

$$L = \sum_{i=1}^{N} \frac{1}{2} m(\dot{x}_i^2 + \dot{y}_i^2) - \sum_{i=1}^{N} \frac{1}{2} m\omega^2 (x_i^2 + (\gamma y_i)^2) - \sum_{i>j} \sum_{j} \frac{k}{\sqrt{(x_i - x_j)^2 + (y_i - y_j)^2}}. \tag{9}$$

$$L = \sum_{i=1}^{N} \frac{1}{2} m\dot{\vec{r}}_i^2 - \sum_{i=1}^{N} \frac{1}{2} m\omega^2 (\vec{r}_i^T \Gamma \vec{r}_i) - \sum_{i>j} \sum_{j} \frac{k}{|\vec{r}_i - \vec{r}_j|} \tag{10}$$

This has generalized momenta of

$$\vec{p}_i \overset{\text{def}}{=} \frac{\partial L}{\partial \vec{r}_j} \tag{11}$$

Where we make use of the abuse of notation $\vec{x} = \frac{\partial Q}{\partial \vec{y}}$ as shorthand for $\vec{x}^{(i)} = \frac{\partial Q}{\partial \vec{y}^{(i)}}$ where $\vec{x}^{(i)}$ denotes the ith component of vector $\vec{x}$. This gives

$$\vec{p}_i = m\vec{r}_j \tag{12}$$

and so the Hamiltonian of the system is given by

$$\boxed{H(\{\vec{r}_i\}, \{\vec{p}_i\}) = \sum_{i=1}^{N} \frac{\vec{p}_i^2}{2m} + \sum_{i=1}^{N} \frac{1}{2} m\omega^2 (\vec{r}_i^T \Gamma \vec{r}_i) + \sum_{i>j} \sum_{j} \frac{k}{|\vec{r}_i - \vec{r}_j|}.} \tag{13}$$

where we will use the shorthands

$$T = \sum_{i=1}^{N} \frac{\vec{p}_i^2}{2m} \tag{14}$$

$$U_h = \sum_{i=1}^{N} \frac{1}{2} m\omega^2 (\vec{r}_i^T \Gamma \vec{r}_i) \tag{15}$$

$$U_c = \sum_{i>j} \sum_{j} \frac{k}{|\vec{r}_i - \vec{r}_j|} \tag{16}$$

to denote the kinetic energy, harmonic potential energy, and Coulomb energy respectively. In this shorthand we have $H = T + U_h + U_c$.

3.2 Fixed points of the Hamiltonian

We now seek fixed points of the Hamiltonian. These satisfy

$$\dot{\vec{r}}_i = \frac{\partial H}{\partial \vec{p}_i} = \frac{\vec{p}_i}{m} = 0, \qquad \dot{\vec{p}}_i = -\frac{\partial H}{\partial \vec{r}_i} = 0. \tag{17}$$

Computing $\frac{\partial H}{\partial \vec{r}_i}$ can be split into two parts, $\frac{\partial U_h}{\partial \vec{r}_i}$ and $\frac{\partial U_c}{\partial \vec{r}_i}$:

$$\left(\frac{\partial U_h}{\partial \vec{r}_i}\right)^{(k)} = \frac{\partial U_h}{\partial \vec{r}_i^{(k)}} \tag{18}$$

$$= \sum_{l=1}^{N} \frac{1}{2} m\omega^2 \frac{\partial}{\partial \vec{r}_i^{(k)}} \sum_p \sum_q \vec{r}_l^{(p)} \Gamma_{pq} \vec{r}_l^{(q)} \tag{19}$$

$$= \sum_{l=1}^{N} \sum_p \sum_q \frac{1}{2} m\omega^2 (\delta_{li}\delta_{pk}\Gamma_{pq}\vec{r}_l^{(q)} + \delta_{li}\delta_{kq}\vec{r}_l^{(p)}\Gamma_{pq}) \tag{20}$$

$$= \frac{1}{2} m\omega^2 \left(\sum_q \Gamma_{kq} \vec{r}_i^{(q)} + \sum_p \vec{r}_i^{(p)} \Gamma_{pk} \right) \tag{21}$$

$$\boxed{\frac{\partial U_h}{\partial \vec{r}_i} = m\omega^2 \Gamma \vec{r}_i.} \tag{22}$$

where we have used the fact that $\Gamma = \Gamma^T$ is a symmetric matrix. Now turning to the Coulomb term we have:

$$\left(\frac{\partial U_c}{\partial \vec{r}_i}\right)^{(k)} = \frac{\partial U_c}{\partial r_i^{(k)}} \tag{23}$$

$$= \sum_{p>q}\sum_{q} \frac{\partial}{\partial r_i^{(k)}}\left[\frac{k}{\sqrt{(\vec{r}_p-\vec{r}_q)^2}}\right] \tag{24}$$

$$= \sum_{p>q}\sum_{q} -\frac{k}{2((\vec{r}_p-\vec{r}_q)^2)^{3/2}}\frac{\partial}{\partial r_i^{(k)}}(\vec{r}_p-\vec{r}_q)^2 \tag{25}$$

$$= -\frac{k}{2}\sum_{p>q}\sum_{q}\frac{1}{|\vec{r}_p-\vec{r}_q|^3}\sum_{j} 2(\vec{r}_p^{(j)}-\vec{r}_q^{(j)})\frac{\partial}{\partial \vec{r}_i^{(k)}}\left(\vec{r}_p^{(j)}-\vec{r}_q^{(j)}\right) \tag{26}$$

$$= -k\sum_{p>q}\sum_{q}\sum_{j}\frac{(\vec{r}_p^{(j)}-\vec{r}_q^{(j)})}{|\vec{r}_p-\vec{r}_q|^3}(\delta_{ip}\delta_{jk}-\delta_{iq}\delta_{jk}) \tag{27}$$

$$= -k\sum_{p>q}\sum_{q}\frac{(\vec{r}_p^{(k)}-\vec{r}_q^{(k)})}{|\vec{r}_p-\vec{r}_q|^3}(\delta_{ip}-\delta_{iq}) \tag{28}$$

$$\frac{\partial U_c}{\partial \vec{r}_i} = -k\sum_{p>q}\sum_{q}\frac{(\vec{r}_p-\vec{r}_q)}{|\vec{r}_p-\vec{r}_q|^3}(\delta_{ip}-\delta_{iq}) \tag{29}$$

$$= -\frac{k}{2}\sum_{p\neq q}\sum_{q}\frac{(\vec{r}_p-\vec{r}_q)}{|\vec{r}_p-\vec{r}_q|^3}(\delta_{ip}-\delta_{iq}) \quad \text{(As symmetric in } p \text{ and } q\text{)} \tag{30}$$

$$= -\frac{k}{2}\left(\sum_{q\neq i}X_{iq}-\sum_{p\neq i}X_{pi}\right) \qquad \left(X_{pq} \overset{\text{def}}{=} \frac{(\vec{r}_p-\vec{r}_q)}{|\vec{r}_p-\vec{r}_q|^3}\right) \tag{31}$$

$$= -k\left(\sum_{q\neq i}X_{iq}\right) \quad \text{(As } X_{pq} \text{ is antisymmetric)} \tag{32}$$

$$= k\left(\sum_{q\neq i}X_{qi}\right) \tag{33}$$

$$= k\left(\sum_{q\neq i}\frac{(\vec{r}_q-\vec{r}_i)}{|\vec{r}_q-\vec{r}_i|^3}\right) \tag{34}$$

$$\boxed{\frac{\partial U_c}{\partial \vec{r}_i} = k\left(\sum_{q\neq i}\frac{(\vec{r}_q-\vec{r}_i)}{|\vec{r}_q-\vec{r}_i|^3}\right)} \tag{35}$$

Putting (22) and (35) together yields a condition for fixed points of the system:

$$0 = -\frac{\partial H}{\partial \vec{r}_i} = -\left(\frac{\partial U_h}{\partial \vec{r}_i}+\frac{\partial U_c}{\partial \vec{r}_i}\right) \tag{36}$$

$$0 = m\omega^2\Gamma\vec{r}_i + k\sum_{q\neq i}\frac{(\vec{r}_q-\vec{r}_i)}{|\vec{r}_q-\vec{r}_i|^3}. \tag{37}$$

That is to say, a fixed point of the system is a set of $\{\vec{r}_i\}$ such that for all $i = 1, \cdots, N$

$$\boxed{0 = m\omega^2 \Gamma \vec{r}_i + k \sum_{q \neq i} \frac{(\vec{r}_q - \vec{r}_i)}{|\vec{r}_q - \vec{r}_i|^3}}. \tag{38}$$

It will also be useful to note that (38) is a simplified form of the general case of the force on each particle given by

$$\dot{\vec{p}_i} = -\left(m\omega^2 \Gamma \vec{r}_i + k \sum_{q \neq i} \frac{(\vec{r}_q - \vec{r}_i)}{|\vec{r}_q - \vec{r}_i|^3} \right). \tag{39}$$

Note also, as we will use it for later:

$$\frac{\partial}{\partial \vec{r}_i} \frac{1}{|\vec{r}_p - \vec{r}_q|} = -\frac{(\vec{r}_p - \vec{r}_q)}{|\vec{r}_p - \vec{r}_q|^3} (\delta_{ip} - \delta_{iq}) \tag{40}$$

3.3 Symmetry properties of the solution set

As a check, suppose that $\gamma = 1$ (i.e. the system is rotationally symmetric). This means that $\Gamma = \mathbb{I}$, the identity matrix. We now expect that if $\{\vec{r}_i\}$ are a solution to (38), we should expect that $\{\vec{r}_i'\}$ are also a solution, where $\vec{r}_i' \overset{\text{def}}{=} R\vec{r}_i$ and R is a rotation matrix. Observe that

$$m\omega^2 R\vec{r}_i + k \sum_{q \neq i} \frac{(R\vec{r}_q - R\vec{r}_i)}{|R\vec{r}_q - R\vec{r}_i|^3} = R \left(m\omega^2 \vec{r}_i + k \sum_{q \neq i} \frac{(\vec{r}_q - \vec{r}_i)}{|\vec{r}_q - \vec{r}_i|^3} \right) \tag{41}$$

$$= 0 \tag{42}$$

as expected. In fact, we notice that the solution set is invariant under the action of any matrix M that commutes with Γ and preserves $(\vec{r}_q - \vec{r}_i)^2$. In other words, any unitary matrix M which commutes with Γ. Suppose $M = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$. The fact that M must commute with Γ implies that either $\gamma = 1$ or $b = c = 0$. In the case of $\gamma \neq 1$ this means that M is a diagonal unitary matrix. This means that each diagonal entry of M (a and d) has complex norm 1. Assuming further that M is real gives that $a = \pm 1$ and $d = \pm 1$. This makes sense, as for $\gamma \neq 1$ the only symmetry transformations we expect on our solution set are similarity transformations of the ellipse, namely reflection about the y-axis ($M = \text{diag}(-1, 1)$), reflection about the x-axis ($M = \text{diag}(1, -1)$), rotation by π ($M = \text{diag}(-1, -1)$), and of course the identity ($M = \mathbb{I}$).

3.4 Special fixed points: equally spaced charges around the circle

Let us consider the special case of $\gamma = 1$. Let us further divide (38) by k and define $x = m\omega^2/k$. Equation (38) now reads

$$0 = x\vec{r}_i + \sum_{q \neq i} \frac{(\vec{r}_q - \vec{r}_i)}{|\vec{r}_q - \vec{r}_i|^3} \tag{43}$$

We conjecture that given N there exists a radius r such that $\vec{r}_j$ defined by

$$\vec{r}_j = r \begin{pmatrix} \cos(2\pi j/N) \\ \sin(2\pi j/N) \end{pmatrix} \tag{44}$$

form a solution to (43). That is to say we conjecture there exists an r such that equally spaced particles on a circle of radius r is a solution. Because the problem is rotationally symmetric, it suffices to check (43) for only one case (i.e. $i = N$) (or $i = 0$ if you prefer an abuse of notation). We may move to the complex plane by associating the x coordinate with the real part and the y coordinate with the imaginary part of a complex function. Thus $\vec{r}_q$ is associated to the scaled root of unity $re^{2\pi iq/N}$. This is equivalent to the claim that the complex function defined below has a root:

$$f(r) \overset{\text{def}}{=} xr + \sum_{q=1}^{N-1} \frac{(re^{2\pi iq/N} - r)}{|re^{2\pi iq/N} - r|^3} \tag{45}$$

$$f(r) = xr + \frac{1}{r^2} \sum_{q=1}^{N-1} \frac{(e^{2\pi iq/N} - 1)}{|e^{2\pi iq/N} - 1|^3} \tag{46}$$

Setting this equal to zero gives:

$$0 = xr^* + \frac{1}{r^{*2}} \sum_{q=1}^{N-1} \frac{(e^{2\pi iq/N} - 1)}{|e^{2\pi iq/N} - 1|^3} \tag{47}$$

$$0 = xr^{*3} + \sum_{q=1}^{N-1} \frac{(e^{2\pi iq/N} - 1)}{|e^{2\pi iq/N} - 1|^3} \tag{48}$$

$$r^* = \left(-\frac{1}{x} \sum_{q=1}^{N-1} \frac{(e^{2\pi iq/N} - 1)}{|e^{2\pi iq/N} - 1|^3} \right)^{1/3} \tag{49}$$

To simplify r^*, define $z_q = e^{2\pi iq/N} - 1$. Now observe that

$$\begin{aligned} |z_q|^2 &= (e^{2\pi iq/N} - 1)(e^{-2\pi iq/N} - 1) && (50) \\ &= 2 - e^{2\pi iq/N} - e^{-2\pi iq/N} && (51) \\ &= 2 - 2\cos(2\pi q/N) && (52) \\ &= 2(1 - \cos(2\pi q/N)) && (53) \\ |z_q|^2 &= 4\sin^2(\pi q/N) && (54) \\ |z_q| &= 2\sin(\pi q/N) && (55) \end{aligned}$$

Thus we have

$$\begin{aligned} r^* &= \left(-\frac{1}{x} \sum_{q=1}^{N-1} \frac{(e^{2\pi iq/N} - 1)}{8\sin^3(\pi q/N)} \right)^{1/3} && (56) \\ &= -\frac{1}{2} \left(\frac{1}{x} \sum_{q=1}^{N-1} \frac{e^{2\pi iq/N} - 1}{\sin^3(\pi q/N)} \right)^{1/3}. && (57) \end{aligned}$$

Now we notice that for each q, the corresponding $N-q$ term has numerator $e^{2\pi i(N-q)/N} - 1 = \overline{e^{2\pi iq/N} - 1}$ and so the imaginary parts cancel as $\sin(\pi q/N) = \sin(\pi(N-q)/N)$. Thus we may write

$$r^* = -\frac{1}{2}\left(\frac{1}{x}\sum_{q=1}^{N-1}\frac{\mathrm{Re}(e^{2\pi iq/N}-1)}{\sin^3(\pi q/N)}\right)^{1/3} \tag{58}$$

$$= -\frac{1}{2}\left(\frac{1}{x}\sum_{q=1}^{N-1}\frac{\cos(2\pi q/N)-1}{\sin^3(\pi q/N)}\right)^{1/3} \tag{59}$$

$$= \frac{1}{2}\left(\frac{1}{x}\sum_{q=1}^{N-1}\frac{2\sin^2(\pi q/N))}{\sin^3(\pi q/N)}\right)^{1/3} \tag{60}$$

$$= \frac{1}{2^{2/3}}\left(\frac{1}{x}\sum_{q=1}^{N-1}\frac{1}{\sin(\pi q/N)}\right)^{1/3} \tag{61}$$

$$\boxed{r^* = \left(\frac{1}{4x}\sum_{q=1}^{N-1}\frac{1}{\sin(\pi q/N)}\right)^{1/3}} \tag{62}$$

The above expression is pretty well approximated by $\left(\frac{N}{2\pi x}\ln(N)\right)^{\frac{1}{3}}$. The above expression can be visualized in Desmos, where it is clear there is always a root. Thus we have shown that for $\gamma = 1$ and all N, there exists r^* such that charges spaced equally around a circle of radius r^* is a fixed point of the system. It remains to be seen whether or not this fixed point is a point of stability or not. I have a conjecture that the above is a position of stability for $N \leq 6$, and is unstable for $N \geq 7$, but I have not succeeded in showing this algebraically.

4 Convergence

To determine the optimal time step at which to run the simulation we look at how the temperature of the system evolves over time. It seems as though the larger the timestep, the faster the temperature of the system increases. For a timestep of $\delta t \approx 10^{-3}$ µs the simulation can run roughly 100 µs before the temperature increases significantly. However for this case, the temperature of the simulation has a tendency to roughly double over the course of 1000 µs. That is, going from around 5 mK to 10 mK

5 Codebase Structure

The codebase consists of the following Python files:

- `natural_units.py` — defines physical constants and conversions.
- `utility_functions.py` — general-purpose numerical helpers.
- `laser.py` — models laser cooling physics.

- simulation_module.py — core simulation logic: initialization, dynamics, and visualization.
- histogram_workers.py — handles histogram production functions.
- parralel_workers.py — handles functions that are later parallelized.
- parralel.py — handles functions that run in parallel.

We now explain each of these in detail.

5.1 natural_units.py

This file defines physical constants in natural units used throughout the simulation. These constants are crucial for scaling energies, forces, and temperatures appropriately. For example:

```
hbar = 0.063507799295889 # Reduced Plank's constant((amu)(um^2)(us^-1))
kB = 1. # Boltzmann constant (in units of kB)
k = 1.38935378902e5 # Coulomb constant ((e^2)(um^3)(us^-2)(amu^-1))
epsilon_0 = 5.7276607423e-7 # Vacuum permitivity ((amu)(us)(um^-3)(e))
electron_charge = 1. # Electron charge (in units of e)
```

This file also includes various functions to convert values from natural units into more standard units. For example, the function theta_to_mK accepts a temperature in natural units of θ and returns the corresponding temperature in units of mK.

5.2 utility_functions.py

This file includes various functions that mainly serve to convert various possible list structures into other list structures. All the functions are well described in the file.

For example, one particular function, base_radius gives an implementation of (62).

5.3 laser.py

This file implements the Laser class, which handles Doppler cooling of the ions. A Laser object may be initialized with a wavelength and various other parameters, and may then be used to compute the Doppler cooling force on a set of ions at a particular time.

5.4 simulation_module.py

INCOMPLETE

5.5 histogram_workers.py

INCOMPLETE

5.6 parralel_workers.py

INCOMPLETE

5.7 parralel.py

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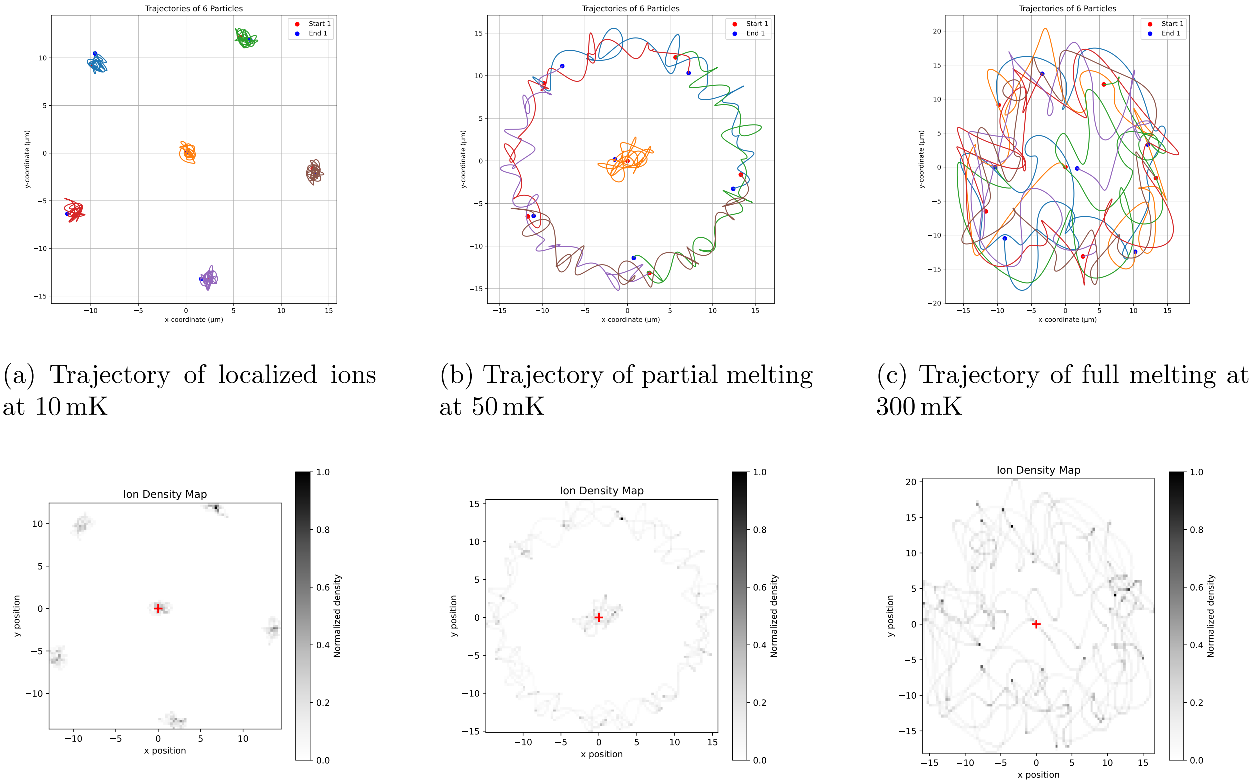
6 Use Examples

6.1 Running A Simple Simulation

The Jupyter Notebook `example_simple_simulation.ipynb` gives a tutorial for using the code to run a simple simulation. As suggested in one of the markdown cells, by changing the initial temperature of the simulation, we can get the crystal of 6 ions to either stay frozen or to melt. Examples of those two conditions are given in Fig. 1. Generally the ion density maps acquired through `SimulationVisualizer().plot_density_map(state)` carry more useful information than the trajectory plots, especially as the length of the simulation gets large. For simulations of length 1000 µs or longer, the ion density maps are always preferred.



(a) Trajectory of localized ions at 10 mK

(b) Trajectory of partial melting at 50 mK

(c) Trajectory of full melting at 300 mK

(d) Density map of localized ions at 10 mK

(e) Density map of partial melting at 50 mK

(f) Density map of full melting at 300 mK

Figure 1: Simulations of 6 ions with an isotropy of 1 over 50 µs. Top row: trajectory maps; bottom row: ion density distributions.

6.2 Running a quench series

The INCOMPLETE Jupyter Notebook `example_quench_series.ipynb` gives a tutorial for using the code to run a series of quenches in parallel and animate the output. This notebook is computationally much more intensive than the one in Section 6.1 and relies on parallelized computation. In my experience, the fact that you will be running this code on a different machine to me means it is likely you will run into some kind of problem with the parallelized computation that might be an issue.

7 Acknowledgements

We would like to thank Boris Blinov for his supervision. We also owe a huge debt of gratitude to Boris Pashinskii for the code that was passed to me. Much of this code grew out of beautiful code written originally by him.

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