

Year 4 Project Report: Direct Simulation of Evaporative Cooling in a Harmonic Trap

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Many thanks to Dr Giovanni Barontini, for his help and advice supervising this project.

1 Abstract

Evaporative cooling has provided the means to cool gasses of atoms down to the low temperature regime required for the formation of Bose-Einstein condensates. The evaporative cooling process dictates the end temperature and phase-space density of the condensate. Simulation can provide a guide for the outcome of experimental evaporative cooling. In this project evaporative cooling within a harmonic trap was simulated using a direct simulation Monte-Carlo method to model collisions. A run was performed to test the thermalisation within a harmonic trap and the gas found to thermalise to the expected Maxwell-Boltzmann speed distribution. An example of an evaporative cooling run was performed where a simulation gas was cooled from $T = 1\mu\text{K}$ to $T = 0.61\mu\text{K}$ in 1s.

2 Introduction

Bose-Einstein condensation, over the last three decades, has brought quantum mechanics into macroscopic view with Bose-Einstein condensates (BECs) providing a rich set of physical phenomena to be investigated. BECs are created when a gas of bosons is cooled past a critical temperature at which point, the quantum mechanical ground state of the gas will become macroscopically occupied [1]. To generate a BEC low temperatures and high phase space density must be reached. To do this the gas requires trapping and cooling.

Evaporative cooling is used in Bose-Einstein condensation experiments to reach temperatures lower than the limits of laser cooling. Laser cooling cools a gas of atoms down using the absorption of photons [2]. As during laser cooling each particle will repeatedly absorb and emit photons it has a fundamental limit set by the temperature increase caused by the recoil of a particle after emission. Another method, therefore, is needed to cool a gas down to the low temperatures required to form a BEC. In 1995 the first BECs were created using rubidium [3], and sodium [4]. Both experiments used evaporative cooling to reach the respective critical temperatures and evaporative cooling remains integral to many ultra-cold atoms experiments today.

Evaporative cooling works on the basis of trapping a gas of atoms in a potential from which the most energetic atoms will be able to escape. This means having a finite potential barrier or pumping surface via which atoms will leave the trap upon overcoming or reaching [5]. This can

be modelled as a trapping potential with a finite trap depth, V_{trap} , after which point the potential is zero. This is the approach taken in this project.

As atoms are lost, collisions between them repopulate the set of atoms at higher energies and the process repeats. As higher energy atoms are more likely to leave the trap, this will decrease the overall temperature within. This process will slow as the temperature decreases as less atoms will have the energy required to leave the trap, and so the depth of the trap must be reduced over time to continue cooling [5]. For this project the ‘cooling ramp’ was defined as the trap depth as a function of time, $V_{\text{trap}}(t)$.

The evaporative cooling process dictates the phase-space density of the final BEC along with the number of atoms lost in the process. Many experiments desire to maximise the end phase-space density for a specified number of atoms [6]. As such the simulation of this process is desirable as it can work hand in hand with experiment in order to predict the results of different experimental cooling ramps.

In this project a trapped gas was simulated using a direct simulation Monte-Carlo (DSMC) method [7]. This method simulates the particles’ positions ballistically, and calculates the collisions based on a Monte-Carlo method. Not long (in 1996) after the first BECs were created this method was used by Wu and Foot to simulate evaporative cooling [8], and more advanced iterations of the method have been used since [9]. This project, in many ways, was simply a repeat of those early simulations.

Section 3 discusses the thermodynamics of a gas in a harmonic trap; **Section 4** describes the DSMC algorithm, its implementation in the simulation and how accurate a model of reality it was; **Section 5** shows two runs of the simulation and **Section 6** gives some concluding remarks.

3 Thermodynamics of a Trapped Classical Gas

During evaporative cooling the temperatures are above the critical temperature for BEC formation and so the regime can be considered classically. More specifically this is true when $n\Lambda^3 \ll 1$, where n is the number density of atoms and $\Lambda = (2\pi\hbar^2/mk_B T)^{1/2}$ the thermal de Broglie wavelength [1]. Additionally bosons at low temperatures interact through s-wave scattering, meaning that collisions will occur and the gas will always tend

to thermal equilibrium.

The phase space density, $n(\mathbf{r}, \mathbf{p})$, of a classical gas at thermal equilibrium will follow a Boltzmann distribution:

$$n(\mathbf{r}, \mathbf{p}) \propto \exp\left(-\frac{\mathcal{E}(\mathbf{r}, \mathbf{p})}{k_B T}\right), \quad (1)$$

$$\mathcal{E}(\mathbf{r}, \mathbf{p}) = \frac{p^2}{2m} + V(\mathbf{r}). \quad (2)$$

In BEC and other cold atoms experiments the traps used are frequently well approximated as harmonic potentials [1]:

$$V(\mathbf{r}) = \frac{1}{2}m(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2). \quad (3)$$

This leads to a three dimensional Gaussian distribution in both position and velocity space:

$$n(\mathbf{r}) \propto \exp\left(-\frac{m}{2k_B T}(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2)\right), \quad (4)$$

$$n(\mathbf{v}) \propto \exp\left(-\frac{m}{2k_B T}(v_x^2 + v_y^2 + v_z^2)\right). \quad (5)$$

Equations 4, 5 are for an infinite harmonic trap. During evaporative cooling the trap has a finite depth, V_{trap} , which is reduced over time. Luiten *et al.* showed that a good approximation for a classical gas undergoing evaporative cooling is a truncated Boltzmann distribution [5]:

$$n(\mathbf{r}, \mathbf{p}, t) \propto \exp\left(-\frac{\mathcal{E}(\mathbf{r}, \mathbf{p})}{k_B T}\right) \Theta(V_{\text{trap}}(t) - \mathcal{E}(\mathbf{r}, \mathbf{p})), \quad (6)$$

Where $\Theta(x)$ is the Heaviside step function: $\Theta(x) = 0$ for $x < 0$ and $\Theta(x) = 1$ for $x \geq 0$. Equation 6 is the kind of distribution expected of the simulation gas during evaporative cooling, and Equations 4 and 5 are the expected distributions for the simulation gas in an infinite trap.

4 Direct Simulation Monte-Carlo

The Direct Simulation Monte-Carlo (DSMC) method was devised by Bird [7] in the 1960s and provides a way to compute multiple particle collisions in a way that is reasonably computationally efficient as it does not require looping over every single particle in the simulation. It has been verified as being an accurate description of experiment [8][10], and it has been shown that DSMC can be used to derive the Boltzmann equation [11]. The efficacy of DSMC in this simulation is discussed in **Subsection 4.3**.

4.1 Method

An explanation of the DSMC algorithm used in the simulation follows. This is based on the article [12] and textbook [7]. A set of simulation particles are created with radius R and the space split up into square cells of side length l . These particles are given an effective particle number that they correspond to; N_{eff} . The number of real particles handled by the simulation can then be made significantly larger. The aim of DSMC is to stochastically sample from a probability distribution that describes how likely it is for a pair of simulation particles within a cell to collide. This probability is equal to:

$$P_{\text{collide}}(\mathbf{v}_{\mathbf{r}}) = \frac{N_{\text{eff}} \pi R^2 |\mathbf{v}_{\mathbf{r}}| \Delta t}{l^3}, \quad (7)$$

Where $\mathbf{v}_{\mathbf{r}} = \mathbf{v}_1 - \mathbf{v}_2$ is the relative velocity between the two particles, and Δt the time of flight over which the probability is taken (i.e. the time step of the simulation). The particles were modelled as hard spheres; the πR^2 in Equation 7 being the total scattering cross section of a hard sphere. This probability can be efficiently sampled from by the following algorithm.

For every cell:

Step 1 Progress the particles for a time step Δt without collision. In this simulation they were in a harmonic potential so at each time step were progressed like:

$$\begin{aligned} \Delta \mathbf{r} &= \mathbf{v} \Delta t, \\ \Delta \mathbf{v} &= -(\omega_x^2 x, \omega_y^2 y, \omega_z^2 z) \Delta t. \end{aligned} \quad (8)$$

Step 2 Pick two particles in the cell at random.

Step 3 Accept the pair as collision partners if $\frac{|\mathbf{v}_{\mathbf{r}}|}{v_{r, \text{max}}} > \mathcal{R}$, where \mathcal{R} is a random number between 0 and 1 and $v_{r, \text{max}}$ is an arbitrary normalising speed that is larger than the maximum relative velocity of two particles in the cell.

Step 4 If the pair is accepted they are ‘collided’ and velocities changed accordingly, explained below.

Step 5 Repeat steps 2 to 4 until the required number of candidates pairs, M_{cand} have been processed, explained below.

The post collision velocities, \mathbf{v}_1' and \mathbf{v}_2' , are calculated such that kinetic energy and momentum are conserved. Conservation of momentum means that the center of mass velocity of particles 1 and 2, \mathbf{v}_{cm} , is constant:

$$\mathbf{v}_{\text{cm}} = \frac{1}{2}(\mathbf{v}_1 + \mathbf{v}_2) = \frac{1}{2}(\mathbf{v}_1' + \mathbf{v}_2') = \mathbf{v}_{\text{cm}}'. \quad (9)$$

Conservation of energy means that the magnitude of the relative velocities is also constant:

$$|\mathbf{v}_r| = |\mathbf{v}_1 - \mathbf{v}_2| = |\mathbf{v}_1' - \mathbf{v}_2'| = |\mathbf{v}_r'|. \quad (10)$$

In spherical polar coordinates the final relative velocity for particles travelling in a certain direction is:

$$\mathbf{v}_r' = |\mathbf{v}_r|(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta). \quad (11)$$

The angles ϕ and θ are chosen randomly. Here the particles are hard spheres and so the relative velocity is uniformly randomly distributed over the unit sphere. The azimuthal angle ϕ is uniformly distributed from 0 to 2π :

$$\phi = 2\pi\mathcal{R}_\phi, \quad (12)$$

Where \mathcal{R}_ϕ is another random number between 0 and 1. The polar angle θ is distributed according to:

$$P(\theta)d\theta = \frac{1}{2}\sin\theta d\theta. \quad (13)$$

Using the change of variables $q = \cos\theta$, as q is uniformly distributed between -1 and 1 (\mathcal{R}_q is another random number between 0 and 1):

$$\begin{aligned} q &= 2\mathcal{R}_q - 1, \\ \cos\theta &= q, \\ \sin\theta &= \sqrt{1 - q^2}. \end{aligned} \quad (14)$$

The two random variables q and ϕ can be used in Equation 11 to generate a relative velocity \mathbf{v}_r' which relates to \mathbf{v}_1' and \mathbf{v}_2' by:

$$\mathbf{v}_1' = \mathbf{v}_{\text{cm}} + \frac{\mathbf{v}_r'}{2}, \quad (15)$$

$$\mathbf{v}_2' = \mathbf{v}_{\text{cm}} - \frac{\mathbf{v}_r'}{2}. \quad (16)$$

The number of collisions that should take place in a cell in one time step M_{coll} is:

$$M_{\text{coll}} = \frac{N_c^2 N_{\text{eff}} \pi R^2 \langle v_r \rangle \Delta t}{2l^3}, \quad (17)$$

Quantity	Unit
Energy	$\hbar\omega_{\text{HO}}$
Distance	a_{HO}
Time	ω_{HO}^{-1}
Velocity	$a_{\text{HO}}\omega_{\text{HO}}$
Frequency	ω_{HO}

Table 1: Table of nondimensional units used in the simulation, where $\omega_{\text{HO}} = (\omega_x\omega_y\omega_z)^{1/3}$ the trapping frequencies of the potential, $a_{\text{HO}} = \left(\frac{\hbar}{m\omega_{\text{HO}}}\right)$ and \hbar is the reduced Planck's constant.

Where $\langle v_r \rangle$ is the average relative velocity in a cell and N_c is the number of particles in a cell. The terms in Equation 17 are discussed in more detail in Chapter 11 of [7]. The number of candidate pairs M_{cand} , is related to M_{coll} by the acceptance/rejection procedure at Step 3 of the algorithm, therefore:

$$\frac{M_{\text{coll}}}{M_{\text{cand}}} = \frac{\langle v_r \rangle}{v_{r,\text{max}}}, \quad (18)$$

$$M_{\text{cand}} = \frac{N_c^2 N_{\text{eff}} \pi R^2 v_{r,\text{max}} \Delta t}{2l^3}. \quad (19)$$

4.2 Implementation

The simulation and results are in nondimensional units relevant to the scale of the system. Two scales have been defined; an angular frequency scale, and a length scale: ω_{HO} and a_{HO} respectively.

$$\omega_{\text{HO}} = (\omega_x\omega_y\omega_z)^{1/3}, \quad (20)$$

$$a_{\text{HO}} = \left(\frac{\hbar}{m\omega_{\text{HO}}}\right). \quad (21)$$

Here ω_i ($i = x, y, z$) are the trapping frequencies of the potential, m the mass of an atom and \hbar the reduced Planck's constant. The length scale a_{HO} is a useful one as the width of the final BEC will be of the order of this length [1]. The other scales of the simulation can be seen in Table 1. The radius of a hard sphere used in this simulation was based on the scattering cross section of Rb87; an isotope which can be used to make a BEC. As the simulated gas was at low energies and Rb87 atoms are bosons the scattering was assumed to be purely s-wave. This leads to a total scattering cross section of $\sigma = 8\pi a^2$ [1]. Equating the cross sections of a hard sphere and a boson the effective hard sphere radius is:

$$R = a\sqrt{8}, \quad (22)$$

Where a is the s-wave scattering length. For a Rb87 atom $a \approx 100a_0$ [13] where a_0 is the Bohr radius. This leads to the radius used in the simulation $R = 0.014a_{\text{HO}}$.

The value of $v_{r,\text{max}}$ in Equation 19 was chosen for each initial distribution to be the maximum relative velocity between two particles in the simulation.

In order to simulate evaporative cooling the trap must have a finite trap depth V_{trap} . This corresponds to the removal of particles with a higher potential energy than V_{trap} from the simulation at every time step. A ‘softer’ version of the trap depth where the particle has a certain probability of leaving the trap that is not simply a step function at V_{trap} has also been implemented and is discussed in Appendix A. Further description of using the simulation can also be found in Appendix A.

4.3 Accuracy

DSMC becomes a better approximation for the Boltzmann equation in the limit of small cells and short time steps [7]. However, if the number of simulation particles in a cell is too small then a non-physical bias occurs [14][15]. Here simulation particles are the particles actually being simulated by the simulation, rather than the N_{eff} real atoms they correspond to. In article [12] Alexander and Garcia recommends a minimum of 20 simulation particles per cell in order to have accurate simulated results.

For fluid simulations the edges of distributions are often the most dilute areas. For a gas in a harmonic trap the edges tend to zero particles exponentially (Equation 4). This means that the tails of the distribution, where multiple cells contain only single particles, may have been inaccurately simulated. This has increased significance for a simulation of evaporative cooling as it is the loss of atoms from these tails that drives the desired reduction in temperature.

The other criterion for accurate simulation is that the side length of the cells, l , is much smaller than the mean free path of the particles, λ [7]. This requirement was easily met by the gas being simulated as the mean free path is inversely proportional to the density:

$$\lambda = \frac{1}{\sqrt{2}\pi R^2 n}. \quad (23)$$

Normalising Equation 4 over the number of atoms, the maximum density (at $\mathbf{r} = (0, 0, 0)$) is:

$$n_{\text{peak}} = \frac{N}{\left(2\pi \frac{k_B T}{m\omega^2}\right)^{3/2}}, \quad (24)$$

Where $\omega_x = \omega_y = \omega_z = \omega$. Figure 1 shows a log plot of the mean free path against temperature for a very high density cloud. Even for such high density parameters λ is only of the order of a_{HO} at the nano Kelvin scale where the simulation is not valid as quantum effects begin to dominate.

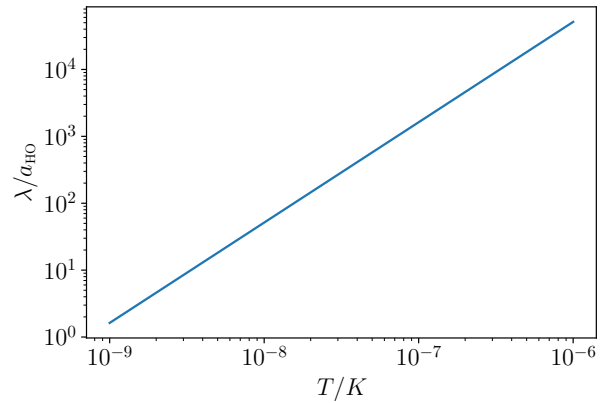


Figure 1: Log plot of the maximum mean free path in the distribution λ against temperature T . Parameters used were: number of atoms $N = 1 \times 10^9$, trapping frequency $\omega = 2\pi 100\text{Hz}$, mass of Rb87 $m = 87 \times 1.66 \times 10^{-27}\text{kg}$, radius $R = 0.014a_{\text{HO}}$. λ is in nondimensional units of a_{HO} .

5 Results

Two runs of the simulation are included here. Subsection 5.1 discusses a run to test if the simulation would thermalise and Subsection 5.2 discusses an example run simulating evaporative cooling.

5.1 Thermalisation

In order to test thermalisation of the DSMC algorithm in this simulation an infinite trapping potential was used. An out of equilibrium cloud was generated; a cubic distribution in both velocity and position space.

The simulation used 100000 simulation particles with $N_{\text{eff}} = 1$ and cells of side length $l = 5a_{\text{HO}}$. It was run for a total time of 0.2s with time steps of $1\mu\text{s}$. The trapping frequencies used were $\omega_x = \omega_y = \omega_z = \omega_{\text{HO}} = 2\pi 100\text{Hz}$. The final and initial distributions in position and velocity spaces can be seen in Figures 7, 8, 9 and 10 respectively which can be found in Appendix B.

If the simulation gas had thermalised the magnitude of its velocity would be distributed as a Maxwell-Boltzmann distribution for speed (which can be derived from Equation 5 using a change of variables from \mathbf{v} to v):

$$P(v) = \sqrt{\frac{2}{\pi}} \left(\frac{m}{k_B T} \right)^{3/2} v^2 \exp \left(-\frac{mv^2}{k_B T} \right). \quad (25)$$

Equation 25 is not in nondimensional units. Figure 2 shows a comparison between the Maxwell-Boltzmann distribution and the speed distribution of the simulation gas at the end of the simulation run. The temperature can be found from the standard deviation of the velocity distribution using Equation 5 and was found to be $T = 0.16\mu\text{K}$. The chi squared statistic was used to quantify the goodness of fit of a Maxwell-Boltzmann curve on the simulated distribution and a small chi squared of $\chi^2 = 0.017$ was found. This indicates the null hypothesis that the simulated distribution does follow a Maxwell-Boltzmann distribution is very likely.

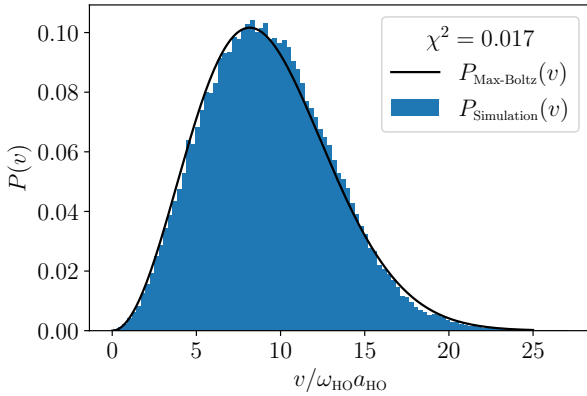


Figure 2: Maxwell-Boltzmann distribution for speed compared with distribution of simulation after 0.2s for an infinite trapping potential. The distribution has a temperature of $T = 0.16\mu\text{K}$.

5.2 Evaporative Cooling

An example of an evaporative cooling simulation run was done using an exponentially decreasing cooling ramp:

$$V_{\text{trap}}(t) = 1800 \exp \left(-\frac{t}{100} \right) + 800. \quad (26)$$

Equation 26 is in nondimensional units. The simulation used 10000 simulation particles with an $N_{\text{eff}} = 100$. The simulation was run for 1s with a time step of $10\mu\text{s}$. The trapping frequencies used were $\omega_x = \omega_y = \omega_z = \omega_{\text{HO}} = 2\pi 100\text{Hz}$. Initially the gas was a thermal cloud (based on Equations 4 and 5) at temperature $T = 1\mu\text{K}$. The number of atoms with respect to time can be seen in Figure 3 and $V_{\text{trap}}(t)$ can be seen in Figure 4. Using the velocity standard deviation of the cloud an approximation (i.e. assuming the cloud is always Gaussian) for the temperature was found from Equation 5 which is plotted against time in Figure 5. Figure 5 shows the reduction in temperature of the distribution over time due to evaporative cooling down to an approximate temperature of $0.61\mu\text{K}$.

It is important to note that while a decrease in temperature was observed this does not mean it can be said with certainty that the simulation is accurately modelling evaporative cooling. For this a comparison with experiment or a molecular dynamics simulation (which processes the result of every actual collision between simulation particles) should be performed.

6 Conclusion

A simulation of the evaporative cooling of a gas of hard spheres was created using the DSMC method. The simulation was shown to thermalise to the expected velocity distribution when in an infinite harmonic trap (Figure 25) with a cubic distribution in real and velocity space thermalising to a Gaussian one with $T = 0.16\mu\text{K}$. A simulation run of evaporative cooling was performed using an exponentially decreasing cooling ramp and the simulation gas shown to have cooled from $T = 1\mu\text{K}$ to approximately $T = 0.61\mu\text{K}$.

The next step for the simulation would certainly be to compare the cooling ramp with experiment to see how accurately the simulation is modelling reality. One of the greatest concerns with the simulation is how significant a non-physical bias is being caused at the edges of the distribution, associated with the low particle number per cell. In addition to a comparison with experiment, an

analysis of this error could be done such as in [15]. Further analysis could be performed investigating the effect of different cooling ramps, and effect of different models describing the edge of the trap (i.e. giving the particles a non-zero chance to remain in the trap even beyond V_{trap}).

The simulation could be improved using a more complicated model for collisions such as in [9]. It could also be improved by using a non-harmonic potential that more accurately describes the trapping potential used in experiment. Different trapping potential shapes could then be compared with one another. Finally, an interesting direction for the project would be to create an optimisation function that trialed different cooling ramps to find the fastest for a specified number of final atoms.

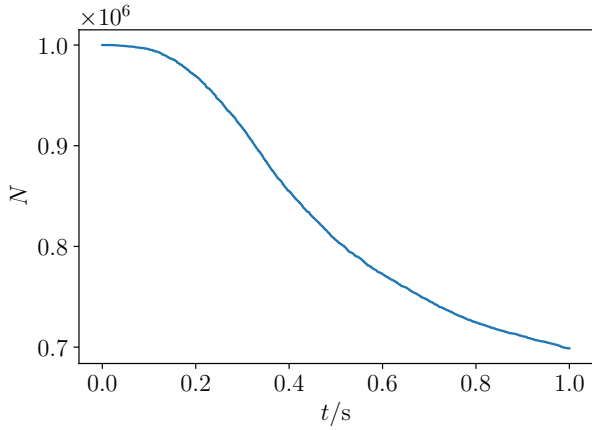


Figure 3: Plot of number of atoms N against t , in units of s, for an evaporative cooling run with an exponentially decreasing trap depth.

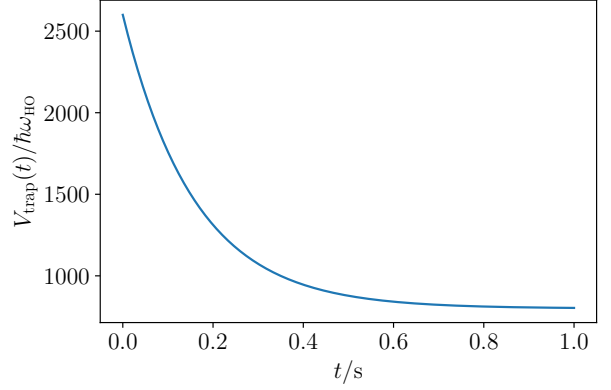


Figure 4: Plot of trap depth V_{trap} , in units of $\hbar\omega_{\text{HO}}$, against t , in units of s, for an evaporative cooling run, with an exponentially decreasing trap depth.

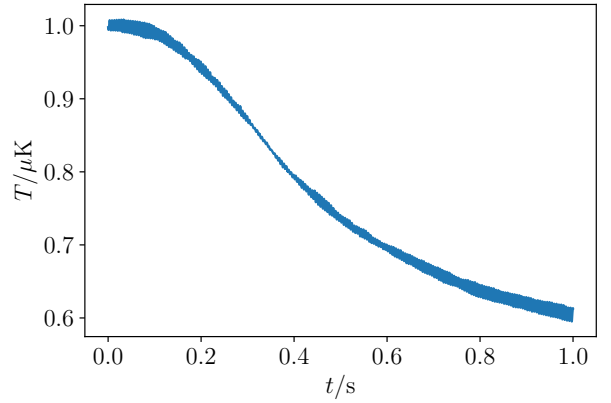


Figure 5: Plot of an approximation for temperature T , in units of μK , against t , in units of s, for an evaporative cooling run with an exponentially decreasing trap depth. T is calculated assuming the velocity distribution is Gaussian using Equation 5.

Appendix A Steps Using the Simulation

Step 1 Specify trapping frequencies ω_x , ω_y and ω_z .

Step 2 Initialise distribution of N_{sim} simulation particles using inbuilt methods. Either a thermal cloud at an inputted temperature or a cubic distribution with an inputted width.

Step 3 Run the simulation inputting: the effective number of atoms N_{eff} ; radius of the atoms R ; max relative velocity (Equation 19) $v_{r,\text{max}}$; number of iterations; length of time step in seconds Δt ; side length of a cell l ; function of trap depth with respect to time $V_{\text{trap}}(t)$ and optionally a function describing the probability of an atom escaping as function of potential energy.

Output A run would output, for every time step, the statistical standard deviations in the x , y and z directions for velocity and position; the number of atoms and an approximation for the temperature based on the assumption that the distribution is described well by Equation 5. Additionally a series of snapshots (the number being specified before the run) could be taken of the full distribution over the run.

Plotting The output arrays could be directly plotted or the distributions plotted using an inbuilt function.

The default for a run was a hard cut off at V_{trap} but the simulation could instead be provided a probability as a function of potential that a particle would escape the trap. For example instead of a step function at the trap height a function like:

$$P(V) = \frac{1}{e^{A(V_{\text{trap}} - V)} + 1}, \quad (27)$$

Could be used, (see Figure 6). This would mean a small chance a particle close but below the trap depth could escape the trap, and a small chance the particle could remain trapped beyond the trap depth. This is likely a more realistic view of the edge of the trapping potential.

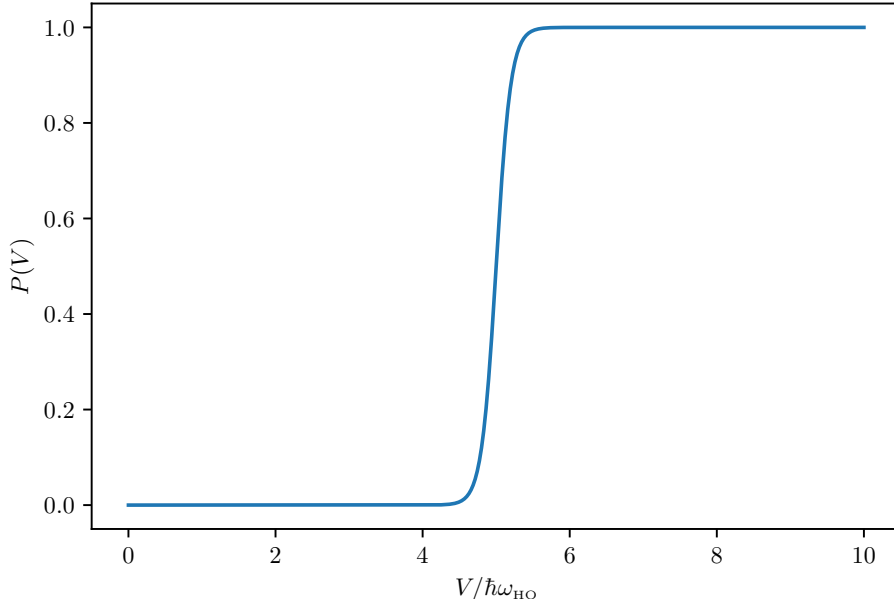


Figure 6: Plot of Equation 27 for $A = 10$, $V_{\text{trap}} = 5$, showing an alternative probability distribution for escaping the trap.

Appendix B Thermalisation Run Figures

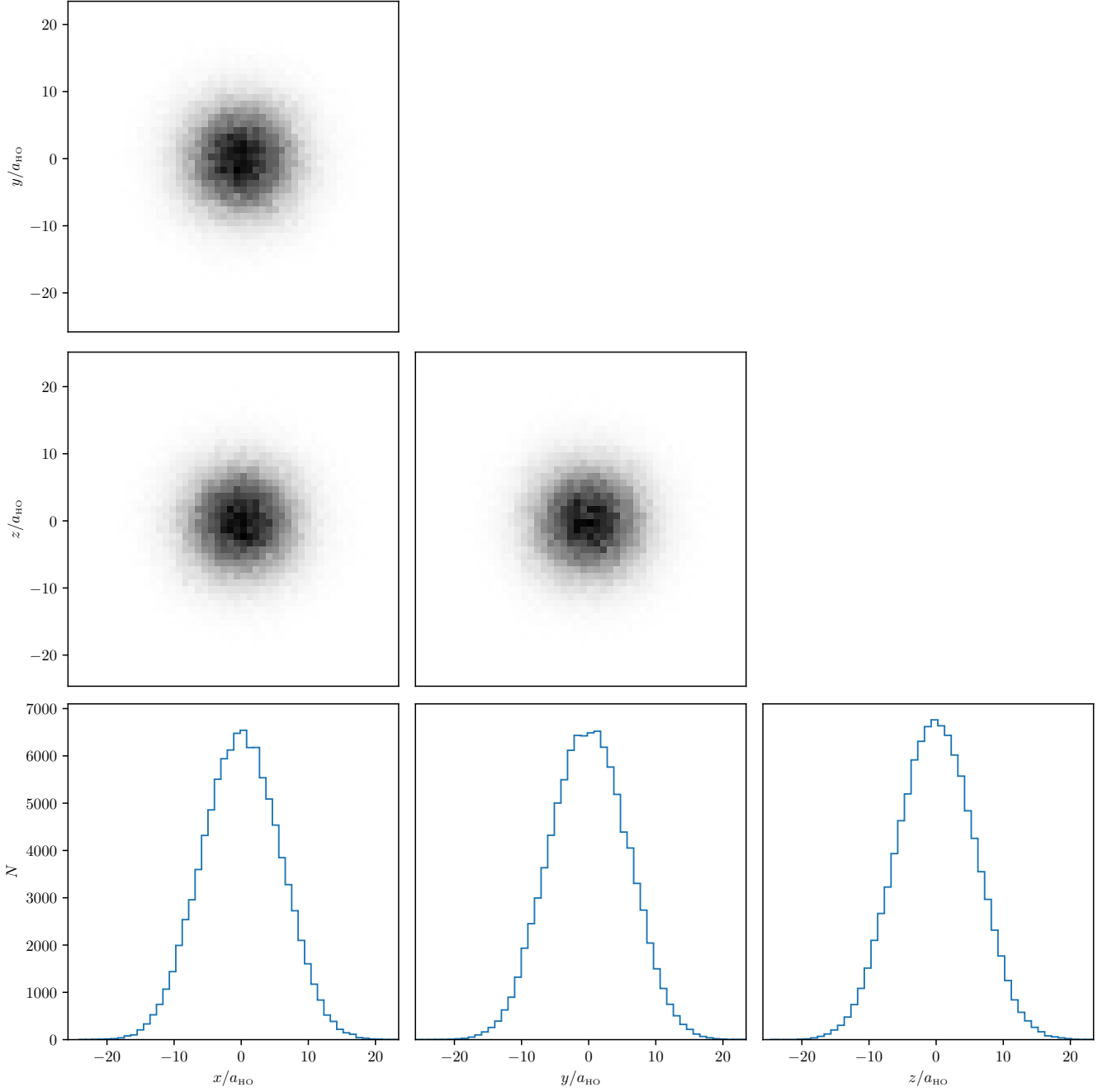


Figure 7: Corner plot of the final (after 20ms) real space distribution for a simulation run testing the thermalisation of the simulation gas using an infinite trapping potential.

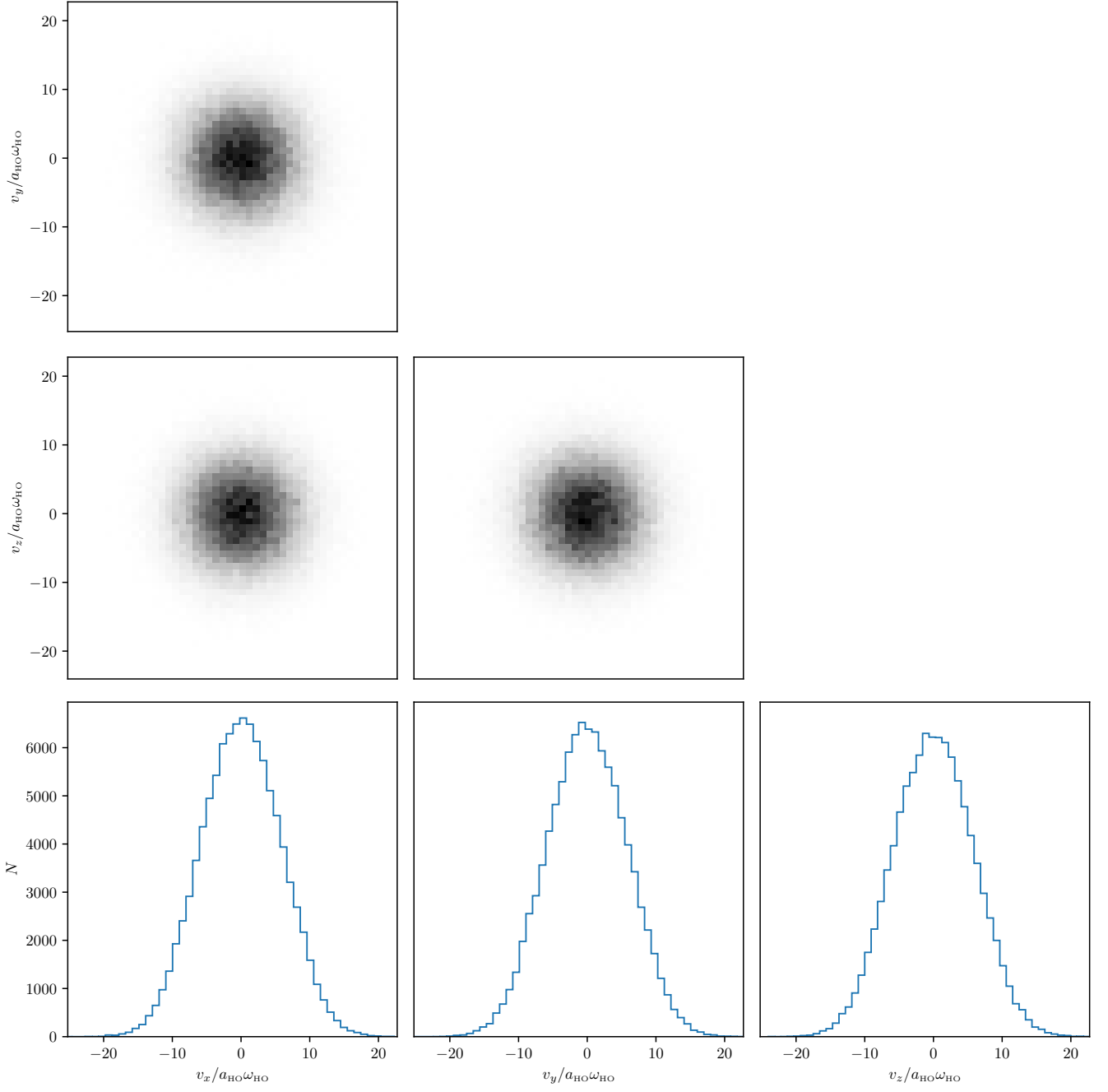


Figure 8: Corner plot of the final (after 20ms) velocity space distribution for a simulation run testing the thermalisation of the simulation gas using an infinite trapping potential.

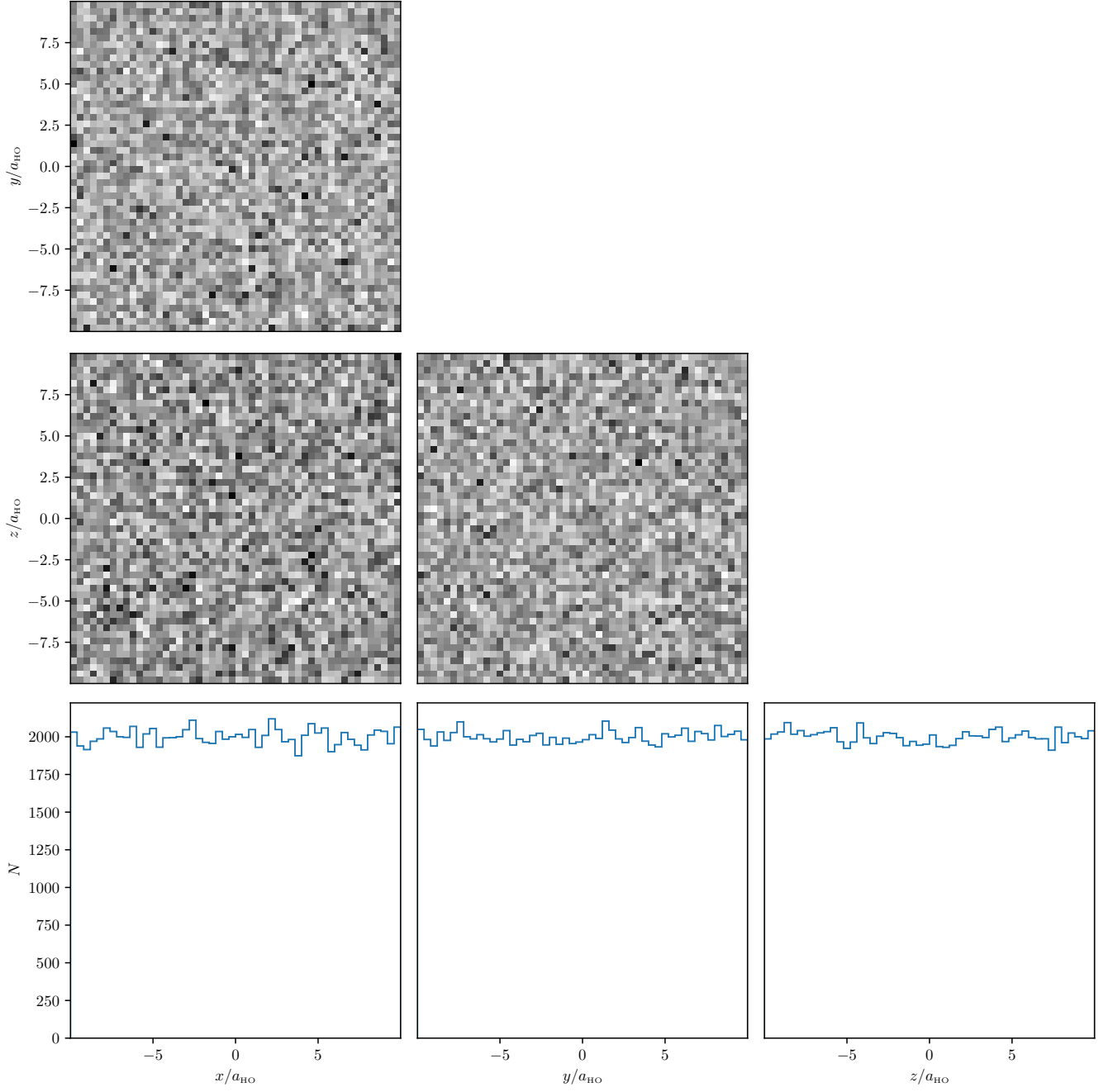


Figure 9: Corner plot of the initial real space distribution for a simulation run testing the thermalisation of the simulation gas. Initial distribution is a cube of side length $20a_{\text{HO}}$.

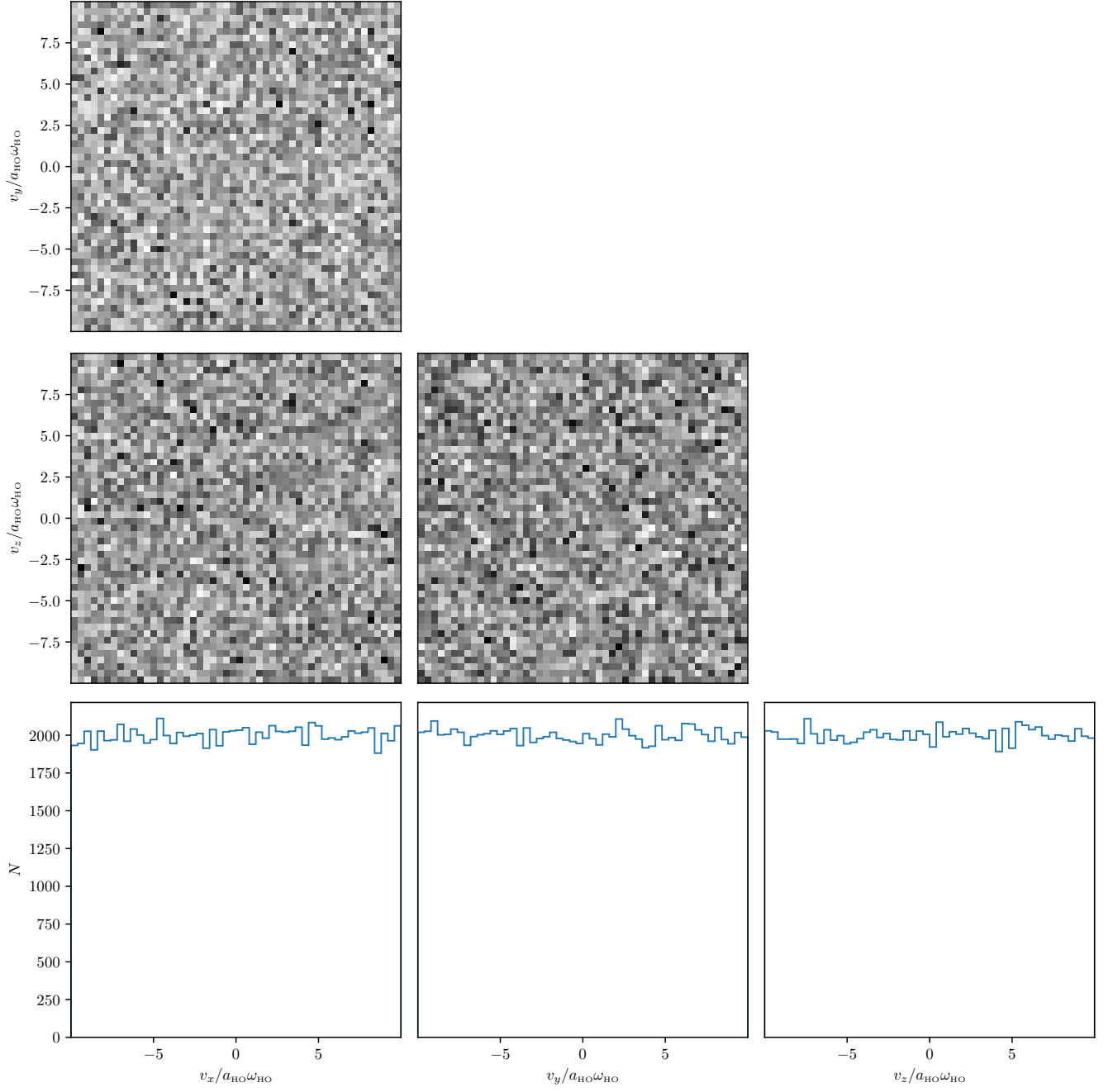


Figure 10: Corner plot of the initial velocity space distribution for a simulation run testing the thermalisation of the simulation gas. Initial distribution is a cube of side length $20a_{\text{HO}}\omega_{\text{HO}}$.

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