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antiprotons using SIMBUCA

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*“We saw brilliance, when the world, was asleep.
There are things that we can have, but can’t keep”¹*

¹Chester Bennington, 2017.

Abstract

This thesis summarises my tasks and efforts during the Technical Student Programme at CERN in 2016/17. First, the main experiment Aegis and its theoretical background are introduced. Aegis is located at CERN's Antiproton Decelerator (AD) and its main scientific goal is to measure Earth's gravitational acceleration on antihydrogen. To enhance the accuracy of this gravitational acceleration measurement a doubly sympathetic cooling scheme was proposed by Michael Doser (CERN) and Alban Kellerbauer (University of Heidelberg), involving antiprotons, a cationic and an anionic species, which are simultaneously confined in a penning trap, with only one actively cooled (cationic) species. The focus of this thesis lies on testing the functionality of this doubly sympathetic cooling scheme using a penning trap simulation program called Simbuca, which calculates the coulomb force on a GPU, what reduces the simulation times significant. Besides, the theoretical physical background is presented, which is necessary to follow the subsequent simulations. The performed Simbuca-simulations are analysed in detail and the behaviour of the trapped, charged particles is described. Furthermore, although a sympathetic cooling effect between the oppositely charged particles was clearly observed, the functionality of the proposed scheme could only be confirmed with severe limitations.

Zusammenfassung

Diese Arbeit fasst meine Tätigkeiten und Bemühungen, während des Technical Student Programm's in 2016/17 am CERN zusammen. Zunächst erfolgt eine Beschreibung des Hauptexperiments Aegis, sowie dessen theoretischer Hintergrund. Aegis ist eines der Experimente, die um den Antiprotonen-Entschleuniger (Antiproton Decelerator) am CERN gebaut sind. Das vorwiegende wissenschaftliche Ziel von Aegis ist eine Messung der Fallbeschleunigung von Anti-Wasserstoff im Gravitationsfeld der Erde. Um die Genauigkeit dieser Gravitationsbeschleunigungsmessung zu verbessern, wurde von Michael Doser (CERN) und Alban Kellerbauer (Universität Heidelberg) ein doppelt sympathisches Kühlungsschema vorgeschlagen, bei dem Antiprotonen, eine kationische und eine anionische Spezies, gleichzeitig in einer Penningfalle eingeschlossen sind, wobei nur die kationische Spezies aktiv gekühlt wird. Der Fokus dieser Arbeit liegt auf der Überprüfung der Funktionalität dieses doppelt sympathischen Kühlungsschemas unter Verwendung eines Penningfallen-Simulationsprogramms namens Simbuca, das die Coulomb-Kraft auf einer GPU berechnet, was die Simulationszeiten signifikant reduziert. Außerdem wird der physikalische Hintergrund vorgestellt, der notwendig ist, um den nachfolgenden Simulationen folgen zu können. Die durchgeführten Simbuca-Simulationen werden im Detail analysiert und das Verhalten der geladenen Teilchen in der Penning-Falle beschrieben. Darüber hinaus wurde ein sympathetischer Kühleffekt zwischen den entgegengesetzt geladenen Teilchen eindeutig beobachtet, allerdings konnte die Funktionalität des vorgeschlagenen Schemas nur mit starken Einschränkungen nachgewiesen werden.

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1 Introduction

This thesis summarizes my work and efforts accomplished during the technical student programme 2016 at the $AE\bar{g}IS$ experiment located at CERN.

The focus of this thesis lies on my simulations, testing a doubly sympathetic cooling scheme for antiprotons with the penning trap simulation programme Simbuca. The goal of this new scheme was to surpass the 100 mK temperature-limit for the produced antihydrogen, which is needed for an actual sign measurement of $\bar{g}$ (the gravitational acceleration on antihydrogen). To accomplish this, an actively cooled species is needed, which cools the antiprotons sympathetically. What makes this sympathetic cooling scheme unique is that it involves three charged particle species (antiprotons, anions and cations), which are simultaneously confined in a penning trap sympathetically cooling each other, whereby the cationic species is actively cooled by a laser-system. The primary goal of my simulations was to observe a sympathetic cooling-effect between the three species. The first two sections will give an overview over the main-experiment $AE\bar{g}IS$ and its theoretical background. In the next three sections, all theoretical facts and information regarding the Simbuca-simulations are given. In the following, an overview over the respective main sections is given.

In section 2 the theoretical background of the $AE\bar{g}IS$ experiment is outlined. Antimatter and some of its important features are introduced. Then, the WEP and CPT-symmetry are briefly theoretically discussed to point out why the experiments performed at $AE\bar{g}IS$ are of importance and to give a better understanding of what they aim to test.

Section 3 shows the $AE\bar{g}IS$ -experiment in detail and explains the different experimental steps, which finally lead to the production of antihydrogen, which is the final test object for all subsequent experiments and tests (like WEP or CPT-symmetry).

The next section 4 contains some theoretical information about the behavior and characteristics of particles confined in a penning trap. This section is of importance since it provides some of the essential physics background, for the main part of the thesis - the Simbuca simulations to test the doubly sympathetic cooling scheme with different particle species simultaneously confined in a penning trap.

Section 5 introduces the simulation program Simbuca and explains why this program is so well adjusted for the penning trap simulations performed. It contains some information over the scheme and techniques implemented and gives some insight into the hierarchy of the code with its sub-programmes.

All the basic and fundamental ideas behind the doubly sympathetic cooling scheme as well as the physical processes that might arise but should be avoided can be found in section 6. This section contains in a way the 'starting-point know-how' at the beginning of my simulations and tests.

The main part of the thesis (section 7) contains amongst other things a brief introduction of the visualization of the data outputted by Simbuca with Wolfram Math-

ematica, as well as the input preparation for Simbuca (also done with Mathematica). Most importantly besides some general tests, which are analysed to learn about the behaviour and interaction of the charged particles in the penning trap, the final simulations are shown, where indeed sympathetic cooling could be registered and the general functionality of the doubly sympathetic cooling scheme could be confirmed (at least to a certain extent). This section includes also a very detailed analysis of individual particles, which was done to draw conclusions regarding the interaction of the different species and the general functionality of the proposed cooling scheme.

Last but not least a summary of the most important conclusions and achievements and an outlook for further tests respectively the general functionality of the scheme is given in section 8.

2 Antimatter - Theoretical background

2.1 Dirac's equation and the postulation of antimatter

The Dirac equation was discovered by the British physicist Paul Dirac in 1927 [1]. This relativistic wave equation not only satisfies the principles of quantum mechanics (as its non-relativistic predecessor the Schrödinger equation), it also is consistent with the principles of special relativity. The Dirac equation is valid for massive spin- $\frac{1}{2}$ particles such as electrons and it was validated and investigated extensively for the hydrogen spectrum and its fine structure. Anyway, since there are not only positive but also negative energy solutions for the Dirac equation, it also predicts a new kind of matter (called antimatter) for every massive spin- $\frac{1}{2}$ particle and indeed in 1931 C. Anderson discovered the *positron*, the positively charged twin-particle of the electron.

In the following section a brief derivation of Dirac's equation is shown, starting by replacing the classical energy E and momentum-vector $\mathbf{p}$ by their quantum mechanical operators which will act on the wavefunction Ψ :

$$\mathbf{p} \rightarrow -i\hbar\nabla \quad \text{and} \quad E \rightarrow i\hbar\frac{\partial}{\partial t} \quad (2.1)$$

It is convenient to introduce four-vectors to simplify the notation:

$$p^\mu = \left(\frac{E}{c}, p_x, p_y, p_z\right) \quad (2.2)$$

where the relativistic energy-momentum relation can be represented by

$$p_\mu p^\mu = \frac{E^2}{c^2} - \mathbf{p}^2 = m^2 c^2 \quad (2.3)$$

The relations in (2.1) can be rewritten in four vector representation as

$$p_\mu \rightarrow i\hbar\partial_\mu \quad (2.4)$$

where

$$\partial_\mu \equiv \frac{\partial}{\partial x^\mu} \quad (2.5)$$

which means

$$\partial_0 = \frac{1}{c} \frac{\partial}{\partial t} \quad , \quad \partial_1 = \frac{\partial}{\partial x} \quad , \quad \partial_2 = \frac{\partial}{\partial y} \quad , \quad \partial_3 = \frac{\partial}{\partial z} \quad (2.6)$$

By inserting these operator in the relativistic energy-momentum relation one finds the Klein-Gordon equation:

$$-\hbar^2 \partial^\mu \partial_\mu \Psi - m^2 c^2 \Psi = 0 \quad (2.7)$$

or

$$-\frac{1}{c^2} \frac{\partial^2 \Psi}{\partial t^2} + \nabla^2 \Psi = \left(\frac{mc}{\hbar}\right)^2 \Psi \quad (2.8)$$

The Klein-Gordon equation is second order in time and is valid for particles with spin 0. Besides, this equation is incompatible with Born's statistical interpretation of the wavefunction, which states that $|\Psi(\mathbf{r})|^2$ is proportional to the probability of finding

the particle at a certain point $\mathbf{r}$. This problem arises from the fact that the equation is second order in time. Thus, Dirac tried to find an equation which is compatible with the relativistic energy momentum relation and yet first order in time. So Dirac factorized the equation in the following way:

$$(p^\mu p_\mu - m^2 c^2) = (\beta^\kappa p_\kappa + mc)(\gamma^\lambda p_\lambda - mc) \quad (2.9)$$

where β^κ and γ^λ are eight coefficients which had to be cleverly chosen and indeed due to Dirac's brilliant idea to assign matrices instead of a number to the γ 's and to choose $\beta^\kappa = \gamma^\kappa$ to avoid terms linear in p_κ , he found

$$(p^\mu p_\mu - m^2 c^2) = (\gamma^\kappa p_\kappa + mc)(\gamma^\lambda p_\lambda - mc) = 0, \quad (2.10)$$

where

$$\gamma^0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \gamma^i = \begin{pmatrix} 0 & \sigma^i \\ -\sigma^i & 0 \end{pmatrix}. \quad (2.11)$$

σ^i ($i = 1, 2, 3$) are the Pauli matrices, 1 represents the 2×2 unit matrix and 0 a 2×2 matrix where all elements are 0. The Dirac equation can be obtained by taking one of the terms of (2.10). The conventional choice is given by

$$(\gamma^\lambda p_\lambda - mc) \quad (2.12)$$

Thus the Dirac equation finally can be derived by substituting the relation (2.4) and let the the equation act on a wavefunction ¹

$$i\hbar\gamma^\mu\partial_\mu\Psi - mc\Psi = 0 \quad (2.13)$$

A detailed analysis of the solution of (2.13) results in the interpretation that the four components are the wavefunctions of spin up and spin down particles respectively antiparticles. Besides, it also can be shown that particles and their respective antiparticles have the same masses and also the same spin, but all internal quantum numbers are inverted, as is the electrical charge [2, 3].

2.2 Testing the WEP and CPT-Symmetry with antimatter

2.2.1 The Weak Equivalence Principle and tests

The weak equivalence principle (WEP) state the universality of the free fall. In other words, all objects in a uniform gravitational field fall with exactly the same acceleration independently of their composition. This means that the inertial mass m_i (which is a measure for an object's resistance to the acceleration by an external force) and the gravitational mass m_g (which measures the gravitational force exerted by or on an object) are completely identical. The strong equivalence principle extends the WEP also for objects which are bound by gravitation, like astronomical objects. The WEP has been tested very accurately with 'ordinary' matter for distances of microscopic to astronomical length scales. The precision of these tests is often given by the Eötvös parameter, which gives a measure to which extend the free fall accelerations g_1 and g_2 are equal for two test masses m_1 and m_2 :

¹it is important to note that Ψ is now a four element column matrix called 'Dirac spinor'

$$\eta_{1,2} = \frac{g_1 - g_2}{(g_1 + g_2)/2} \quad (2.14)$$

For ordinary matter, precisions for the Eötvös parameter between several pairs of elements at the order of 10^{-13} were achieved. Since gravity is described by general relativity (which is a classical theory) it does not include a model for the existence of antimatter [4].

Theoretical physicists focused on two broad classes of possibilities out of which an asymmetry between matter and antimatter could arise and were able to establish bounds on this eventual asymmetries with the help of precision Eötvös experiments, which were performed with ordinary matter.

The first possibility leads to the fact that fundamental principles of general relativity and quantum field theory are violated and a theoretical formulation has to be found, which derives this asymmetries in a consistent way. In that case, antimatter just behaves differently under gravity than ordinary matter. To establish a bound for this kind of violation, contributions to the inertial masses of atoms were considered, since there are processes in perturbative QED which contribute to the inertial mass of particles, like vacuum polarization effects and the antiquark content of nucleons. Thus, these processes encode the presence of antimatter. For both cases, it can be estimated to which degree these kind of contributions are needed to satisfy the equivalence principle. Followed by the assumption that that any asymmetry respectively deviation of g_H (gravitational acceleration on hydrogen) from $g_{\bar{H}}$ (gravitational acceleration on antihydrogen) would be a violation of the equivalence principle for these contributions at the same level. In this way, the precision Eötvös experiments can be used to establish bounds on $|g_H - g_{\bar{H}}|/g_H$.

The second possibility to explain this eventual asymmetry is to introduce a new long range forces of gravitational strength mediated by scalar and/or vector particles. This 'fifth force' could have been not yet spotted in the previous matter-matter experiments because it could be many orders weaker than gravity or another possibility is that the force contribution could be cancelled due to the matter-matter interaction but seen for matter-antimatter interactions. [5, 6, 7]

The essential point is that the eventual asymmetry of the free fall of matter respectively antimatter in the gravitational field, can be constrained by precision Eötvös experiments, due to the compositeness of atoms and the nature of scalar and vector interactions. This bound could be estimated to be less than 10^{-7} [5].

One should notice, that the argument that gravity has an impact on virtual particles is though strongly questioned by the cosmological constant problem. Since there should also be a coupling between gravity and the virtual particles and antiparticles that constitute to the vacuum energy (vacuum fluctuations), what in turn would result in a deviation of 120 order of the cosmological constant [6].

2.2.2 CPT-Symmetry and Tests with Antimatter

Symmetries play an important role with respect to the laws of physics and of nature. Mathematically, a symmetry is found, if the laws of physics are invariant with respect to a respective symmetry transformation. In a physical experiment a symmetry suggests that something is conserved respectively remains constant, during the experiment. So conservation laws and symmetries are strongly connected, since to every symmetry of nature corresponds a conserved current, which is also known as Noether-Theorem.

In general, we distinguish between continuous and discrete symmetries. The invariance of a system under a continuous symmetry transformation leads to a conservation law, like the invariance under space and time translations results in momentum and energy conservation. Discrete symmetries are also a topic of interest in modern particle physics, especially three of them play a fundamental role:

- charge conjugation, C: an operation which converts each particle into its antiparticle $\rightarrow C|p\rangle = |\bar{p}\rangle$, by changing the sign of all internal quantum numbers of a particle state $|p\rangle$, while motion and spin stays unaffected.
- Parity, P: a transformation which performs a reflection of the coordinates in space (but not in time) at the origin $\rightarrow (\vec{r} \rightarrow -\vec{r})$. This leads to a change of sign for the position and momentum, while spin of the particle is unchanged.
- Time reversal, T: an operation which replaces the time coordinate t by $-t$. Here also the spin changes its sign, additionally momentum, velocity and angular momentum.

These discrete symmetries do individually usually, but not always hold. Thus, also composed symmetries were investigated like CP or CPT, where the operations are performed after each other. For a long time physicists thought that CP was an exact symmetry, but its violation was found in 1964 in the neutral kaon system. Until now, the combination of all three operations CPT still holds as a symmetry and its tests are a field of recent investigations and experiments [2, 8, 9].

The CPT theorem is one of the deepest results of quantum field theory and it is based only on the most general assumptions like Lorentz invariance, quantum mechanics and the interpretation that interactions are represented by fields. It states that the combined CPT operation (here the order of the individual operators is irrelevant), applied on a particle state is an exact symmetry of any interaction. More importantly, it is simply impossible to build up a quantum field theory one the principles mentioned before in which CPT is not conserved. The CPT theorem also implies that inertial masses of particles and antiparticles, the lifetimes and the energy levels are identical.

Many precision tests of Lorentz and CPT symmetry have already been performed in atomic systems, where the predominant interactions are described by quantum electrodynamics. An examples is, the Hughes-Drever type experiments, which compare two clocks or high-precision magnetometers tested with different atomic species. Another example are tests with leptons and baryons confined in Penning traps. These experiments measure the g -factor (a dimensionless quantity that characterizes the magnetic moment and gyromagnetic ratio of a particle) of e.g. electrons and positrons and obtain a bound on the g -factor difference to a precision of 2×10^{-12} .

A special interest CPT symmetry-tests arises since CPT-violation could be a clear evidence for physics beyond the standard model. The standard model can be extended

into a more general theory (SME), where Lorentz and CPT symmetry can be spontaneously broken [10]. Thus, SME allows CPT and Lorentz violations and it is based on an argument that any CPT-violating interaction must manifest itself by a term in the Dirac equation that has the dimension of mass or energy. This theory is used to study how effects of eventual violations could show up in, for example $\bar{H}$ experiments.

While testing CPT in the frame of SME, the highest sensitivity can be obtained by reaching the highest precision in terms of absolute energy. Besides SME is the only model that allows a comparison of CPT tests in different systems. Until now, the measured mass difference between the neutral kaon and antikaon is often referred to as most significant test of CPT since a relative precision of 6×10^{-19} could be achieved. The antihydrogen hyperfine transitions could be a major sensitive test for CPT violations, see figure 1. [10, 11]

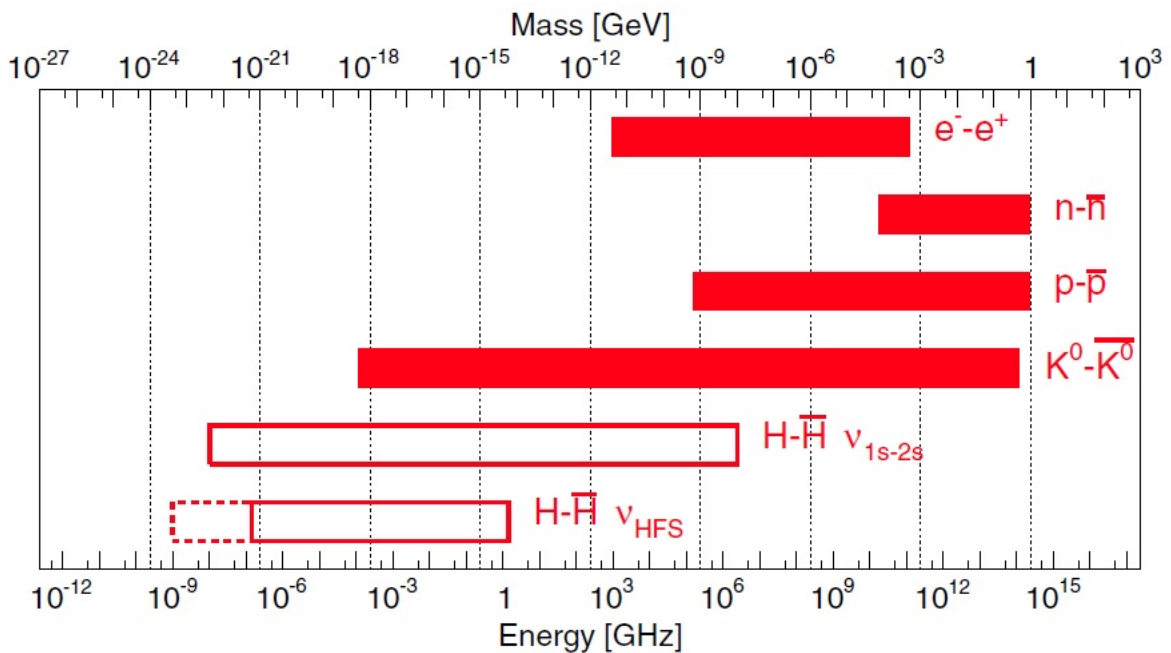


Figure 1: Precisions of different CPT-tests. Here the right end of the bar represents the absolute value of the measured quantity, the length the relative precision and the left end of the bar the sensitivity on an absolute scale. In comparison are the masses of different elementary particles, the transitions in antihydrogen (1S-2S and hyperfine). The dashed shows the limit theoretically reachable in an atomic fountain experiment, [13].

There are two compelling reasons to compare antihydrogen and hydrogen measurements to achieve most sensitive CPT symmetry tests. First, antihydrogen is the simplest atom consisting entirely of antimatter and second, its matter-counterpart is the most precisely measured and investigated atom until now.

The laser spectroscopy of the 1S-2S transition of antihydrogen is dominated by the electromagnetic interaction and the energy levels are in first order sensitive to the well known positron mass. The HFS of the antihydrogen on the other side, is caused by the spin-spin interaction and since correction terms arise from the finite antiproton charge and magnetic radius play the comparison between hydrogen and antihydrogen is at a precision of 10^{-5} also sensitive to eventual difference in the structure

of protons and antiprotons caused by the strong-interaction. [12, 13]

3 AEGIS

The Antihydrogen Experiment: Gravity, Interferometry, Spectroscopy (AEGIS) is located at CERN's Antiproton decelerator (AD). Its primary scientific goal is to measure the gravitational acceleration of antihydrogen at a precision of 1 % and therefore to test the WEP with antimatter. Additionally as a long term goal, the AEGIS collaboration aims to test the CPT symmetry by measuring the ground state hyperfine splitting of antihydrogen. An overview of the different steps which lead to antihydrogen-production, the experimental setup and the gravitation measurement with antihydrogen is given in the next subsections.

3.1 The Antiproton decelerator - Antiproton production

The Proton Synchrotron (PS), one of the pre-accelerators of CERN's Large Hadron Collider (LHC) is the starting point for producing the $\bar{p}$'s used in the experiments connected to the AD. The high energetic protons (26 GeV) are fired into a block of metal, where they interact with the nucleus of the metal atom (Cu, Ir), producing a proton-antiproton pair through pair creation. The $\bar{p}$'s are guided by magnets towards the AD-beamline where they get decelerated by stochastic cooling and electron cooling. Then, the $\bar{p}$'s with energies at 5.3 MeV are guided through titanium degrader foils before they are lead towards the AEGIS beamline and the antiproton traps [14].

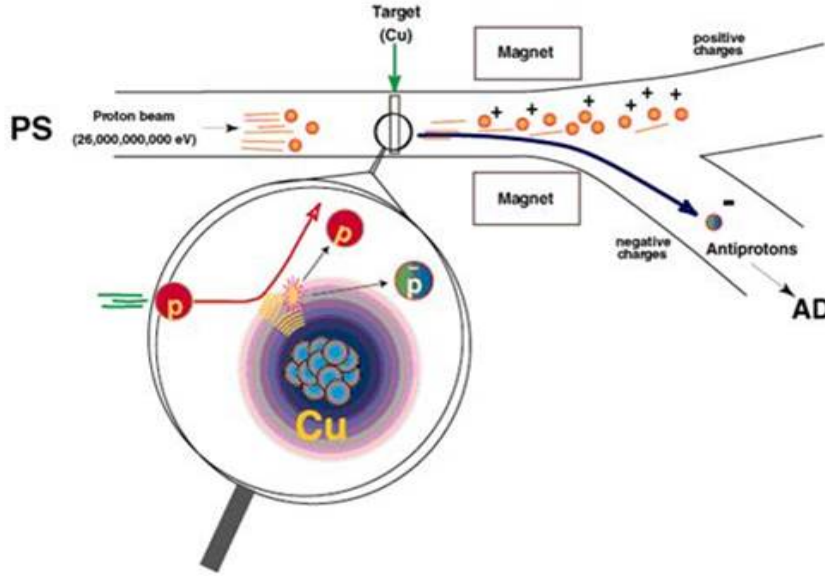


Figure 2: $\bar{p}$ -production at the AD, Source: Landua, R. CERN.

3.2 Antihydrogen production

The Aegis collaboration aims to produce cold antihydrogen via "Resonant Charge Exchange". For this, the antiprotons are electron cooled separately to the temperature of the cryogenic environment. Then, the highly excited positronium ($n_{PS^*} = 18 - 25$) mixes with the ultracold antiprotons forming Rydberg antihydrogen ($\bar{H}^*$).



Subsequently the $\bar{\text{H}}^*$ -atoms are stark accelerated toward the deflectormeter and the detector using electric field gradients, as shown in figure 3.

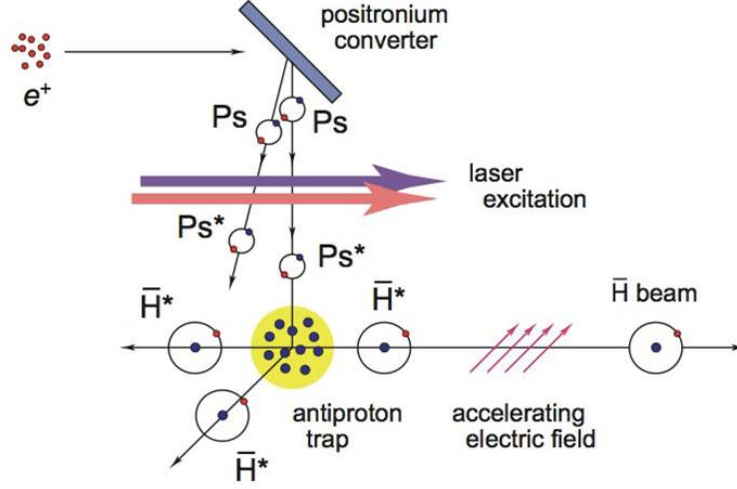


Figure 3: Antihydrogen-production through resonant charge exchange, [16].

In the next sections a more detailed view into the production of antihydrogen is given, from the catching and cooling of the antiprotons to the positronium formation and excitation. The content is mainly based on [7, 15, 17].

3.2.1 Catching and cooling of antiprotons

The $\bar{p}$'s from the AD are caught by a Penning-Malmberg trap, which uses a superconducting solenoid magnet, producing a magnetic field of 5 T and high voltage electrodes which are tunable up to 20 kV, what corresponds to the highest kinetic energy of the $\bar{p}$'s eventually captured in the trap. While catching the antiprotons in the 5 T Penning-Malmberg trap they are mixed with electrons. Since electrons emit cyclotron radiation which reduces their kinetic energy efficiently, they are able to cool $\bar{p}$'s through collisions down to kinetic energies of some eV. For antiprotons, this effect of emitting cyclotron radiation is negligible since their mass is much heavier.

Additionally to cooling the $\bar{p}$'s with electrons a technique called the 'rotating wall' is used to compress the plasma radially by applying a rotating electric field. After the cooling process the electrons are kicked out of the trap by applying short voltage pulses which do not significantly effect the $\bar{p}$'s since they are much heavier.

Then, the cold and compressed plasma is led to a second Penning-Malmberg trap where the production of antihydrogen takes place. A smaller magnetic field increases the efficiency of cyclotron cooling since the plasma is less magnetised, therefore the magnetic field of the second trap is chosen to be 1 T. In the 1 T trap the plasma is again cooled through cyclotron radiation and radially compressed using the rotating wall and Sideband cooling. To reach the desired $\bar{p}$ -temperature of 100 mK, which is needed for a measurement of the gravitational free fall of antihydrogen at a precision of 1 %, a dilution refrigerator can be used to lower the temperature of the walls of the 1 T trap down to 100 mK. Additionally, Resistive cooling can be applied. Here a RLC circuit is connected to two of the traps ring electrodes, so that the axial motion of the

ions/electrons induces a current in the circuit. So the ions/electrons kinetic energy (in axial direction) is reduced since it is absorbed by the resistor, while the resistor is heated in the process. [18]

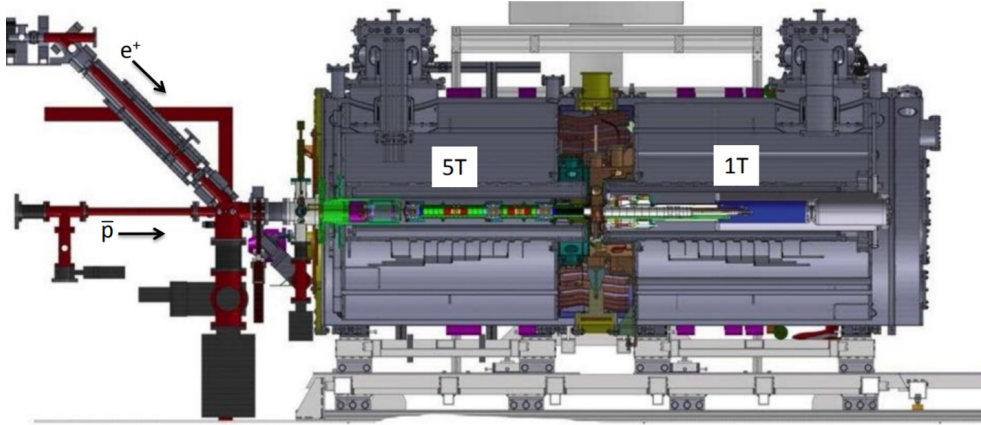


Figure 4: Sketch of the 1 T and 5 T magnets and the Penning-Malmberg traps at the Aegis experiment, [19].

3.2.2 Positronium production and excitation

The positrons (e^+ 's) for the Positronium (Ps) production are produced through a ^{22}Na source with an activity of 50 mCi. The fast isotropically emitted e^+ 's are slowed down by a solid Ne moderator to energies of several eV. Then, the e^+ 's are led by a magnetic field into a Surko-type trap with three stages. Inside the Surko-trap, the (e^+ 's) are cooled by collisions with N_2 molecules and in the following, get trapped in the third stage of the system in less than 1 ms. In this potential minimum at stage three the gas pressure of the N_2 molecules has a minimum in order to avoid that the electrons gain kinetic energy through collisions [15, 20, 21].

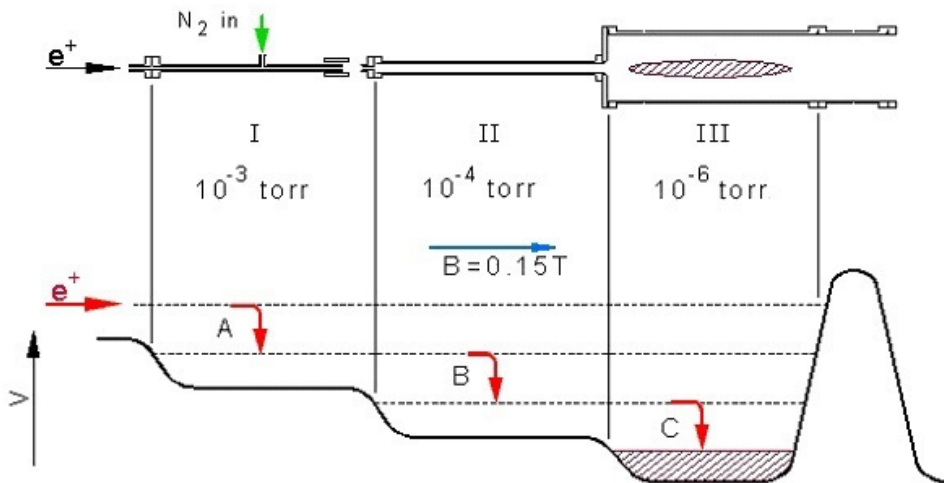


Figure 5: Positron-System, sketch of the system and electric potential, [21].

After catching and cooling the e^+ 's, the nitrogen is pumped out of the trap and the

positrons are guided towards the 5 T trap. In the 5 T region the positrons loose kinetic energy through cyclotron radiation and cool themselves to the temperature of the trap surface (around 4 K). After crossing the 5 T region the e^+ 's reach the 1 T region, where they get accelerated by some kV and shot against a nanoporous silica material, which is as a efficient e^+ /Ps-converter. The positrons are scattered by atoms and electrons of the converter material and therefore slowed down to eV energies within ps. Then, the slow positrons bind themselves either to bound electrons or electrons which were released in prior collisions.

The Ps which accumulates in the pores of the converter material repeatedly bounces off the cavity walls in the pores and thermalize with the material. Therefore, the temperature of the produced Ps depends on the temperature of the converter material. There are two constrain for the optimal Ps temperature. First, the Ps should have enough kinetic energy to leave the pores in the ground state and reach the laser system before the exotic atom decays. Second, the cross section of antihydrogen formation reaches a maximum, if the center of mass velocity of the positronium-antiproton system is close to the orbital velocity of the positron inside the positronium. Out of these two constraints a Ps temperature of 100 K to 150 K and therefore a poresize of 12 nm is favorable.

The ground state positronium is produced in two different states, which occur with an equally large probability. First, there is the singlet state (also called para-Positronium) with antiparallel spins of the components (what means spin 0 for the Ps) and a lifetime of 125 ps. Secondly, the exotic atoms can be formed in a triplet state (ortho-Positronium), with parallel spins of the components, what means that the atom has spin 1 and a longer lifetime of 142 ns. The lifetime of the para-Ps is in general too short to reach the laser system and to get excited before decaying (respectively self-annihilating), mainly into two γ 's at 511 keV. Since the ortho-Ps on the other side annihilate into three γ 's or more (with a total energy of $2 \cdot 511$ keV), it has a long enough lifetime to perform laser excitation.

The excitation of the positronium to a Rydbergstate is implemented primarily because the cross section for antihydrogen formation via 3-body interaction with Ps is proportional to n^4 , where n denotes the principal quantum number. Besides, another reason is that the lifetime of the excited state Ps is longer than the ground state lifetime. The laser excitation is performed in two steps. First the Ps will be excited from the $n = 1$ to the $n = 3$ ($\lambda = 270$ nm) state, followed by a second excitation from $n = 3$ to $n = 35$ ($\lambda = 1650$ nm–1700 nm). The excitation is performed in two steps, since there is no laser commercially available ($\lambda = 180$ nm) to perform the direct excitation from $n = 1$ to $n = 35$. Besides, the middle step $n = 3$ is chosen because the lifetime of this state is longer than the lifetime of the $n = 2$ state.

3.2.3 Antihydrogen production and acceleration

Simulations of the charge-exchange process show that the mean value of the principal quantum number of the antihydrogen atoms ($n_{\bar{H}}$) and the Ps principal quantum number are related by $n_{\bar{H}} \approx \sqrt{2}n_{Ps^*}$.

When the Rydberg excited positronium enters the Penning trap with the cold antiprotons through a 90 % transparent grid it binds to antihydrogen via resonant charge exchange. Since $\bar{H}$ is a neutral atom it will leave the trap in all directions with velocities from 25 to 80 m/s and is stark accelerated towards the deflectometer and the detection zone. For the stark acceleration an electric field gradient is used which exerts

a force on the electric dipole moment of the anti-atom. Since the dipole moment scales with the square of the principal quantum number, highly excited Rydberg atoms are required. With this method, a horizontal beam of $\bar{\text{H}}$ atoms with a velocity of around 400 m/s^{-1} will be guided towards the experimental section.

3.3 Gravitation measurement and Moiré deflectometer

For the free fall measurement of the $\bar{\text{H}}$ -beam, a Moiré-deflectometer is used. Like shown in figure 6, a Moiré-deflectometer consists out of three plates, which are placed at an equally distance L (25 mm) from each other. There are two identical gratings with a periodicity of $40 \mu\text{m}$ and a position sensitive emulsion detector. The following text is mainly based on [22, 23].

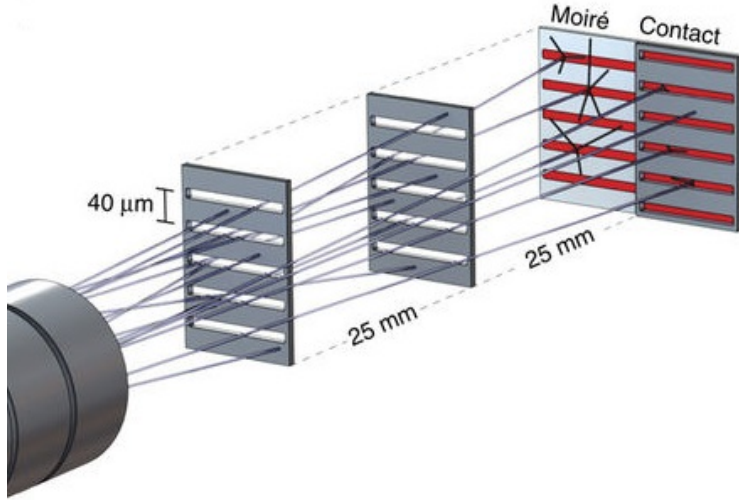


Figure 6: Moiré deflectometer used for the free fall measurement, [22].

With a de-Broglie wavelength of about 1 nm at 400 m/s the $\bar{\text{H}}$ s behave like classical particles. The shadow of the particles on the position sensitive detector forms the slit positions with a vertical shift because of the gravitational force.

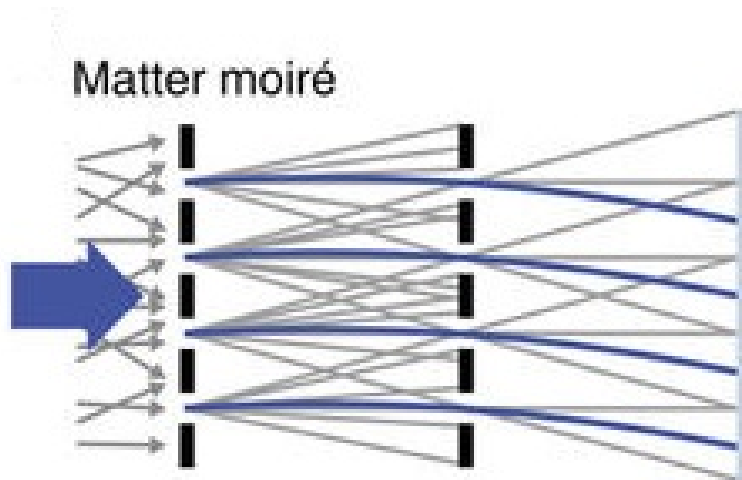


Figure 7: The uncollimated beam of $\bar{\text{H}}$'s passing the Moiré deflectometer, [22].

Like shown in figure 7, the beam of $\bar{H}$'s passing through the two first grating gets collimated to make a more precise measurement. Since also the exact positions of the grating slits are essentially for a gbar measurement with a precision at 1 %, the pattern of the Moiré deflectometer operated with light is used as a reference. This so called Laué-Talbot interferometer produces a slit pattern according to the slit positions on the detector, see also figure 8.

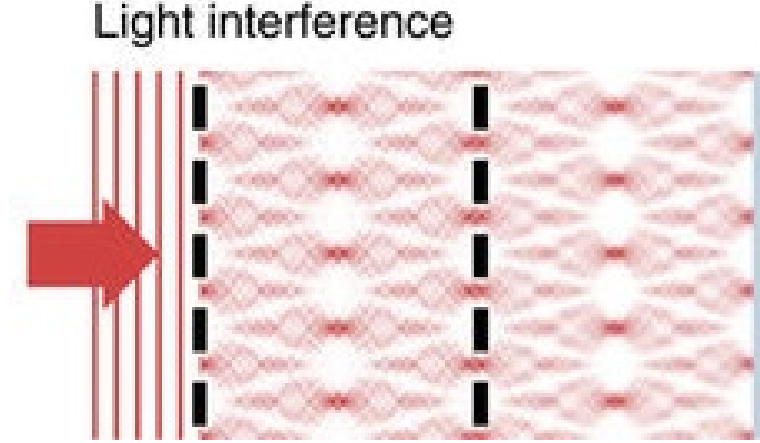


Figure 8: The pattern of the Moiré deflectometer operated with light, [22].

The positions of the $\bar{H}$ s hitting the detector material will be measured in an emulsion, mostly through pions which were produced in pbar annihilations, the positrons on the other side, will interact with electrons of the material and annihilate into photons.

To determine the trajectories of the particles flying through the deflectometer Newtons second law of mechanics is used:

$$F(t) = m \frac{dv}{dt} \quad (3.2)$$

where m denotes the mass of the particle and $v = (v_x, v_y, v_z)$ the velocity at a certain time t . In the case of the gravitational force this leads to:

$$F = mg \quad (3.3)$$

where g is the gravitational acceleration. To estimate the vertical $\bar{H}$ trajectory one has to solve this differential equation for the relevant coordinate which leads to

$$z(t) = z_0 + v_{z_0}t - \frac{1}{2}gt^2 \quad (3.4)$$

here z_0 denotes the initial, vertical position of the particle and v_{z_0} its initial, vertical velocity.

Lets look at the conditions for a atom to pass the slits of the first respectively second grating, let z_1 be a set of vertical values, which are inside a slit of the first grating and z_2 a set for the second grating and z_d the set of the atoms vertical positions at the detector. Lets t be the time a particle needs to travel to the first grating:

$$z_1 \in S_1 \quad (3.5)$$

and

$$z_2 \in S_2 \tag{3.6}$$

then, for the conditions follows:

- first grating: $z_1 = z_0 + v_{z_0}t - \frac{1}{2}gt^2$
- second grating: $z_2 = z_0 + v_{z_0}2t - \frac{1}{2}g2t^2$
- detector: $z_d = z_0 + v_{z_0}3t - \frac{1}{2}g3t^2$

After expressing the initial velocity through the grating conditions by

$$v_0 = \frac{1}{2}(z_1 - z_2) - \frac{3}{2}gt \tag{3.7}$$

the set of the atoms vertical positions is given by

$$z_d = -z_1 + 2z_2 + gt^2 \tag{3.8}$$

As can be seen in (3.8) the shadow of the particles on the detector is patterned according to the slit positions of the gratings, though shifted due to the gravitational force [23].

For the estimation of $g_{\bar{H}}$, besides the relative distance between the light pattern and the annihilation point, the velocities of the $\bar{H}$'s are required. To acquire the velocities of the $\bar{H}$'s a time of flight measurement is done. The starting point of the measurement is the time when the electric field, used for the stark acceleration is switched on, the endpoint is registered via scintillating fibres behind the emulsion. With these information the relative precision of 1 % for $g_{\bar{H}}/g$ the to 100 mK precooled $\bar{H}$'s can be estimated.

4 Particle motion in a penning trap

In this section, an overview over the most important and fundamental physics and formalism of particle confinement in penning traps is given. The content is mainly based on [24, 25, 26].

A Penning trap is a device in which charged particles can be stored and manipulated. Also rare particle species like antimatter can be collected and stored, single particles can be observed and a high variety of high precision measurements can be done. A particle with charge q and mass m in a Penning trap is held in a specific region through a magnetic field.

$$\vec{B} = B\hat{e}_z \quad (4.1)$$

and an electrostatic field

$$\vec{E} = -\nabla\Phi \quad (4.2)$$

4.1 Cyclotron motion and guiding center motion

A particle with mass m and charge q , moving in a magnetic field experiences the Lorentz force,

$$\vec{F}_L = q\vec{v} \times \vec{B} \quad (4.3)$$

for a particle which moves perpendicular to the magnetic field lines ($\vec{v} \perp \vec{B}$) the trajectory of the particle will be a circle. In the general case, the particle has arbitrary velocity components perpendicular and parallel to the magnetic field, so the trajectory of the particle will be spiral shaped. To find the angular velocity of the particle moving perpendicular to a uniform magnetic field $\vec{B}$, one can equal the Lorentz force and the centripetal force,

$$qvB = m\omega^2 r \quad (4.4)$$

where m is the mass of the particle and r is the particle's circular path radius. By using the relation $\omega = \frac{v}{r}$ one finally finds,

$$\omega = \frac{qB}{m} \quad (4.5)$$

This frequency is called cyclotron frequency and it doesn't depend on the velocity of a particle.

Since there is not only a magnetic but also an electric field in the penning trap exerting a force on the charged particle, there is in addition to the very fast circular motion also a slow drift of the guided center (the center of the cyclotron motion) observable. For the case that $\vec{E} \parallel \vec{B}$ the guided center is accelerated in field direction, as can be seen in figure 9 (second image).

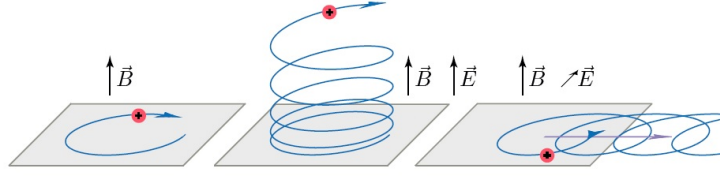


Figure 9: Particle moving perpendicular to the magnetic field axis (l), particle moving in a magnetic and parallel electric field (m), particle moving in a magnetic and orthogonal electric field, [25].

In the case that $\vec{E} \perp \vec{B}$, the particle gets accelerated and again decelerated as it moves along and against the electric field lines. This causes the circular path radius of the particle to increase as it moves along the electric field and decrease it completes its orbit against the field lines. This change in radius leads to a drift of the guided center perpendicular to the electric and magnetic field, which is also called $\vec{E} \times \vec{B}$ -drift ($\vec{E}$ cross $\vec{B}$ -drift). Inside a Penning trap one can assume a superposition of the two last cases $\vec{E} \perp \vec{B}$ and $\vec{E} \parallel \vec{B}$.

4.2 Penning trap electrodes

The charged particles inside a Penning trap are axially confined through an electric field which corresponds to a potential of the form

$$\Phi(\rho, z) = \frac{U_0}{d} \left(\frac{1}{2} \rho^2 + z^2 \right) \quad (4.6)$$

with

$$\rho^2 = x^2 + y^2, \quad (4.7)$$

$$z(\rho)^2 = z_0^2 + \frac{\rho^2}{2} \quad (4.8)$$

and

$$d^2 = \frac{1}{2} \left(z_0^2 + \frac{\rho_0^2}{2} \right) \quad (4.9)$$

To create a potential of this form, at least three cylindrically symmetric electrodes are needed, which are placed along the equipotential lines of Φ , like shown in figure 10. Two endcap electrodes along the hyperbola of revolution $z(\rho) = \pm \sqrt{z_0^2 + \frac{\rho^2}{2}}$ and one ring electrode which follows the hyperbola of revolution $\rho(z) = \pm \sqrt{\rho_0^2 + 2z^2}$. Here, z_0 and ρ_0 are the minimal axial respectively radial distances to the electrodes, as can be seen in figure 10.

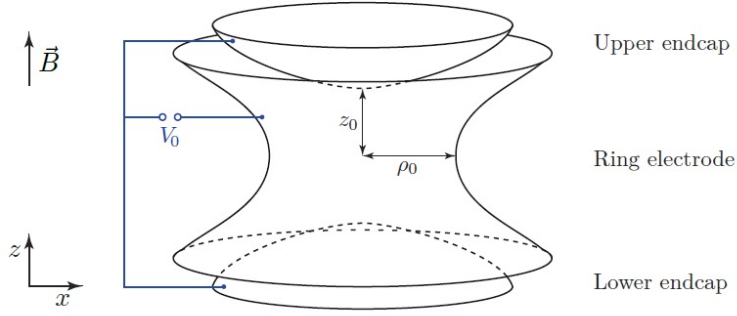


Figure 10: Sketch of the electrode configuration of a Penning trap, [25]

4.3 The particles Penning trap frequencies

The Penning trap frequencies result from the equation of motion

$$\ddot{\vec{r}} = \frac{q}{m}(\vec{E} + \dot{\vec{r}} \times \vec{B}) \quad (4.10)$$

Where $\vec{B}$ has only a component along the z-axis $\vec{B} = B\hat{e}_z$. By inserting the potential (4.6) inside equation (4.2) follows

$$\begin{pmatrix} \ddot{x} \\ \ddot{y} \\ \ddot{z} \end{pmatrix} = \frac{q}{m}B \begin{pmatrix} \dot{y} \\ -\dot{x} \\ 0 \end{pmatrix} + \frac{qU_0}{2mz_0^2} \begin{pmatrix} x \\ y \\ -2z \end{pmatrix} \quad (4.11)$$

By solving this differential equation for the z-component, which has the same form like the well known undamped, harmonic oscillator one can find

$$z(t) = \hat{z}_0 e^{i\omega_z t} \quad (4.12)$$

with

$$\omega_z = \sqrt{\frac{qU_0}{mz_0^2}} \quad (4.13)$$

ω_z is called axial frequency. To derive the other Penning trap frequencies one has to solve the differential equation (4.11) for the radial part. Using the definitions of ω_c and ω_z the equation for the radial components looks like

$$\begin{pmatrix} \ddot{x} \\ \ddot{y} \end{pmatrix} = \omega_c \begin{pmatrix} \dot{y} \\ -\dot{x} \end{pmatrix} + \frac{1}{2} \begin{pmatrix} x \\ y \end{pmatrix} \quad (4.14)$$

By introducing the complex function $u(t) = x(t) + iy(t)$, the equation can be written as

$$\ddot{u} = -i\omega_c \dot{u} + \frac{1}{2}\omega_z^2 u \quad (4.15)$$

With the Ansatz $u(t) = u_0 e^{-i\omega t}$ two independent solutions can be found

$$\omega_{\pm} = \frac{1}{2}(\omega_c \pm \sqrt{\omega_c^2 - 2\omega_z^2}) \quad (4.16)$$

where ω_+ is called the reduced cyclotron frequency and ω_- the magnetron frequency. For usual trap parameters ω_+ is close to ω_c , what means that the frequency is rather

high. The magnetron motion is a slow rotation of the guiding center around the central axis of a penning trap which arises from the $\vec{E} \times \vec{B}$ -drift.

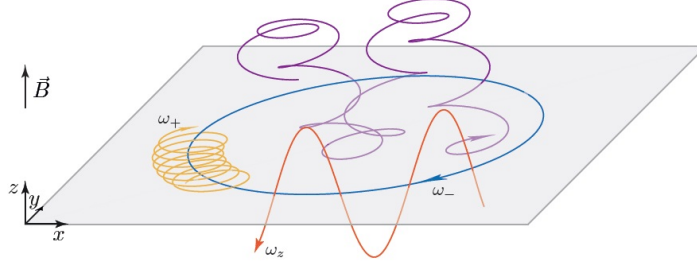


Figure 11: The three decoupled motions and the overall motion (purple) of a particle caught inside a Penning trap. The axial motion ω_z which harmonic oscillating (red), the reduced cyclotron motion ω_+ is a fast motion around the magnetic field lines and the magnetron motion ω_- is a slow drift around the trap center. The particle movement is a superposition of these motions, [25].

To obtain real-valued, physical frequencies of the trapped particles the square root in (4.16) has to be real valued and the condition $\omega_c^2 > 2\omega_z^2$ has to be met. This expression can be rewritten as

$$B > \sqrt{2 \frac{m U_0}{q} \frac{1}{z_0^2}} \quad (4.17)$$

This trapping condition has to be met in order to confine the particles radially in the trap through the magnetic field. For the Penning trap frequency the typical hierarchy looks as follows,

$$\omega_- \ll \omega_z \ll \omega_+ < \omega_c \quad (4.18)$$

Other important relations between the independent trap eigenfrequencies are

$$\omega_c = \omega_+ + \omega_- \quad (4.19)$$

$$\omega_c^2 = \omega_+^2 \omega_-^2 + \omega_z^2 \quad (4.20)$$

$$\omega_+ \omega_- = \frac{1}{2} \omega_z^2 \quad (4.21)$$

The first two relations can be derived by using (4.16) and (4.13) and the third relation results directly from (4.16).

5 Simbuca

This section introduces Simbuca, the program used for the simulations, which build the main part of my thesis. The content is mainly based on [27, 28, 29].

Simbuca is a Penning trap simulation program written in C++ and CUDA by Simon Van Gorp and Pierre Dupré. Originally it was developed for CERN's WITCH experiment which is a sub-experiment at ISOLDE. What makes Simbuca unique is that it uses a graphics card (GPU) instead a conventional CPU to calculate the Coulomb force between the charged particles inside the trap. This is important because simulations with charged particles are mostly restricted by the long computation time due to the Coulomb interaction calculations. Since the Coulomb interaction, as a long range force, has to be calculated between all N particles, the simulation times scale in general with $\mathcal{O}(N^2)$.

Although, approximation methods like the Barnes-Hut tree or the FFM algorithm exist, which reduce the computation time to $\mathcal{O}(N \log N)$, they reduce the calculation time at the cost of accuracy. In principle these methods divide the three-dimensional-space into cubic cells and let only close distant particles interact individually. All other cells are grouped together to a single particle at the position of their center of mass. But never the less, the calculation of the coulomb-interaction still affects the simulation time severely.

5.1 The Chamomilescheme adapted for coulomb interactions

To improve the simulation speed, the Coulomb interaction is calculated on the GPU, since the structure of GPUs, with parallel stream-processors and threads, is convenient to calculate parallelizable algorithms, leading e.g. to the calculation of the Coulomb interaction between charged particles. Here parallelism is straight forward because each particle interacts with every other particle. The main reasons to use a GPU for simulating charged particle interactions are listed below.

- The calculations and instructions on the GPU can be executed on multiple data blocks during the same time cycle.
- The calculation of the Coulomb-force between two particles is relatively simple with around 20 floatingpoint operators.
- In 2007, CUDA, a NVIDIA's GPU programming language similar to C was released, making use and programming of GPUs much more user friendly.

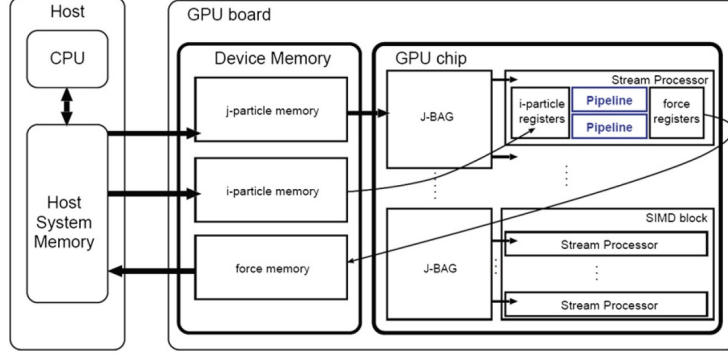


Figure 12: Schematic sketch of the Chamomile scheme, [28].

The Chamomile scheme was originally designed by Hamada and Iitaka to calculate the gravitational N-body-interaction on a graphics card. They implemented the code to the *Cunbody-1*-library, where a function called *cunbody1_force*($x_j, m_j, x_i, eps, a_i, n_{max}$) can be found. $x_i = x_j$ are the positions of the particles written in two dimensional arrays, m_j are the particle masses and eps is a softening factor to avoid divisions by zero. n_{max} is the total number of particles and a_i is the acceleration of the bodies due to the gravitational force and calculated by the library with $\vec{a}_i = \vec{F}_i/m_i$. The force on the i -th particle exerted by the j -th particles is,

$$\vec{f}_{ij} = G \frac{m_i m_j}{|\vec{r}_{ij}|^2} \hat{r}_{ij} \quad (5.1)$$

where G is the gravitational constant, m_i and m_j are the masses of the i -th respectively j -th body, $\vec{r}_{ij} = \vec{r}_j - \vec{r}_i$ and $\hat{r}_{ij} = \vec{r}_{ij}/|\vec{r}_{ij}|$. For the total force acting on the i -th particle follows

$$\vec{F}_i = \sum_{j=1}^{n_{max}} \vec{f}_{ij} \quad (5.2)$$

Figure 12 shows a schematic sketch of the Chamomile scheme and the *cunbody-1* function implemented on a GPU. The function calculates the force that one group of particles (j -particles) exerts on the other group (i -particles). At first, the particle positions are copied from the host computers memory to the device memory on the GPU (j -particle memory and i -particle memory). The J-BAGs are blocks of j -particles with the size of each shared memory and the i -particles are also divided into blocks with the total number of pipelines (called I-POTs). Then, the first J-BAG is transferred from the device memory to the shared memory in each stream processor and in parallel, the force on the first IPOT is accumulated. This blockwise process is repeated for all J-BAGs (as the outer loop) and the IPOTs (as the inner loop), to sum the fragments of the total force up, like shown in (5.2).

Since the equation of Coulomb-force is very similar to the gravitational force equation, see (5.1) and

$$\vec{f}_{ij} = -k_e \frac{q_i q_j e^2}{|\vec{r}_{ij}|^2} \hat{r}_{ij} \quad (5.3)$$

the output of the *cunbody-1* function (a_i) can be scaled in order to calculate the Coulombforce. Here, k_e is the Coulomb constant, e the elementary charge, and q_i and

q_j are charge numbers of the i -th respectively the j -th particle. Thus, the Coulomb-force between the charged particles can be estimated by scaling the gravitational acceleration $a_i[i]$ in the form:

$$a_{Coulomb}[i] = -\frac{e^2 k_e}{m_j[i]} a_i[i] \quad (5.4)$$

where the minus sign states that equally charged particles repel each other.

5.2 The Simbuca Code

The Penning trap simulation programme Simbuca is written in C⁺⁺. It consists out of a variety of sub-programms, the most important ones are briefly discussed in this section and their hirarchy is shown in figure 13. For further information, see [28, 29].

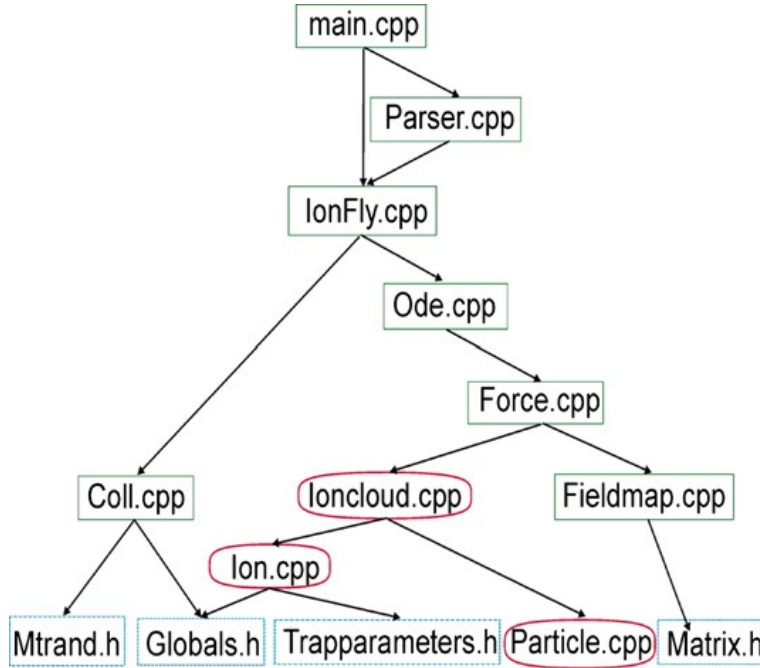


Figure 13: Hirarchy and overview of the Simbuca-files written in C⁺⁺. The rectangular (green) boxes refer to implementation files, ovals to classes and the blue boxes to header files, [27].

- *globals.h* - all physical constants are contained in this file
- *trapparameters.h* - all the characteristic trap parameters like the magnetic field or the depth of the trap (U_0/d^2) can be found here
- *particle.cpp* - this class contains the positions and velocities of the particles in x,y and z direction
- *ion.cpp* - this class contains the masses of the charged particles and the Penning trap frequencies ω_+, ω_- and ω_c are estimated here
- *ioncloud.cpp* - this class mainly contains two arrays with the information of the particles from *ion.cpp* and *particle.cpp*

- *force.cpp* - this file is splitted in two parts. One part calculates the Coulombforce on the CPU and second part on the GPU, depending on what processing unit is chosen in the Makefile. Independently of the processing unit, also the forces due to the magnetic and electric fields of the Penning trap are estimated.
- *ode.cpp* - the integrators for the differential equations are implemented here, see also next section
- *ionFly.cpp* - in this file important variables like the integrator, or when the program starts are initialised here
- *main.cpp* - in this file different parameters like Coulomb interaction, boundary inclusion, and many more can be set
- *Makefile* - this file compiles the actual Simbuca code. Also the processing unit (CPU/GPU) and the compiler (g++/icpc) can be changed in this file

6 Doubly sympathetic cooling scheme

This section introduces the cooling scheme, which I tested with my simulation. The doubly sympathetic cooling scheme was proposed by Michael Doser (CERN) and Alban Kellerbauer (University of Heidelberg) [30] to minimize and control the divergence of the slow horizontal beam of antihydrogen required for the antimatter gravity experiment performed by Aegis. The divergence of the beam is dominated by the velocity distribution of the formed antihydrogen atoms and this in turn depends on the temperature of the initial antiproton plasma. The goal of this cooling scheme is to cool antiprotons down to the mK-region to enhance the precision of the gravitational acceleration measurement at Aegis.

6.1 Possible particle loss mechanisms

The doubly sympathetic cooling scheme uses three species: antiprotons, anions and cations, which are all simultaneously confined in a Penning trap. Furthermore, the cations are laser cooled, sympathetically cooling the anions, which in turn cool the antiprotons. The anionic species acts hereby as a buffer species which is included to prevent annihilations between the cations and the antiprotons. In principle, any pair of cation and anion could be used but there are also some processes which can lead to particle losses. These processes are discussed in the next following points.

- Annihilation of antiprotons with cations

Since the cations and the antiprotons are oppositely charged, they will attract each other, whereas in the end the heavier cation will capture the antiproton forming a metastable exotic atom, which will very fast de-excite and annihilate. To avoid annihilations of the antiprotons it is therefore important to separate them from the cations by a negatively charged buffer species.

In general, charged plasma in a magnetic field forms rotation spheroids. If more than one species are radially confined in a magnetic field, the different species separate radially into concentric shells due to the rotationally induced centrifugal migration. The antiprotons, with the highest q/m ratio are ending up in the center.

To avoid interactions between the antiprotons and the cations a certain charge-to-mass must be obtained, where the antiprotons are the innermost, the cations the outermost and the buffer-species form a shell in between.

Besides, it is important to keep in mind that, the anion and cation plasmas will rotate in opposite directions, due to their opposite charges.

- Charge exchange between anions and cations

The next problem to address, are the different processes which can lead to neutralization of the anion and cation plasmas. Since the anion carries an additional electron and the cation is lacking an electron, interactions between this species can lead to an exchange of charge and thus to neutralization. Since this process depends on the relative values of cations electron affinity and the binding energy

of the anion, the species have to be chosen very carefully. With an ionization energy of 3.89 eV, the cation with the lowest electron affinity is Cs^+ . But the species has to be laser-cooled in a Penning-trap, therefore the choice fell on the rigorously studied Ba^+ [31]. Even though the ionization energy of Ba is 5.21 eV. The anion on the other side should have a very high binding energy. With an electron affinity of 3.61 eV, Cl^- should be a promising candidate. But looking deeper in the matter, one finds that, even with the optimal combination of Cs^+ and Cl^- , the process of mutual neutralization is exothermal by 0.28 eV. This means that the energy balance of the system is after the neutralization lower than before, what makes the process quite likely to happen and therefore Cl^- to an unsatisfying choice. Since there is no atom with a higher binding energy than Cl^- , one has to look for an molecular anion, so-called superhalogen anions, which exhibit vertical detachment energies (ionization energies) up to 14 eV [32]. These superhalogens are i.a. tri-atomic molecules consisting of an atom of Na or Li, and the other two atoms of F, Br, I or Cl. The lightest superhalogen is LiF_2^- , with a molecular mass of $m_{\text{LiF}_2^-} = 45 \text{ u}$, what is quite a bit less than the mass of Ba^+ with $m_{\text{Ba}^+} = 137 \text{ u}$. Here u corresponds to the atomic mass unit.

- Collisional neutralization

LiF_2^- has an electron detachment energy of 6.5 eV [33]. Therefore this combination of species ensures that mutual ionization is endothermal by 1.3 eV and therefore, the system needs additional energy for the process to occur. Thus, the neutralization of the LiF_2^- and the Ba^+ is energetically not allowed, if the species are at rest with respect to each other.

Since this is not the case because of the relative rotational and thermal energy of the species, mutual neutralization through collisions is still possible.

Around temperature of 100 K, the cations have energies at 1 meV. The relative energy of the counter-rotating species depends on the rotational frequencies and therefore on the Penning trap and plasma parameters.

At the Brillouin limit, which is an equation for the maximum possible radial electric field that still allows plasma confinement, the relative energies at the interface of the plasma species are comparable to the reaction energy. However, it is possible to choose the plasma dimensions and densities in a way that ensures that the kinetic energies of both species will be below the threshold for mutual ionization.

- Formation of neutral molecules

Another possible process and loss mechanism for the trapped, charged particles is due to formation of a molecular bound state. For example if the molecule LiF_2^- breaks down into $\text{LiF} + \text{F}^-$, with a dissociation energy of 3.01 eV and then binds with the Ba^+ cation into a neutral final state like $\text{BaF} + \text{LiF}$ (which is endothermic by 1.22 eV). Where the bond-dissociation energy is a measure of the strength of a chemical bond [34].

The binding energy of the molecule must be released in the process of formation and is given by the difference between the electron detachment energy of the

anion (F^-) with 0.82 eV and the electron affinity of the cation (Ba^+).

In the case of atoms, there are two processes possible to release this energy difference of initial and final state. First, radiative recombination, where the binding energy is released through an emitted photon and second, three-body recombination, where the binding energy is transferred to a spectator particle. For molecules it is also possible that the binding energy is released through ro-vibrational excitations.

To estimate the reaction rate of anion-cation recombination, one can have a closer look at antihydrogen production at temperatures around 10 K through three-body recombination and radiative recombination with a ratio of $10^3 : 1$. This ratio is comparable to the ratio of anion-cation recombination to radiative recombination [34].

For the hydrogen respectively antihydrogen atom the processes look as follows: $p + e^- \rightarrow H + \gamma$, for the radiative recombination and $p + 2e^- \rightarrow H + e^-$, the three-body recombination [35, 36].

Thus the rates of particle losses for the cation and the molecular anion while interaction should also be comparable to the (anti)hydrogen production rates (for similar plasma parameters), and therefore the recombination rate of the ions can be estimated at approximately $10^{-3} s^{-1}$, for a density of $10^8 cm^{-3}$ and a total number of 10^6 ions.

6.2 Removal of unwanted species

To avoid interactions between the coolant species and the positrons respectively antiprotons during the antihydrogen formation process, it is convenient to remove the coolant before the antiatom-formation. Since the Barium cation is the heaviest species they are positioned in the outermost shell. To remove the laser-cooled cations a static quadrupole potential can be applied, in addition to the electrode potential of the trap. If the amplitude of this potential is high enough, the motion and trajectories of the Barium cations get unstable in radial direction and the particles will shortly afterwards hit the electrodes. To remove the anionic buffer species, a laser-pulse with the respective amplitude and characteristics can be used to photodetach the additional electron of the anionic buffer species and therefore to neutralize it.

7 Simulating the doubly sympathetic cooling scheme

7.1 Mathematica files - Input preparation and adaption, data visualization

In this subsection, the visualization of the data outputted by Simbuca and the data preparation for the input shall be discussed. As mentioned in the introduction, Wolfram Mathematica is used for the input preparation, the output visualization and the output analysis. In the next figures the most important extracts of the Input-Creator-file are shown and explained.

In figure 14 some of the initialization parameter of a Simbuca-simulation are shown. Next to the folder path, the important Integrator settings are chosen. The integrator is set to 5, this means that the chosen integrator is Dormand Price (5th order). Next to Dormand price, also Runge Kutta (4th order), Gear method and the Velocity Verlet integrator are available. In this example the time steps are chosen to be adaptive. The initial time step can be guessed (in this case 10^{-10} sec), afterwards the steps will be adapted automatically. The simulation time is set to 1 ms and data are saved every $10 \mu\text{s}$.

Simulation initialization:

```
Specify relative folder for simulation files:  
  
In[139]:= FolderPath = "TestFolder";  
  
Integrator settings:  
  
In[140]:= IntegratorNumber = 5;  
          AdaptiveTime = 1;  
          InitTime = 10-10;  
  
Length of simulation:  
  
In[143]:= SimTime = 10-3;  
  
Data output timesteps:  
  
In[144]:= DOutTime = 10-5;
```

Figure 14: Initialization parameters for a simulation with Simbuca.

In figure 15 (left), the input data for the penning trap settings are shown. The B -field is always parallel to the z -axis and in this example set to 1 T, the trap potential is set to -10 V and the harmonic factor is set to 30000. The anharmonic factors are set to zero, therefore the potential is of harmonic shape in this example. The radius of the electrodes is also given with 2 cm. The electrostatic potential has the following form:

$$V(r, z) = U_0 c_0 + U_0 c_2 (z^2 - r^2/2) + U_0 c_4 (z^4 - 3r^2 z^2 + 3/8 r^4) + U_0 c_6 (z^6 - 15/2 r^2 z^4 + 45/8 r^4 z^2 - 5/16 r^6) \quad (7.1)$$

where c_2 is the harmonic factor, c_4 and c_6 anharmonic factors and U_0 the potential difference between endcap- and ring-electrodes.

Trap potential settings:

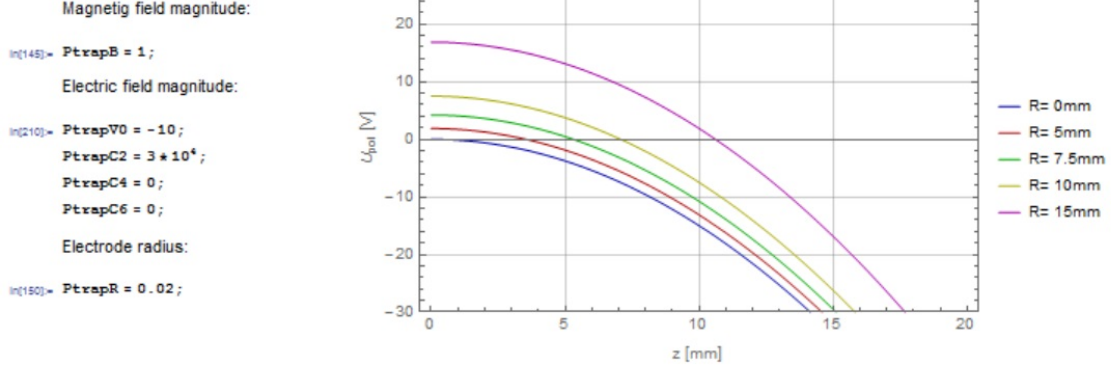


Figure 15: Trap potential settings and visualization.

The right side of figure 15 shows the visualization of the trap potential along the trap axis (z). The different colors show the potential for the respective radial position at 0, 5, 7.5, 10 and 15 mm.

In figure 16, the general plasma parameters are listed. The number of particles simulated by Simbuca and the number of particles simulated considering the Coulomb-factor. This means that Simbuca scales the Coulombforce to simulate more particles with less computational costs. This scaling factor, the so-called Coulomb factor, the ratio between these particle numbers is also shown in figure 16. Besides, the plasma density, the plasma species (negatively charged magnesium isotopes and hydrogen, which can be interpreted as antiprotons), the masses of the different species (u stands for atomic mass unit), the ratio of the particle species, the initial plasma temperature (here 1 K), as mentioned before the Coulombfactor (Cf). The simulation density of the actually simulated plasma (nSim) and the interparticle distance l and the particle number vector (PNumbers).

```

Particles simulated by Simbuca:

In[156]> NSim = 210;
Number of particles that should be simulated:

In[157]> Ntotal = 105;
Density of the plasma:

In[158]> n = 5 × 1011;
Names of the species as vector:

In[159]> PNames = {"24Mg1-", "1H1-"};
NSpecies = Length[PNames];
Masses of the species as vector:

In[161]> PMasses = {24 u, 1 u};
Ratios of the species in plasma:

PRatios = {10, 10};
PRatios = PRatios / Total[PRatios];
Initial plasma temperature:

In[165]> PTemp = {1, 1};
Coulomb factor:

Cf = Ntotal / NSim;
Simulation density and initial inter particle distance:

In[168]> nSim = n / Cf;
l = nSim-1/3;
Particle number calculation:

In[170]> PNumbers = Table[Floor[NSim PRatios[[n]]], {n, 1, NSpecies - 1}];
PNumbers = Append[PNumbers, NSim - Total[PNumbers]]
Out[171]> {512, 512}

```

Figure 16: General plasma parameters.

The plasma positions are generated using a cylindrical shaped 3 dimensional grid as can be seen in figure 17. The Length of the plasma is given with 40 mm and the radius is calculated by equalling

$$V_{\text{cyl}} = r^2 * \pi * h \quad \text{and} \quad V = \frac{n}{\rho} \quad (7.2)$$

where n represents the particle-number and ρ the particle density. Thus, expressing r one finds

$$r = \sqrt{\frac{n}{\rho \pi h}} \quad (7.3)$$

Then, a grid is initialized with grid points according to the inter particle distance (l). The function CylGrid selects the grid point positions which are within a cylindrical volume (V_{cyl}) according to the plasma volume (V).

Length and radius of cylindric plasma:

PLength = 0.040;

$$PRad = \sqrt{\frac{NSim}{nSim \pi PLength}}$$

0.00126157

```
RawGrid = Flatten[Table[{m1, m2, m3}, {m1, Floor[-1.0 PRad], Ceiling[1.0 PRad]}, {m2, Floor[-1.0 PRad], Ceiling[1.0 PRad]}, {m3, Floor[-1.0 PLength/2], Ceiling[1.0 PLength/2]}], 2];
CylGrid = Select[RawGrid, RegionMember[Cylinder[{0, 0, -1.3 PLength/2}, {0, 0, 1.3 PLength/2}], 1.3 PRad], #] &;
NGrid = Length[CylGrid];
```

Distribution of the particles on the positions:

```
SampleTable = Range[1, NGrid];
SampleList = Range[1, NSpecies];
For[i = 1, i <= NSpecies, i++, SampleList[[i]] = RandomSample[SampleTable, PNumbers[[i]]];
SampleTable = Select[SampleTable, NoneTrue[SampleList[[i]], Function[v, v == #] &];]
```

Position list:

```
PositionList = Table[CylGrid[[n]], {n, 1, NSpecies}, {n, SampleList[[m]]};
Graphics3D[{Blue, Sphere[PositionList[[1]], 1/3], Red, Sphere[PositionList[[2]], 1/3]}]
```

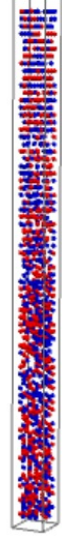


Figure 17: Initialization of the particle positions.

Next, the particles are distributed to the positions of the cylindrically shaped grid and a position list is created with all positions for all different species of particles. Additionally, on the right side of figure 17 the initialized plasma is visualized. In the plasma configuration shown in figure 17, LiF_2^- is plotted in blue and Ba^+ in red. The plasma length is chosen to be 40 mm and the radius is about 1.3 mm. Besides, in this example the two species are distributed randomly to all gridpoints.

```
AbsVelList = Table[RandomVariate[ProbabilityDistribution[mbd[v, PMasses[[n]], PTemp[[n]], {v, 0, \infty}], PNumbers[[n]], {n, 1, NSpecies}];
RandAngleList = Table[{RandomReal[{0, 2 \pi}], PNumbers[[n]], RandomReal[{0, \pi}], PNumbers[[n]]}^T, {n, 1, NSpecies}];
VelocityList = Table[{#[[1]] {Cos[#[[2, 1]] Sin[#[[2, 2]]], Sin[#[[2, 1]] Sin[#[[2, 2]]], Cos[#[[2, 2]]]} & /@Transpose[{AbsVelList[[n]], RandAngleList[[n]]}], {n, 1, NSpecies}];
In[80]:= Histogram[Evaluate@Table[VelocityList[[1, 1 ;; n]], {n, 1, 3}]]
```

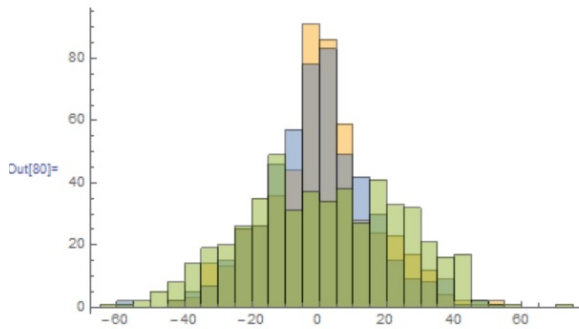


Figure 18: Initialization of the particle velocities: v_x (yellow), v_y (blue), v_z (green) and the overlap regions (grey).

In figure 18 the particle velocities are initialized via Maxwell-Boltzmann distributions and random angle generators and assigned to the particles. The different colors

indicate the absolute velocities in the respective spatial direction, v_x in yellow, v_y in blue, v_z in green and the grey areas represent the overlap of v_x and v_y .

After feeding the generated data to Simbuca, the simulation can be executed.

7.2 Plasma-preparation and thermalization

The first step for testing the doubly sympathetic cooling scheme was to find a suitable plasma configuration for the LiF_2^- and Ba^+ . Although the cooling scheme was of course designed to cool antiprotons, the third species was neglected in the testing phase to save simulation time. For the sake of simplicity the plasma is initialized already in a cylindrical shape, where the Ba^+ -cations are placed axially in the middle and the LiF_2^- -anionic molecules in the outer cylinder-ends, like shown in figure 19. This way the particles can be caught without any turbulences by the double well potential applied on the two different species, imitating the potential of the penningtrap-electrodes.



Figure 19: Initialized plasma-shape.

In figure 20, the double-well potential along the trap axis z is illustrated, for $z \geq 0$, where $z = 0$ corresponds to the trap center. After initializing the plasma and applying a respective electric-potential and magnetic field, the plasma needs to thermalize inside the simulated trap, to avoid unphysical behaviour due to simulation effects. An example of a thermalized plasma is shown in figure 21. A plasma is thermalized, if the mean temperature respectively the mean kinetic energy doesn't severely change anymore and the velocity distribution follows a Maxwell-Boltzmann distribution. Besides, the axial velocity component approaches the radial velocity component. The plasma radius should also stabilize, since the plasma volume has to be constant. In figure 21 the visualization of the initialized plasma and its development is shown. Here, the columns contain arbitrary many timesteps up to 10 ms (the simulation end), and the rows the different spatial planes, the radial plane in the first row, and x/z , respectively y/z in the second and third row. The axial direction is again described by the z -coordinate. LiF_2^- is here plotted in blue and Ba^+ in orange. Besides, in the first column, it can be observed how the plasma is initialized on a cylindrically shaped grid before the charged particles are experiencing any forces, with the cations in the trap center and the anions axially outermost on both sides.

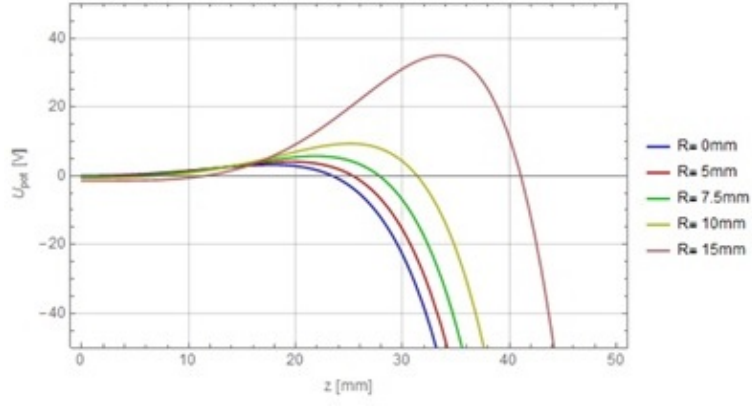


Figure 20: Double-well potential for $z \geq 0$.

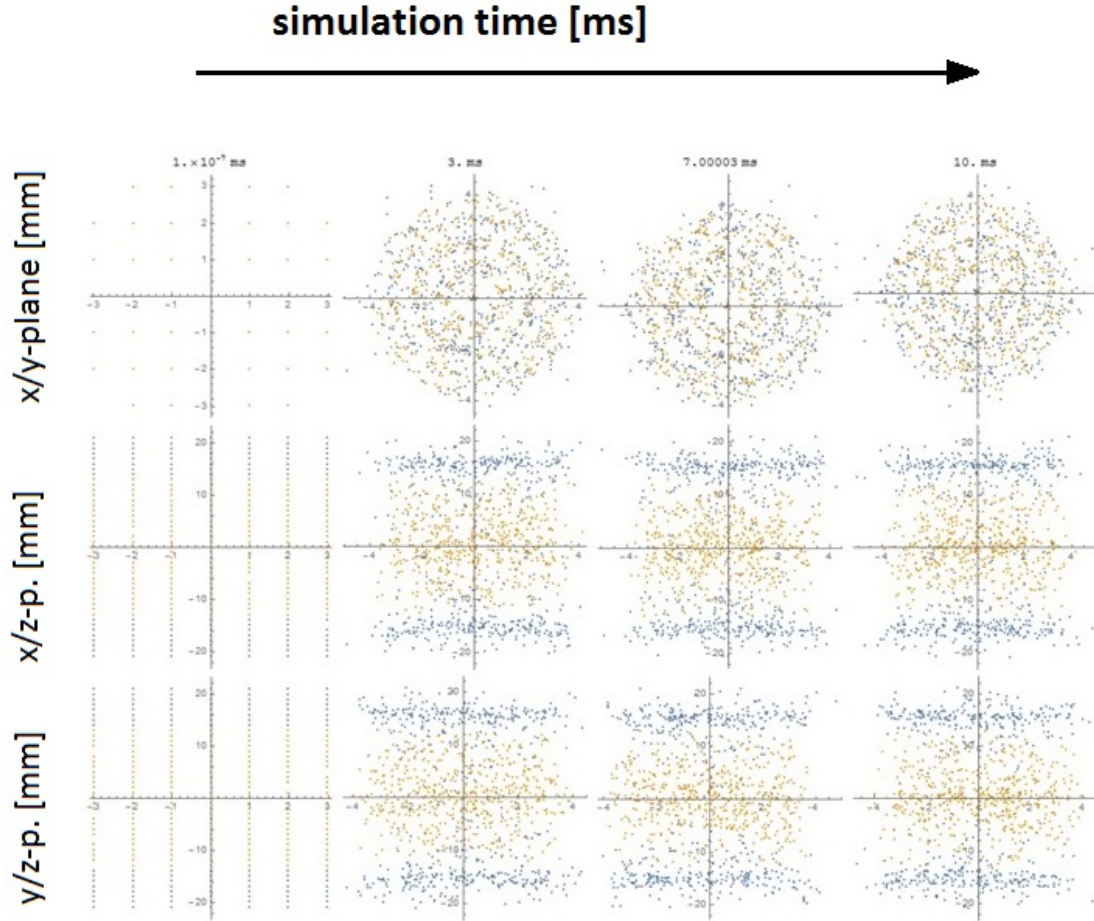


Figure 21: Development of the plasma-shape: LiF_2^- in blue and Ba^+ in yellow. In the three rows, the respective spatial-planes are visualized, where the units of the axes are given in mm . In the columns, the arbitrarily chosen timesteps are shown.

Anyhow, the double well potential was not arbitrarily chosen. The idea behind it is, to ensure and control the strength of the interaction of the two species by ramping the electric potential to lower absolute values. Besides, since the proposed doubly sympathetic cooling scheme also includes the idea that the plasma-species should separate

radially into concentric shells due to the rotationally induced centrifugal migration, it seemed straight forward to test this configuration. Since the LiF_2^- crosses the Ba^+ plasma from both sides in this configuration, also a certain stability should be maintained.

7.3 Laser-force and potential-ramping implementation

The strength of the laserforce, acting on the Barium cations to cool them down to temperatures close to the Doppler-limit is estimated in the following. The formulism and content is based on [37].

Since the absorbed photon gives the atom a kick in the direction opposite to its motion, the scattering effect of many photons exerts an average force, which slows the Ba^+ cations down.

The force in 7.4 describes the magnitude of the scattering force induced by the laser.

$$F_{\text{scatt}} = (\text{photon momentum}) * (\text{scattering rate}) \quad (7.4)$$

The scattering rate is given by

$$R_{\text{scatt}} = \frac{\Gamma}{2} \frac{\Omega^2/2}{\delta^2 + \Omega^2/2 + \Gamma^2/4} \quad (7.5)$$

where $\delta = \omega - \omega_0 + kv$ denotes the frequency detuning from resonance, with the laser frequency ω , the atomic resonance frequency ω_0 and the doppler shift kv . Ω is the Rabi-frequency and Γ is the natural linewidth of the excited state. Since the Rabi-frequency and the saturation intensity I_{sat} are related by $I/I_{\text{sat}} = 2\Omega^2/\Gamma^2$ and the photon momentum is given by $\hbar k$, for the scattering force it follows:

$$F_{\text{scatt}} = \hbar k \frac{\Gamma}{2} \frac{I/I_{\text{sat}}}{1 + I/I_{\text{sat}} + 4\delta^2/\Gamma^2} \quad (7.6)$$

For a detuning of $\delta = -\Gamma/2$ and $I = 2I_{\text{sat}}$, the scattering-force can be estimated by

$$F_{\text{scatt}} \simeq \hbar k \frac{\Gamma}{4} \quad (7.7)$$

Ba^+ has two interesting transitions in respect to lasercooling. An optical transition from $S_{1/2}$ to $P_{1/2}$, at 493 nm ($\Gamma \approx 15$ MHz) and a second transition at 649 nm, from $P_{1/2}$ to $D_{3/2}$ ($\Gamma \approx 5$ MHz)[38]. Since the Doppler-cooling limit for the $S_{1/2} \rightarrow P_{1/2}$ transition lies at $\sim 40 \mu\text{K}$, which was considered as low enough for these test-simulations, only this transition was used for the laserforce-implementation.

Thus, the absolute value of the wave k can be estimated through:

$$k = |\vec{k}| = \frac{2\pi}{\lambda} = \frac{2\pi}{493 * 10^{-9} \text{m}} \quad (7.8)$$

After inserting the Ba^+ -specific values for k and Γ and dividing the result through the Barium-mass, one finds:

$$F_{\text{scatt}} \simeq \left(\frac{1}{4}\Gamma\hbar k\right) = 5.04011 * 10^{-21} \frac{\text{m} * \text{kg}}{\text{s}^2} \quad (7.9)$$

$$a_{\text{scatt}} = F_{\text{scatt}}/m_{\text{Ba}} = 22154.9 \frac{\text{m}}{\text{s}^2} \quad (7.10)$$

The laser-force was implemented directly in the force-file of the Simbuca code and the value of the strength of the force calculated in 7.10 was inserted as can be seen in figure 7.4. Besides, unless otherwise stated, only two lasers in axial direction were implemented for all following simulations.

```

//Implementation of an averaged laser cooling force in z
    if(_cloud.mass[j_]>1e-25){
        if((-0.05>vz)&&(vz>-600)){
            (*forcev).derivs[j_][2]+=2.2e4;    //axial
        }
        if((600>vz)&&(vz>0.05)){
            (*forcev).derivs[j_][2]-=2.2e4;
        }
    }

//Implementation of an averaged laser cooling force x
    if(_cloud.mass[j_]>1e-25){
        if((-0.05>vx)&&(vx>-600)){
            (*forcev).derivs[j_][2]+=2.2e4;
        }
        if((600>vx)&&(vx>0.05)){
            (*forcev).derivs[j_][2]-=2.2e4;
        }
    }

//Implementation of an averaged laser cooling force y
    if(_cloud.mass[j_]>1e-25){
        if((-0.05>vy)&&(vy>-600)){
            (*forcev).derivs[j_][2]+=2.2e4;
        }
        if((600>vy)&&(vy>0.05)){
            (*forcev).derivs[j_][2]-=2.2e4;
        }
    }

```

Figure 22: Laser-force implemented in Simbuca.

The example shown in 22 imitates in a very general form six lasers adjusted along the three spatial axes. Since the main goal of testing the doubly sympathetic cooling scheme was to find a general proof of principal, this laserforce-imitation was enough for my purpose. Anyhow, as illustrated the laser-force acts only on the Ba^+ cations, with a mass $m_{\text{Ba}} \approx 2.27 \times 10^{-25}$ kg, since the LiF_2^- -superhalogens are excluded with a mass of $m_{\text{LiF}_2} \approx 7.47 \times 10^{-26}$ kg. Additionally, the laserforce is implemented as a constant force, which acts on the Ba^+ -atoms of certain velocity range.

The velocity range was chosen arbitrary during the testing phase due to simulation-time and simplicity reasons, since the main focus at this point was to find the suitable trap and plasma parameters to test the proposed cooling scheme.

The force, applied on the charged particles due to the electrode potential is shown in figure 23. The boolean flag *UseIdealTrap*, is set to *true* by default and includes the calculation executed for a harmonic potential and *trap_config* == 1 includes the anharmonic terms. The relation between the induced force on a particle and the electrostatic potential is

$$\vec{F}_{\text{pot}} = -q\vec{\nabla}U \quad (7.11)$$

The force terms for the anharmonic correction factors $c4$ and $c6$ can be estimated via a Taylor series. Besides, U_0 is the voltage applied between endcap- and ring-electrodes at the beginning of the simulation and U_t is the desired voltage at the end of the

simulation or after a chosen timespan, the ramping of the potential is integrated as a linear function. In figure 24 the code for the voltage variation and the corresponding function is shown.

```

if(UseIdealTrap){
  (*forcev).derivs[j_][0] = w_z2m *x*0.5*Ut;
  (*forcev).derivs[j_][1] = w_z2m *y*0.5*Ut;
  (*forcev).derivs[j_][2] = -w_z2m * z*Ut;
  if(Bfield){
    (*forcev).derivs[j_][0] += w_cm*vy;
    (*forcev).derivs[j_][1] += -w_cm*vx;
    (*forcev).derivs[j_][0] -= delta*vx;
    (*forcev).derivs[j_][1] -= delta*vy;
  }
  if(trap_config==1)
  {
    //c4
    r2 = x*x+y*y;
    z2 = z*z;
    r4 = r2*r2;
    z4 = z2*z2;
    qDmassa= _cloud.charge[j_]*el_charge/_cloud.mass[j_];
    (*forcev).derivs[j_][0] += qDmassa*U0*Ut*c4*(6.*x*z2-1.5*x*r2);
    (*forcev).derivs[j_][1] += qDmassa*U0*Ut*c4*(6.*y*z2-1.5*y*r2);
    (*forcev).derivs[j_][2] += qDmassa*U0*Ut*c4*(-4.*z2*z+6.*r2*z);
    //c6
    (*forcev).derivs[j_][0] += qDmassa*U0*Ut*ct*c6*(15.*x*z4 + 45./2.*z2*x*r2 -15./8.*x*r4);
    (*forcev).derivs[j_][1] += qDmassa*U0*Ut*ct*c6*(15.*y*z4 + 45./2.*z2*y*r2 -15./8.*y*r4);
    (*forcev).derivs[j_][2] += qDmassa*U0*Ut*ct*c6*(-6.*z*z4 + 30.*r2*z*z2 -45./4.*r4*z);
  }
}

```

Figure 23: Code example: Electrostatic potential induced by the electrodes.

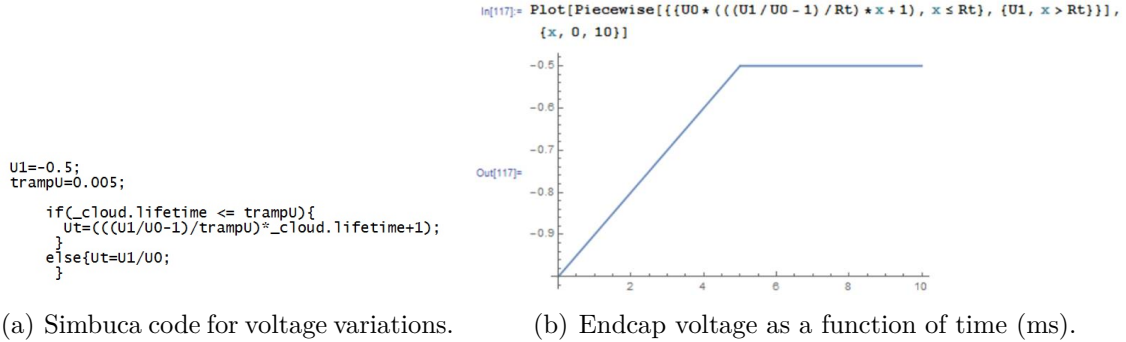


Figure 24: Example for ramping of the electrode potential from -1 to -0.5 V in 5 ms and a simulation time of 10 ms.

7.4 First tests - testing different parameters and plasma configurations

The first tests were mainly designed to find a suitable plasma configuration and trap parameters for the observation of interaction respectively radial-shell-formation. For example a plasma configuration with LiF_2^- in the middle of the trap and Ba^+ in the potential sidebags, turned out to be an unpromising candidate for observing any interaction not to mention sympathetic-cooling between the species. The main problem arose, when the absolute value of the potential was lowered to allow interaction between the species. In this configuration, the LiF_2^- leaves the trap in axial direction during the 'ramping-phase' since it is not the actively coolable species. To be more precise, no

cooling effect was observed for the LiF_2^- -anions, no sympathetic cooling effect and of course no cooling effect due to a laser, since only the cations are lasercooled. Thus, the anions leave the trap in axial direction, at the time when the potential hill confining the particles can be overcome by the particles due to their kinetic energy.

Since a configuration with LiF_2^- in the trap-center could be excluded, I focused on the configuration with Ba^+ in the trap-center, for all further simulations. This way particle losses could be avoided, since the Barium cations are lasercooled to far lower temperatures in comparison to the anionic species.

The Ba^+ ions were for the following simulations pre-cooled via the implemented lasersystem, before the interaction of the species was initiated. The LiF_2^- was also assumed to be pre-cooled, mostly down to a range from 200 K to 40 K, which could be in practice realised by for example electron cooling.

Hunting for evidence of interaction respectively of sympathetic cooling

In the following examples two very interesting physical effects can be observed and important statements over the behaviour of the plasma due to simulation-time and potential-variations can be concluded.

Figure 25 shows the spatial shape of the plasma for different time-steps on the left side and the mean temperature of the charged particles, as well as the particle number and radius on the right side. Furthermore, the temperature calculation for T_{ax} and T_{rad} (the axial and radial temperature) is based on the mean velocities of the charged particles ($\bar{v}_{rad}$ and $\bar{v}_{ax}$), which follow from the 1 dimensional Boltzmann-distribution for the axial temperature and reads as follows

$$\bar{v}_{ax} = \sqrt{\frac{2k_B T_{ax}}{\pi m}} \quad (7.12)$$

and from the 2 dimensional distribution for the radial temperature

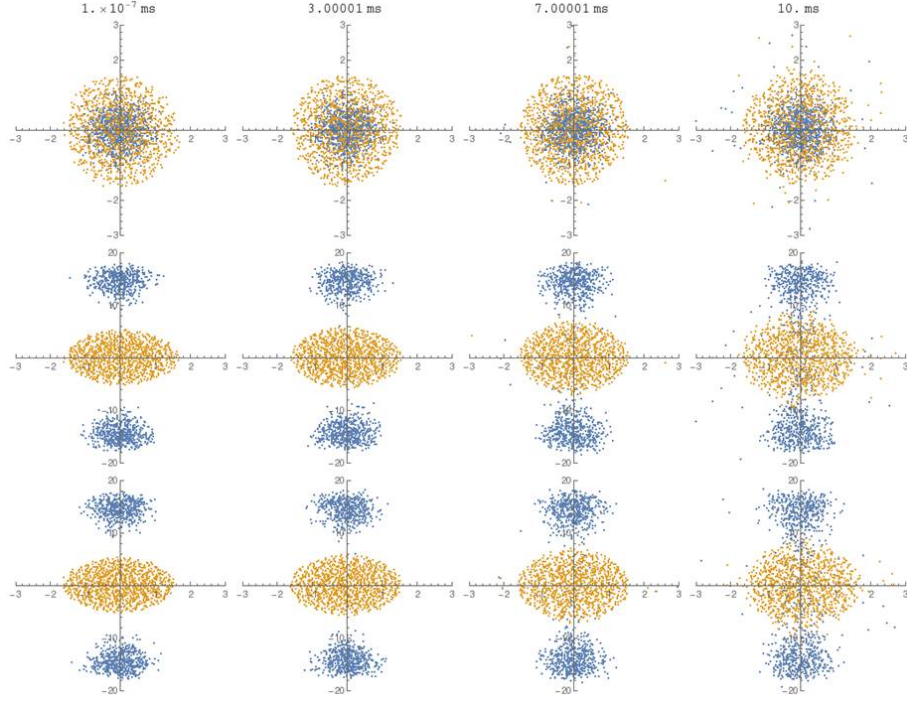
$$\bar{v}_{rad} = \sqrt{\frac{\pi k_B T_{rad}}{2m}} \quad (7.13)$$

where k_B denotes the Boltzmann constant and m the particle mass.

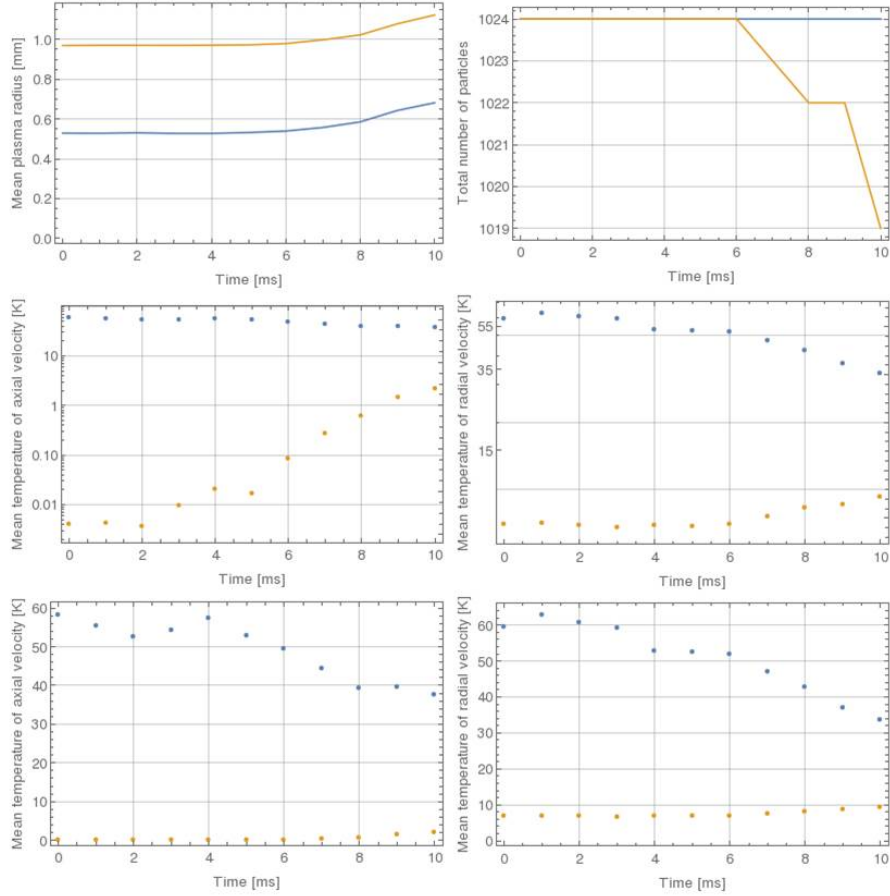
As a reminder, the LiF_2^- is again held in blue and Ba^+ in orange. In this example, a B -field of 1 T was used and the simulation-time was set to 10 ms. The potential was ramped down from -0.5 V to -0.2 V in 10 ms. For clarification, it should be noted that in this and in all further cases, the term 'ramped down' refers to the absolute value of the applied potential.

The first thing clearly observable is that the mean temperature of the LiF_2^- anionic molecules is cooling down by ~ 20 K. Unfortunately it would be hasty to bring ones hope up, that already clear evidence for sympathetic cooling was found. In later simulations, I will show and discuss, that this cooling effect is attributable to the potential alteration. Besides, two LiF_2^- were lost during the simulation, which is unexpected, since the LiF_2^- in contrast to the Ba^+ ions should be confined stably by the electrostatic potential and the B -field.

In figure 26 the result of a 7 ms-simulation with a constant potential at -0.15 V and a magnetic field of 1 T is shown. Interesting here is that the plasma gets unstable and starts to rotate. The reason for these rotations is probably that the magnetron motion

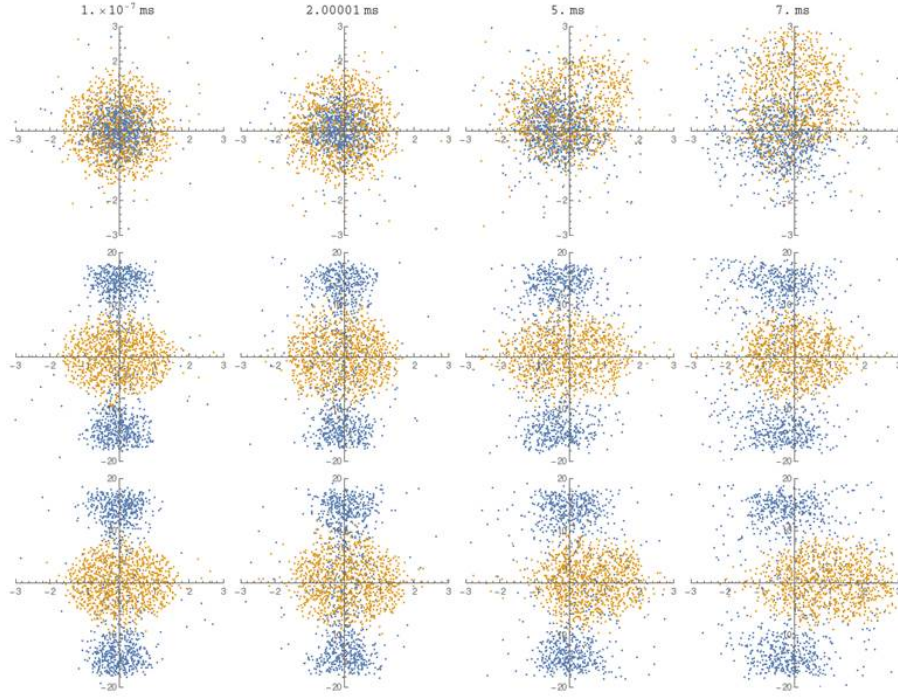


(a) Development of the plasma-shape: LiF_2^- in blue and Ba^+ in yellow.

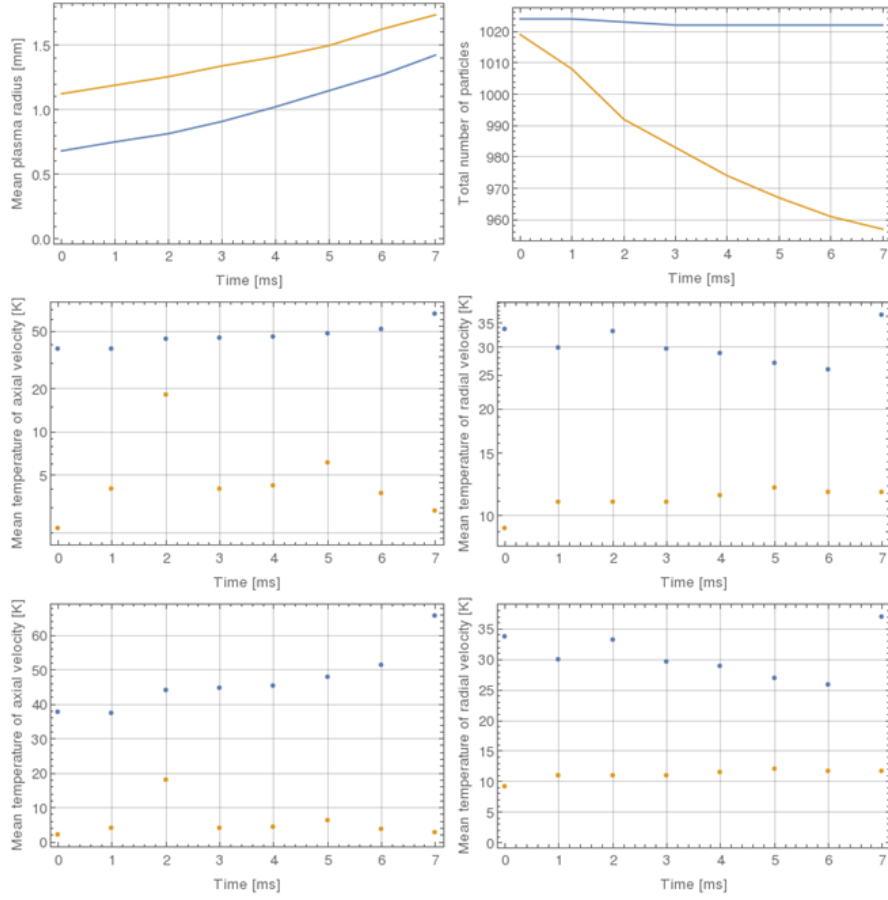


(b) Plasma-temperature in logarithmic (middle column) and linear scale (last c.), -number and -radius. The temperature calculation is based on the mean velocities of the charged particles, which follow from the 1 dim. Boltzmann-distribution for the axial and the 2 dim. MBd for the radial temperature.

Figure 25: Example-1, a test-simulation to find suitable plasma and penning-trap parameters.



(a) Development of the plasma-shape: LiF_2^- in blue and Ba^+ in yellow.



(b) Plasma-temperature in logarithmic (middle column) and linear scale (last column), -number and -radius.

Figure 26: Example-2, a test-simulation to find suitable plasma and penning-trap parameters.

of the two species oppose each other in direction. Therefore it is likely that kicks between the LiF_2^- -ions and the Ba^+ -cations are responsible for this instability. In later simulations these kind of rotations could be prevented through an appropriate choice of plasma parameters (density and plasma form) as well as by cooling the Ba^+ -cations down to lower temperatures.

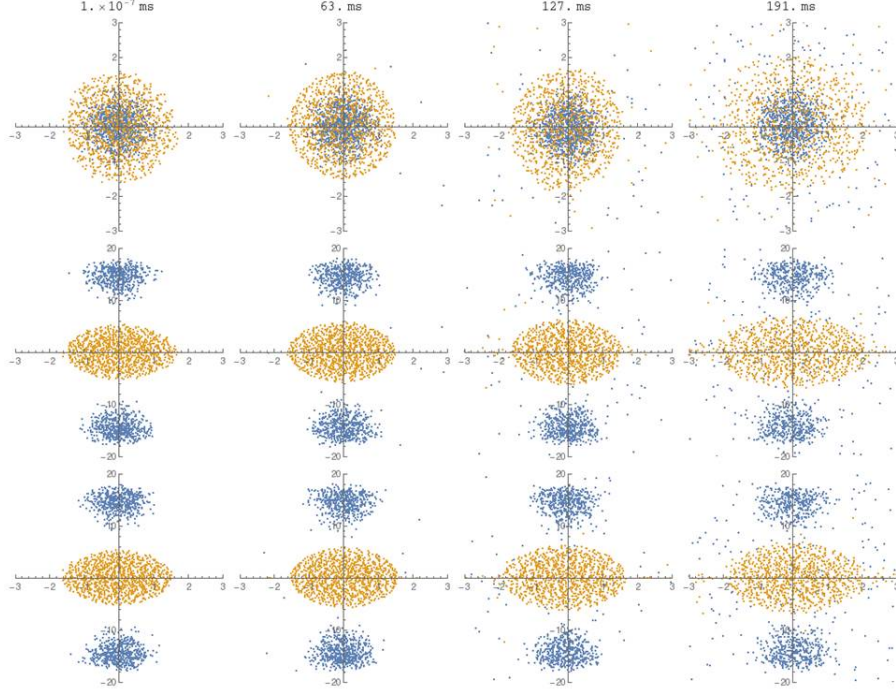
For the 3rd example, shown in figure 27, a long simulation and ramping time of 200 ms was chosen. The potential was lowered from -0.5 to -0.2 V and the magnetic field is again set to 1 T. The total number of particle plot shows clearly that the LiF_2^- and Ba^+ leave the trap together as pairs (radially) and the plasma radii show a similar increase. It also should be noticed, that shortly after the radii increase the first particle(s) leave the trap (radially). The most likely explanation for these particles losses is that the cation and the ion form a bound state called guiding center drift atom, respectively a drifting pair, see the conclusion of this subsection for further details (7.4.1).

Testing if the species separate radially into concentric shells

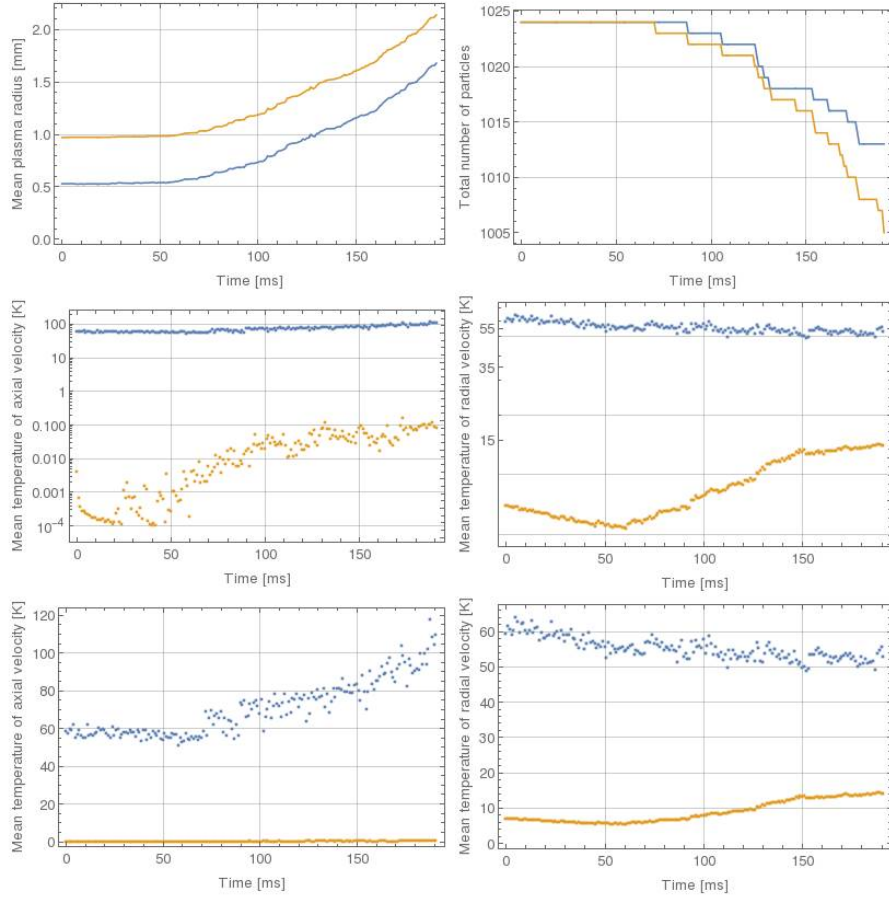
In the following, some simulations are shown and analyzed, trying to observe the formation of concentric shells, with the heavier species (Ba^+) in the outer radial shell and the lighter species (LiF_2^-) in the center.

Figure 28 shows a 10 ms simulation, with a magnetic field of 1.5 T. The potential was ramped down from -0.1 V to -0.08 V in 10 ms. Again plasma rotations are observable. In this case, not only the Barium-cations but also the LiF_2^- -cloud starts to rotate.

The next test, shown in figure 29 was another try to achieve a separation of the two species while avoiding any additional rotation-effects. To stabilize the plasma as good as possible four additional laser in x - and y -direction were included. All other parameters are exactly as in example-4.

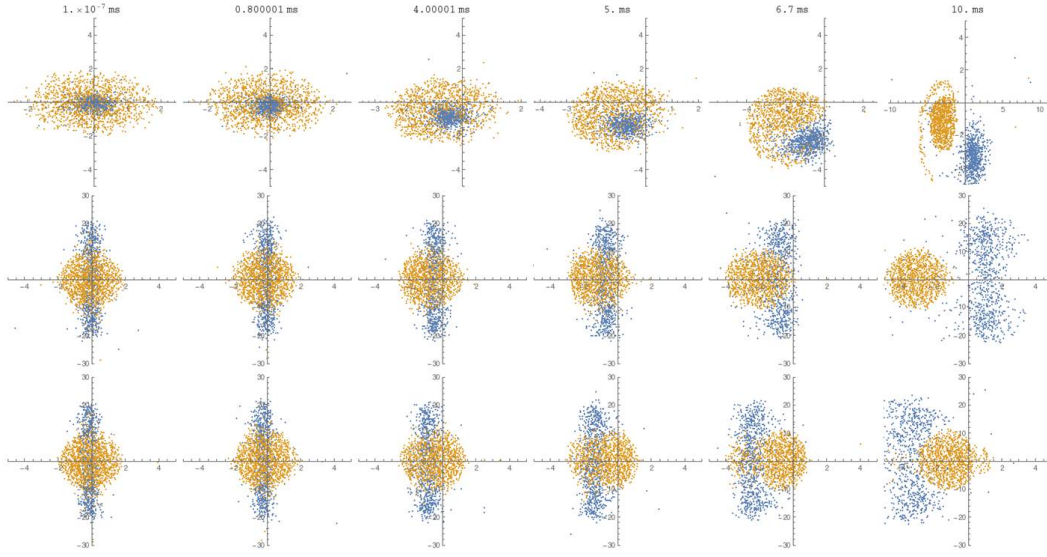


(a) Development of the plasma-shape: LiF_2^- in blue and Ba^+ in yellow.

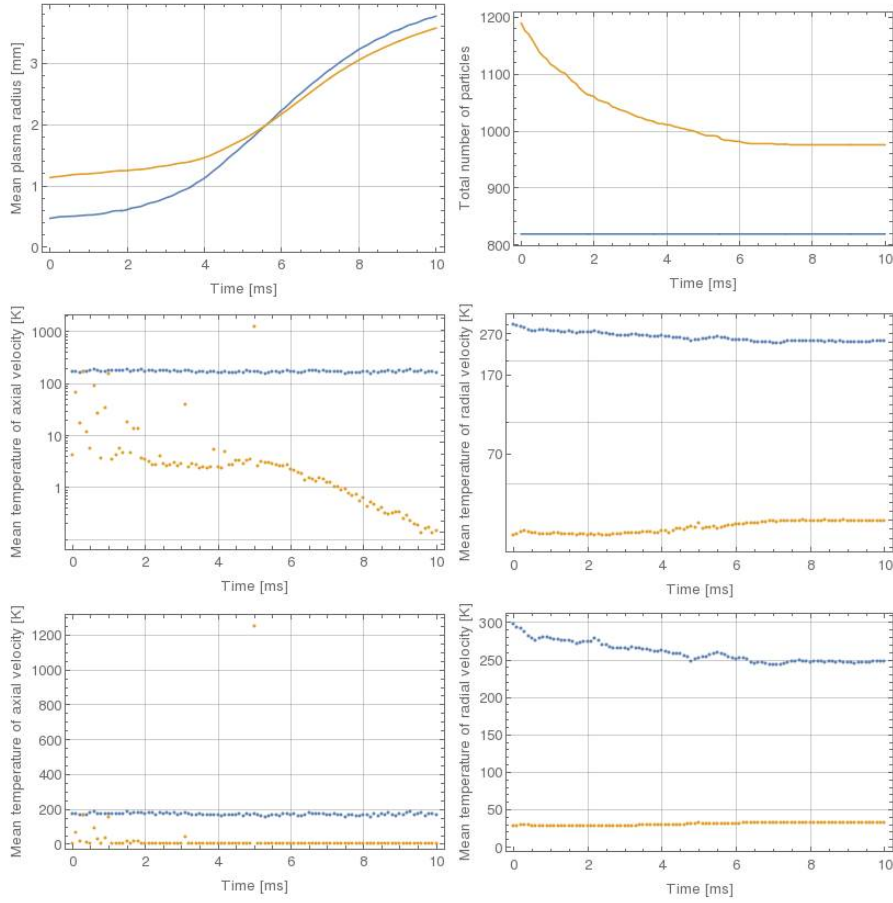


(b) Plasma-temperature, -number and -radius.

Figure 27: Example-3, a test-simulation to find suitable plasma and penning-trap parameters.

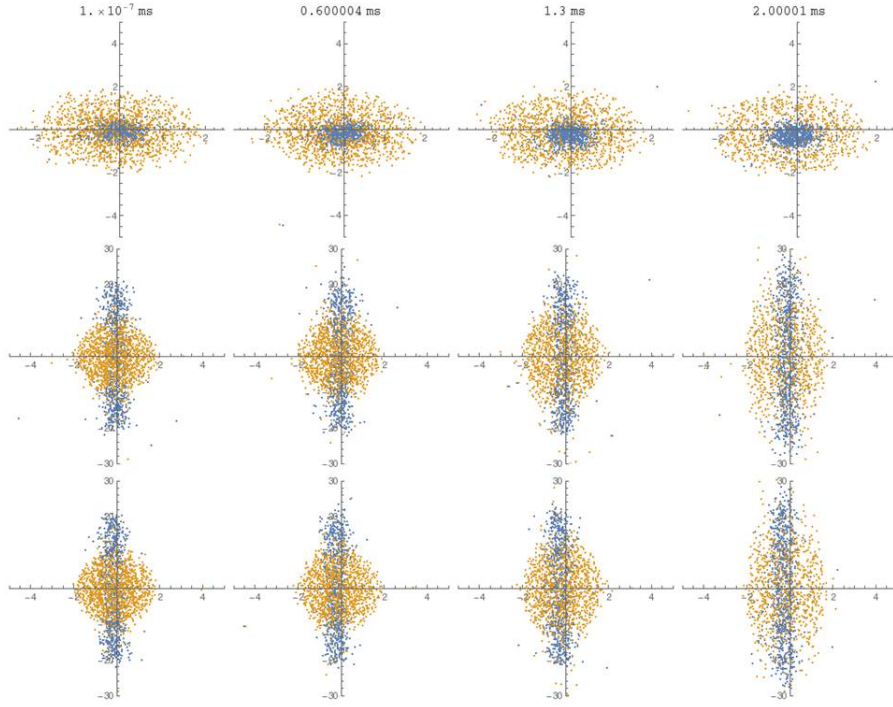


(a) Development of the plasma-shape: LiF_2^- in blue and Ba^+ in yellow.

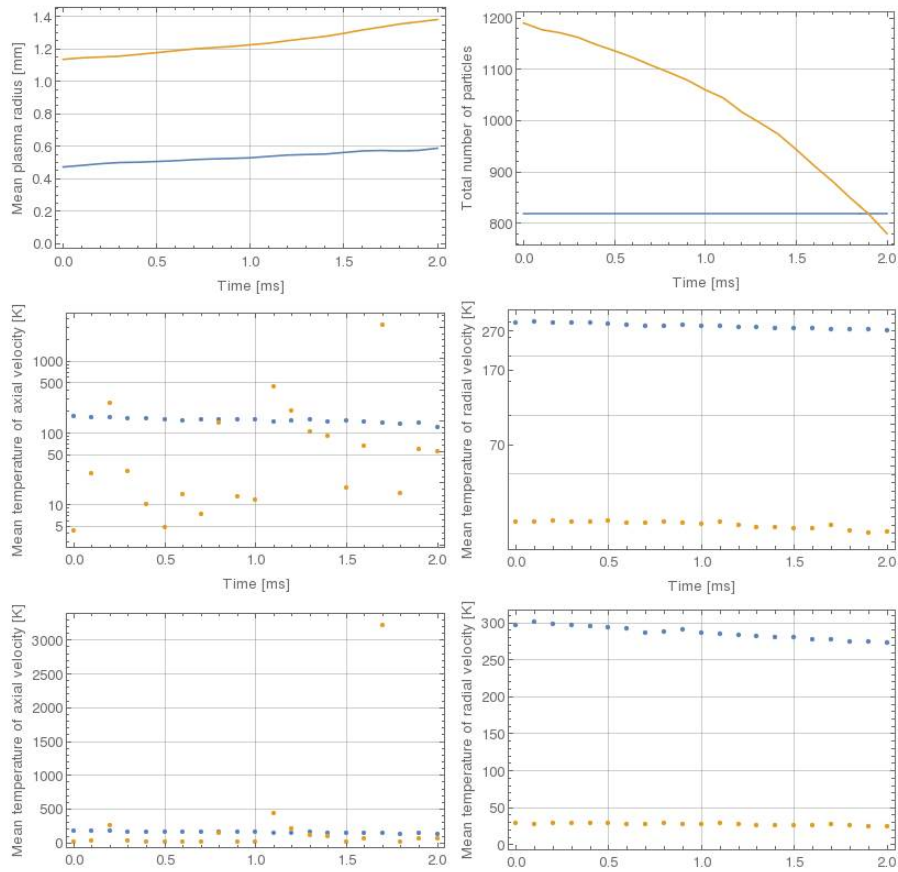


(b) Plasma-temperature, -number and -radius.

Figure 28: Example-4, a test-simulation to find suitable plasma and penning-trap parameters.



(a) Development of the plasma-shape: LiF_2^- in blue and Ba^+ in yellow.



(b) Plasma-temperature, -number and -radius.

Figure 29: Example-5, a test-simulation to find suitable plasma and penning-trap parameters.

Even though the spatial shape of the plasma looks promising regarding a radial separation due to rotationally induced centrifugal migration, the histograms in figure 30 show no evidence of controlled concentric shell formation. More precisely, there is no sign of any redistribution of the radial positions of the Barium cations from the left to the right. It appears that the Ba^+ gets kicked out of the trap while interacting with LiF_2^- in the mixing region since the potential is too low to confine the heated barium axially. These Barium losses continue until the density of the cations is too low to observe any further interaction between the species.

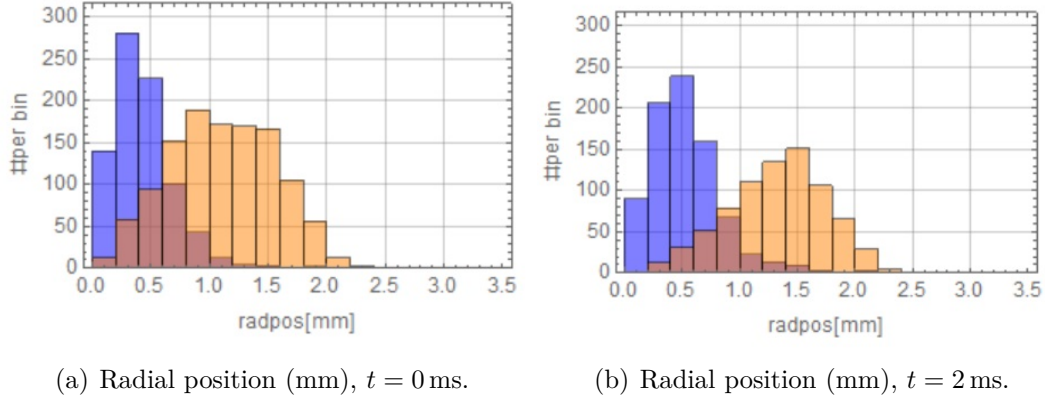
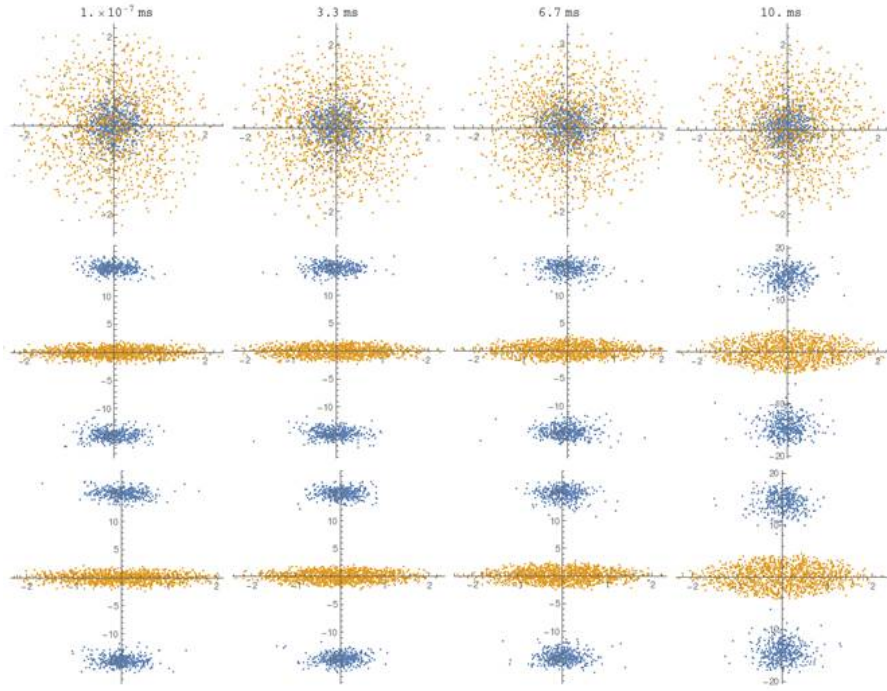


Figure 30: radial position (mm) of the particles for $t=0$ ms and $t = 2$ ms. The positions of the LiF_2^- are held in blue, the Ba^+ -positions in yellow and the brown areas indicate an overlap of the two species.

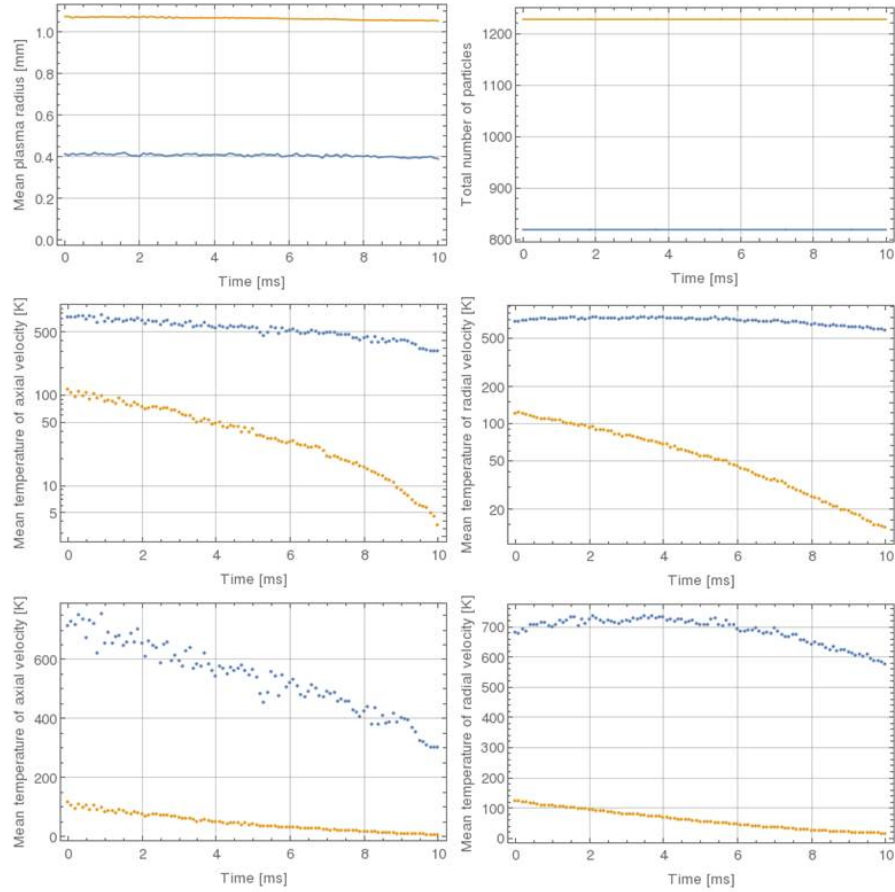
To avoid these uncontrolled plasma-rotations and to simplify the penetration of the LiF_2^- through the cold Ba^+ -cloud, it was concluded that the Ba^+ -plasma-shape should be axially fattened and the magnetic field increased.

Testing the relation between cooling-observations and potential variations

Like mentioned in the previous section, the cooling-observations as shown in figure 31 are not clearly assignable to an interaction between the two species. Further tests indicated, that the visible cooling-effects are connected to the potential-ramping-process.



(a) Development of the plasma-shape: LiF_2^- in blue and Ba^+ in yellow.



(b) Plasma-temperature, -number and -radius.

Figure 31: Example-6, a test-simulation to find suitable plasma and penning-trap parameters.

In figure 31 it can be seen that the LiF_2^- cools down from around 700 K to 300 K in 10 ms in axial and about 100 K in radial direction, while the potential is ramped down from -10 V to -1 V in 10 ms. The magnetic field is set to 1.5 T. The temperature of the laser-cooled Ba^+ goes down from around 100 K to 3 K in axial and also about 100 K in radial direction. As can be seen in figure 32 the densities of both species decrease, since the charged particles of both species occupy a larger volume in axial direction, due to the decreasing absolute value of the potential. This increase of volume causes an adiabatic cooling-effect, which is clearly visible for the not lasercooled LiF_2^- . The next example underlines, why a sympathetic cooling effect can be ruled out in this case. Since the plasma radii are still constant no LiF_2^- - Ba^+ -pairs have yet coupled to each other.

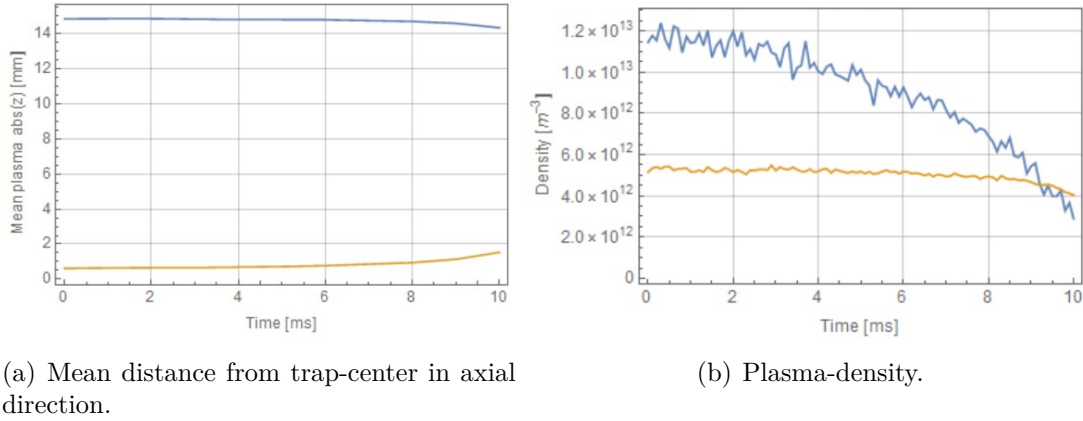
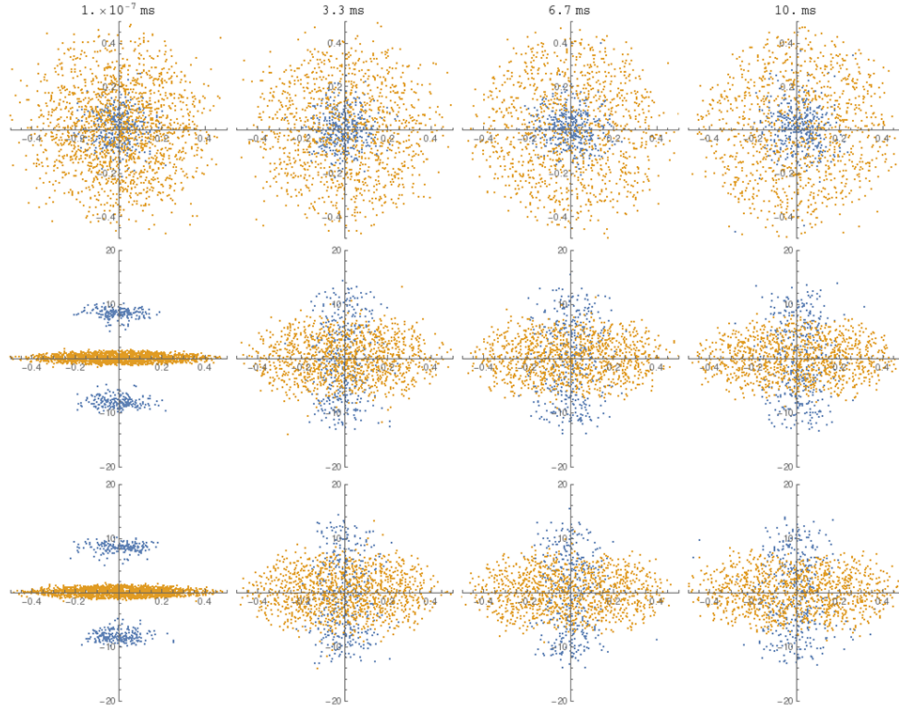
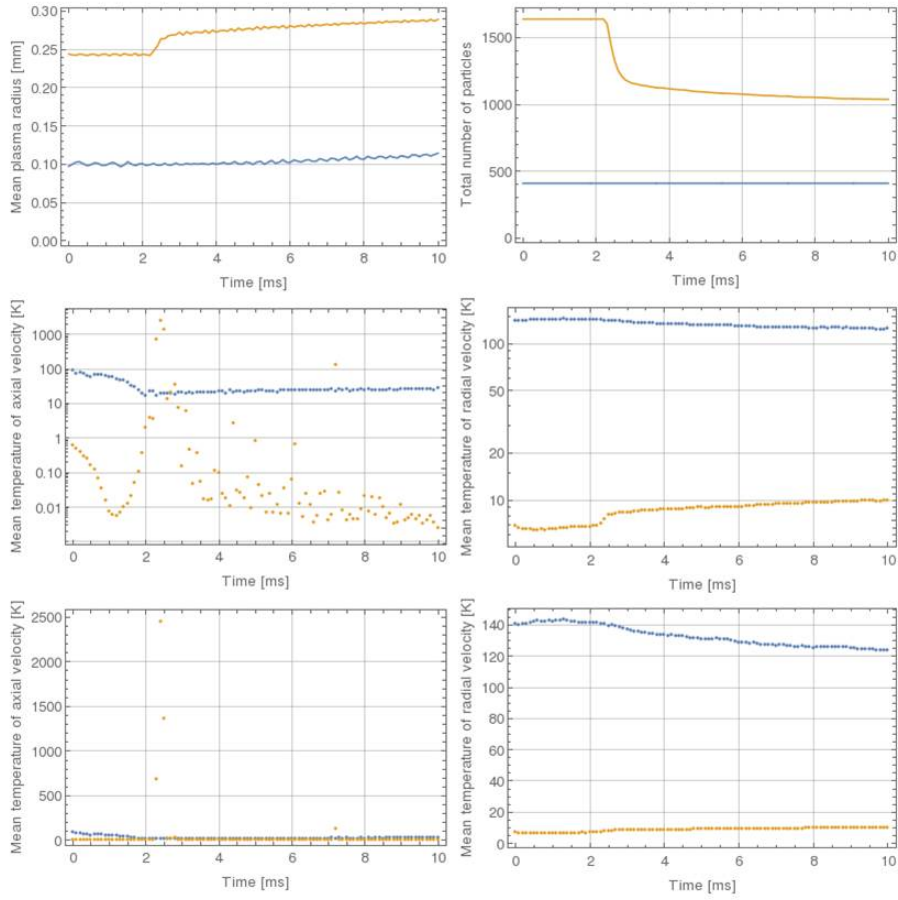


Figure 32: Example-6, further analysis.

The next example shows a very clear evidence for the relation between cooling-observations and potential variation.



(a) Development of the plasma-shape: LiF_2^- in blue and Ba^+ in yellow.



(b) Plasma-temperature, -number and -radius.

Figure 33: Example-7, a test-simulation to find suitable plasma and penning-trap parameters.

In figure 33 the ramping-phase of the potential is completed in 2 ms, from -1 V to -0.01 V and the B -field is set to 2 T. What can be learned from example-7 is that the axial cooling-phase of the LiF_2^- -anions stops with the ramping of the potential after exactly 2 ms. The Ba^+ ions gain energy due to the interaction with the LiF_2^- and the ramping phase and leave the trap in axial direction. After the heated Barium left the trap, the Barium cloud stabilizes and the lasers cool the cloud down again. Besides, in radial direction the LiF_2^- is cooled down about 15 K probably by interacting with the cold Barium cloud.

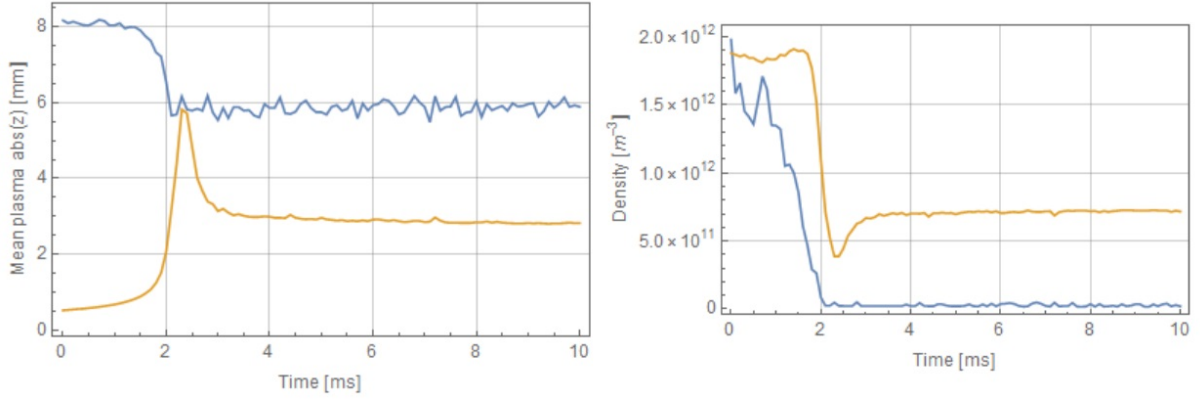
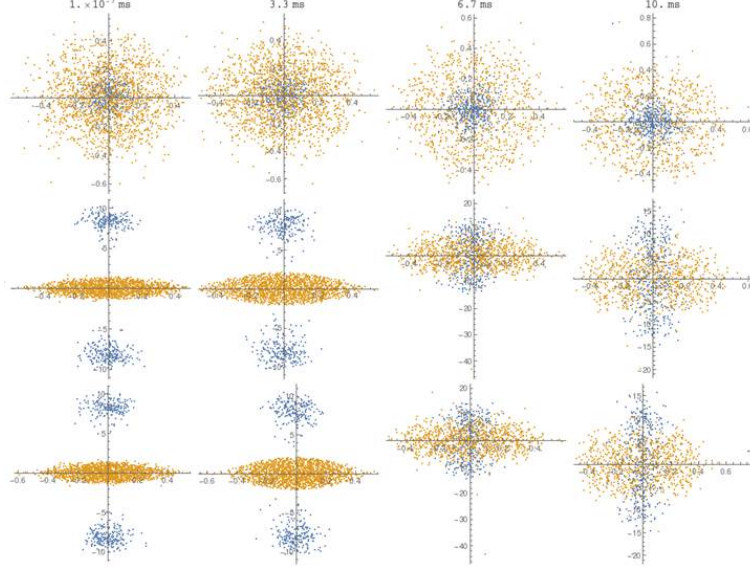
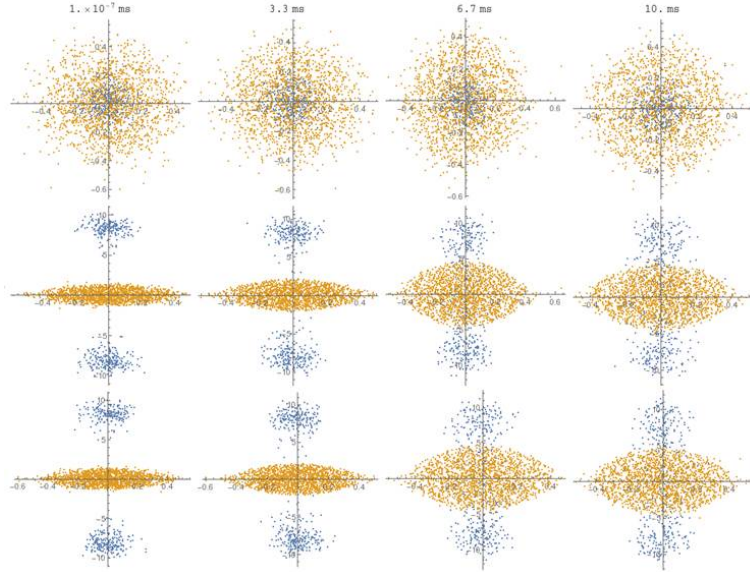


Figure 34: Example-7, further analysis: mean axial plasma distance from the trap center (left) and plasma densities (right).

One last test to learn about the effects caused by the potential-variations is shown in figure 35. For this comparison the same ramping velocity (~ -1.99 V/ms) was used to see if any unexpected effects occur. On the left side, the potential was lowered from -1 V to -0.005 V in 5 ms and on the right side to -0.05 V in 4.77 ms. The B -field was in both cases set to 2 T.



(a) Spatial shape, -1 V to -0.005 V.

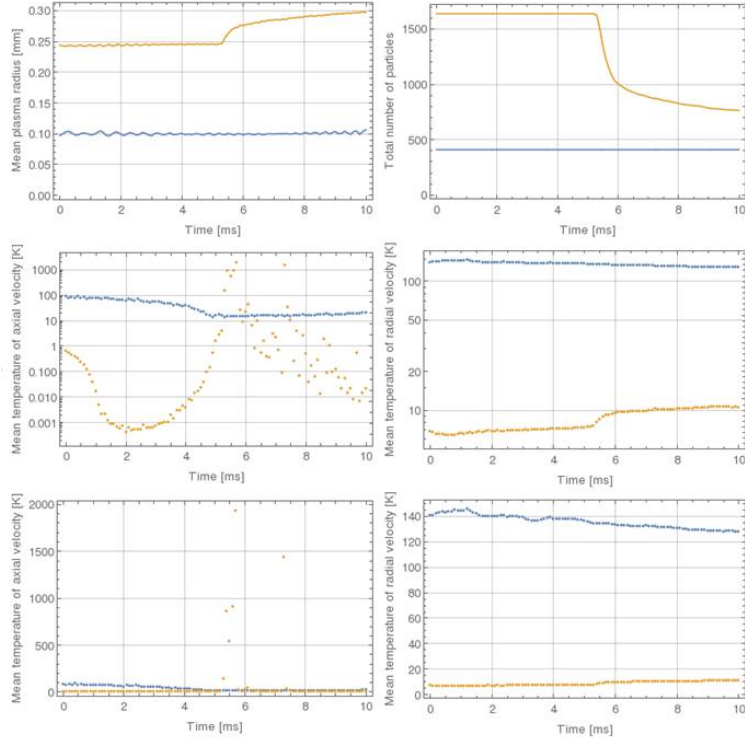


(b) Spatial shape, -1 V to -0.05 V.

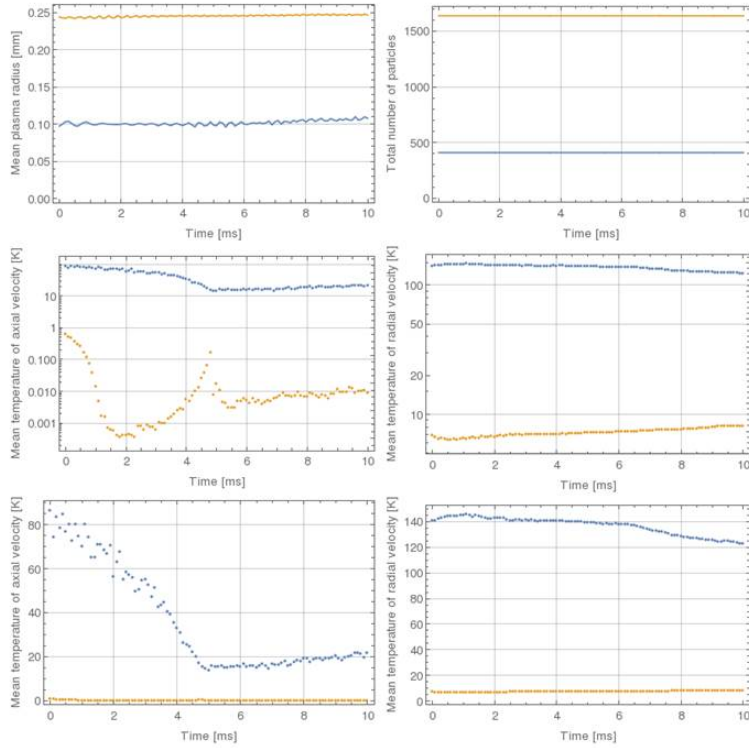
Figure 35: Example-8, a comparison of two simulations with the same ramping velocity but different simulation times.

This example confirms that the built-in ramping function does what it is supposed to do. As expected a similarity in the axial mean velocity plots is observed, see figure 36. Besides, it can be seen that the potential in the left case is already too low to confine the Ba^+ -ions axially, in contrary to the right example. Therefore there are many Ba^+ -losses in the left case. It's also worth noting, that the mean plasma radius increases sharply after the ramping phase. This can be explained with the fact that

the LiF_2^- interacts with the radial inner Ba^+ ions, while penetrating the cloud. These cation-losses lead to an increase of the mean radius. Radial losses or pair-formation are not observed.



(a) -1 V to -0.005 V : Plasma-temperature, -number and -radius.



(b) -1 V to -0.05 V : Plasma-temperature, -number and -radius.

Figure 36: Example-8, further analysis.

As expected the density of case b, see figure 37, falls down considerably less than the density in case a, especially for the cations.

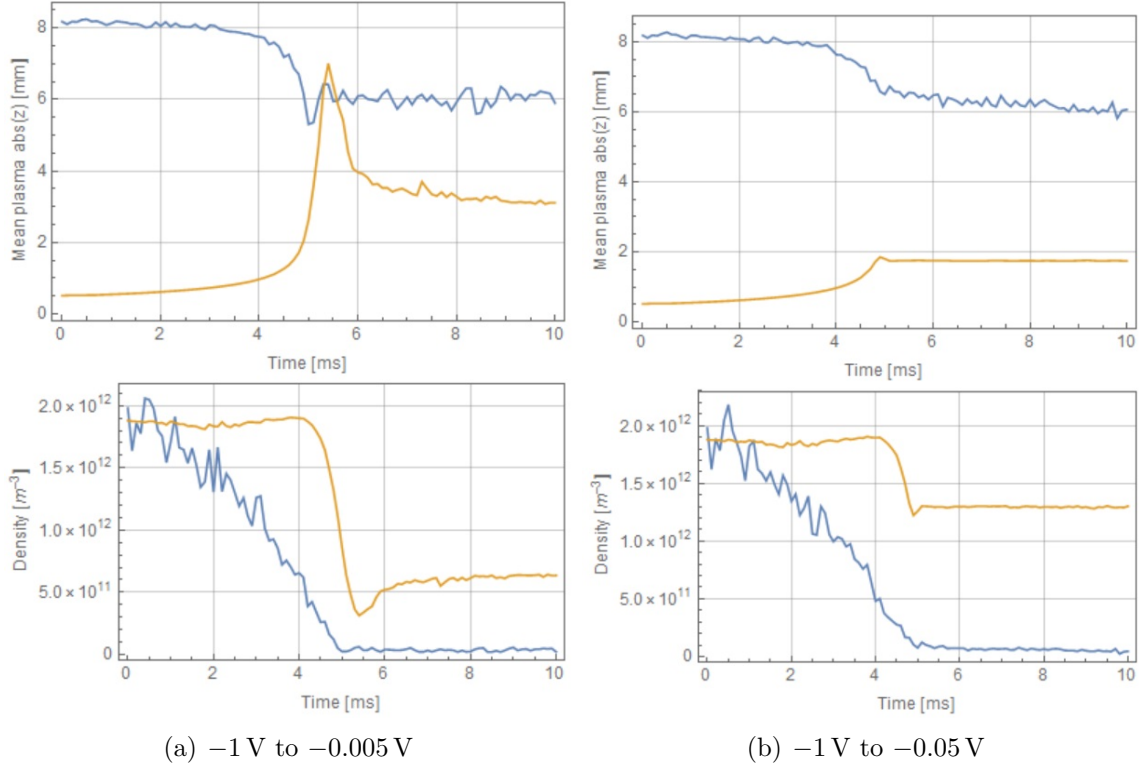


Figure 37: Example-8, Mean distance from trap-center in axial direction and plasma density.

7.4.1 Conclusion of the previous simulations

The previous tests and simulations suggest that a formation in concentric shells of the two and in the further course three species is hard to implement. Even though a shell formation was achieved, the losses of Ba^+ -ions are significant in axial direction, there is also no clear evidence for a sympathetic cooling effect observable. In radial direction a potential cooling-interaction could be observed between the species. This cooling effect could also arise due to the fact, that the axial motion of the particles equilibrates with the radial motion. Though, a sympathetic cooling effect is more likely since the radial Ba^+ -temperature is increasing while the radial LiF_2^- -temperature is decreasing, see for example figure 36.

The uncontrolled plasma-rotations could be avoided by initializing the Ba^+ -cloud very dense, cold and compact in axial direction and by increasing the magnetic field.

A cooling-effect for the LiF_2^- -ions in axial direction was observed which could be related to the variation respectively decreasing of the absolute value of the potential U_0 . This adiabatic cooling effect arises, since the density of the charged particle cloud decreases while ramping down the potential.

Besides, long simulation times have proven to cost particle losses through the formation of LiF_2^- - Ba^+ -pairs ("drifting pairs"), which escape the trap radially. This effect was also observed by ATRAP for antiprotons and positrons during the antihydrogen-production [39]. In general, a guiding center drift atom (a weakly bound electron-ion pair) is formed, if the electrons cyclotron frequency is the largest of the dynamical frequencies, due to a sufficiently strong magnetic field. Besides, the smallest length scale is given by the cyclotron radius of the electron. Under these circumstances, the rapid cyclotron motion can be averaged out and the dynamics of the electron can be treated with guiding center drift theory. These pairs are weakly bound and strongly magnetized.

Figure 38 shows a sketch of a possible kind of motion for a guiding center atom, a so-called drifting pair, where the binding energy is comparatively low. In this case, the ion $E \times B$ drifts in the field of the electron and the electron $E \times B$ drifts in the field of the ion. Further, the electron and the ion move together perpendicular to the magnetic field. This kind of weakly bound state formation and its typical drift effect seems to be comparable to the bound state between the LiF_2^- and Ba^+ occurring in the previous simulations, also regarding the observed behaviour of the pair (radial drift).

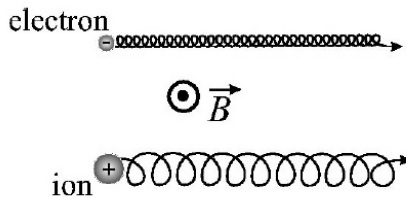


Figure 38: Sketch of drifting ion-electron pair,[39].

This effect can be delayed by applying a higher magnetic field since this increases

the cyclotron motion and therefore a bound state is more difficult to form.

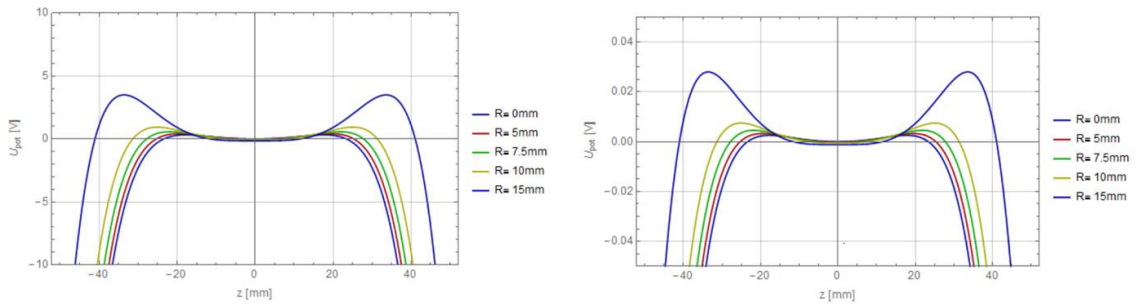
7.5 Final sympathetic-cooling simulations

To finally see a clear sympathetic cooling effect between the species, the simulation work-flow was slightly changed. Instead of initializing the LiF_2^- -ions at the beginning of the simulations together with the Ba^+ -cations, just the Ba^+ -cloud was initialized and cooled down close to the doppler-limit. The trap-potential is ramped down as far as possible, still confining the particles.

In the next step, the LiF_2^- is initialized directly into the center of the cold Ba^+ -rotation-spheroid by replacing Ba^+ cations as LiF_2^- anions in the input-data for Simbuca. The ratio is held at 1:50, so 40 LiF_2^- -anionic molecules were initialized in a cold cloud of 2005 cations. Additionally, the coulomb factor was set to one. This way, rotation effects, which occurred in the previous simulations as well as effects arising from the potential-ramping could be avoided respectively clearly distinguished.

7.5.1 Initialization of Ba^+ , thermalization and laser-cooling

For this simulations a magnetic field of 3 T was chosen and two lasers were applied cooling the Ba^+ in axial direction. The trap-potential can be seen in figure 39, on the left side the potential at the initialization of the cations at -10 V and on the right side the potential with the lowest possible absolute value still confining the cations axially.



(a) -10 V: trapping and cooling Ba^+ .

(b) -0.08 V: Lowest possible potential still keeping the Ba^+ cations.

Figure 39: Trap-potential.

Figure 40 shows the spatial shape of the laser-cooled Ba^+ -cloud, figure 41, the respective plots with the mean distance of the particle to the trap center in axial direction, the mean plasma radius, the density, the number of particles and again the temperature of the particles. Not to be confused, **in this and all following examples the colors representing the particles are switched, which means that Ba^+ is painted blue and LiF_2^- yellow.**

The particle-temperature-calculation is in this example based on the standard deviation of the velocity histograms. This way, the magnetron motion of the particles can be subtracted since the magnetron motion can be seen as a general offset of the

Maxwell-Boltzmann distribution in each time-step, which does of course not effect the shape of the distribution. With this fact in mind and using

$$\sigma = \sqrt{\frac{k_B T}{m}} \quad (7.14)$$

the particle temperature can be calculated without the magnetron-offset to give a more precise result.

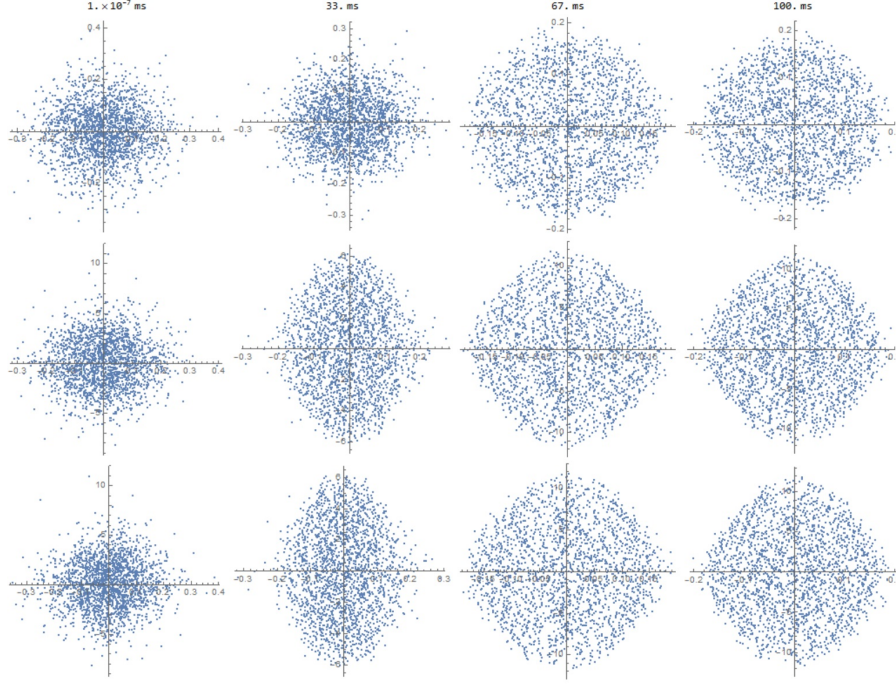


Figure 40: Spatial shape: Ba⁺ only.

As can be seen in 41, the axial temperature of the cations has cooled down to about $54 \mu\text{K}$ (the doppler-limit lies at $40.37 \mu\text{K}$). The radial temperature is splitted up in the velocity component in $\hat{\phi}$ -direction and in the velocity component in $\hat{r}$ -direction (polar coordinates), where

$$\hat{r} = (\cos(\phi), \sin(\phi)) \quad (7.15)$$

and

$$\hat{\phi} = (-\sin(\phi), \cos(\phi)) \quad (7.16)$$

are the respective unit vectors,

$$r = \sqrt{x^2 + y^2} \quad (7.17)$$

and

$$\phi = \arctan y/x \quad (7.18)$$

where x and y denote the Cartesian coordinates.

The potential was in this 100 ms simulation ramped down from -1 V to -0.08 V in 50 ms.

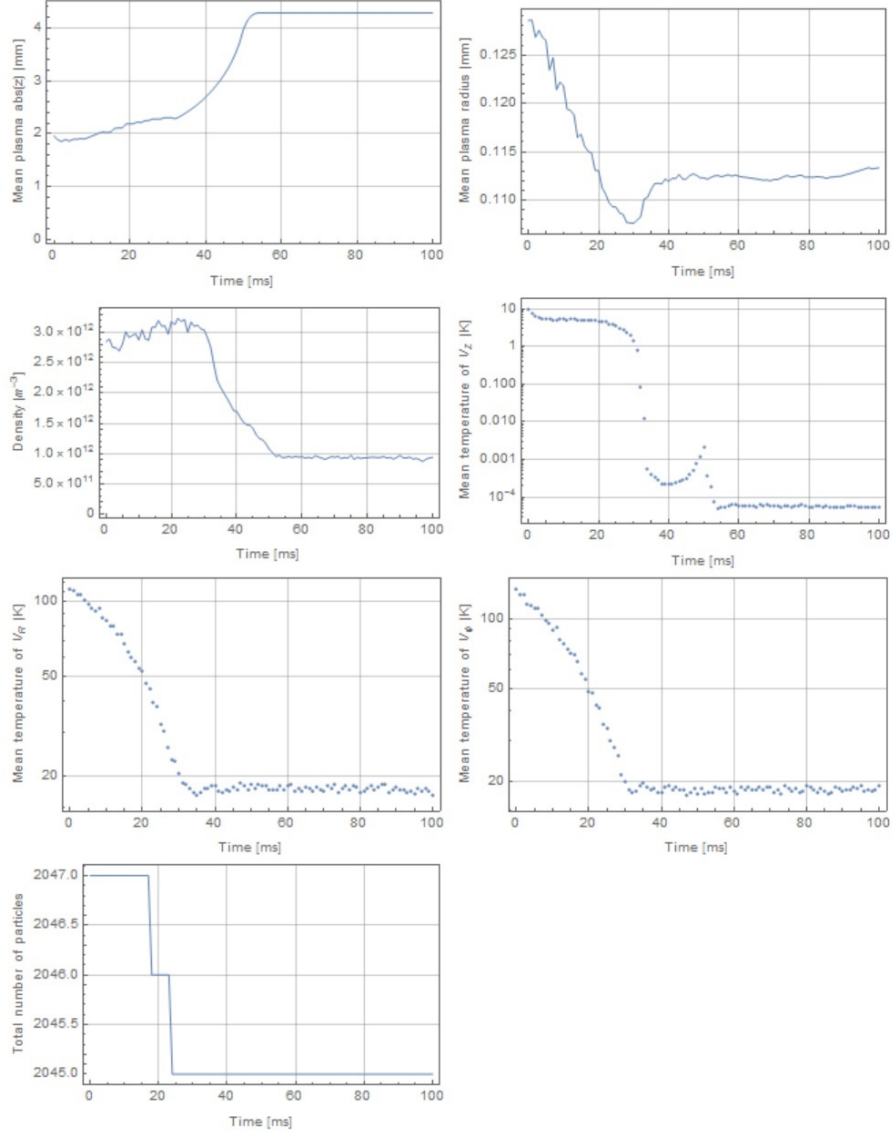


Figure 41: Final simulations: plasma-temperature (without magnetron motion), -density, -radius, -axial distance from trap-center and -number.

Also interesting to see in 41 is that the peak in the axial temperature plot of the cations at around ~ 50 ms also occurs without a second species initialized. This means, that this typical peak (see also figures 37 or 33) can not be related to the species interacting but is an effect clearly resulting from the potential variations.

After preparing the Barium-plasma, the next simulation step could be performed.

Initialization of LiF_2^- in the center of the Ba^+ -cloud

The following figures show the plasma after initializing the LiF_2^- -ions. The 40 ions replaced the randomly selected cations within an cylindrically shaped volume inside the Ba^+ -cloud.

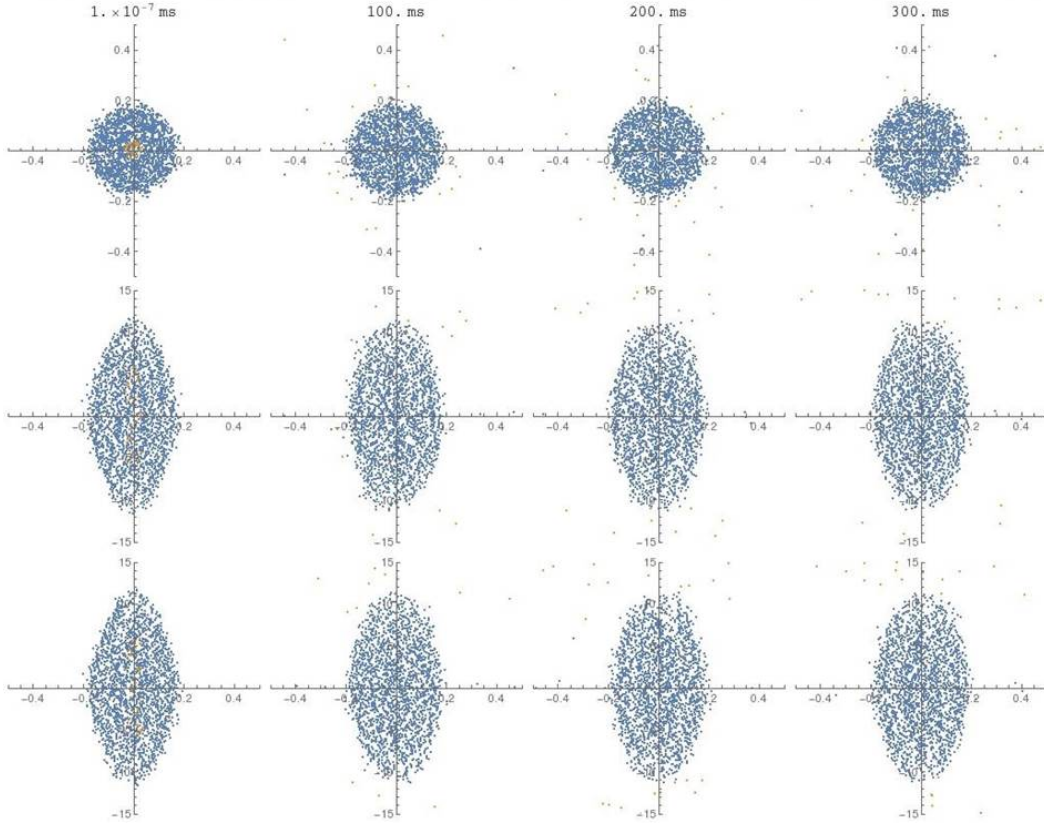


Figure 42: Spatial shape: 40 Ba^+ -cations (blue) are replaced by LiF_2^- (yellow) in the cloud-center.

As can be seen in 43 the LiF_2^- -ions are cooled down from 102 K to 6 K (axial) and from 98 K to 33 K (radial). It should be pointed out again, that no potential variations were implemented during this 300 ms simulation, which means that the observed cooling effect is due to coulomb-interaction between the species. It also can be observed that the most effective cooling occurs in the first 50 ms. After this period, the mean radius of the LiF_2^- -ions has increased significant, which is probably the reason for the decreasing cooling-efficiency.

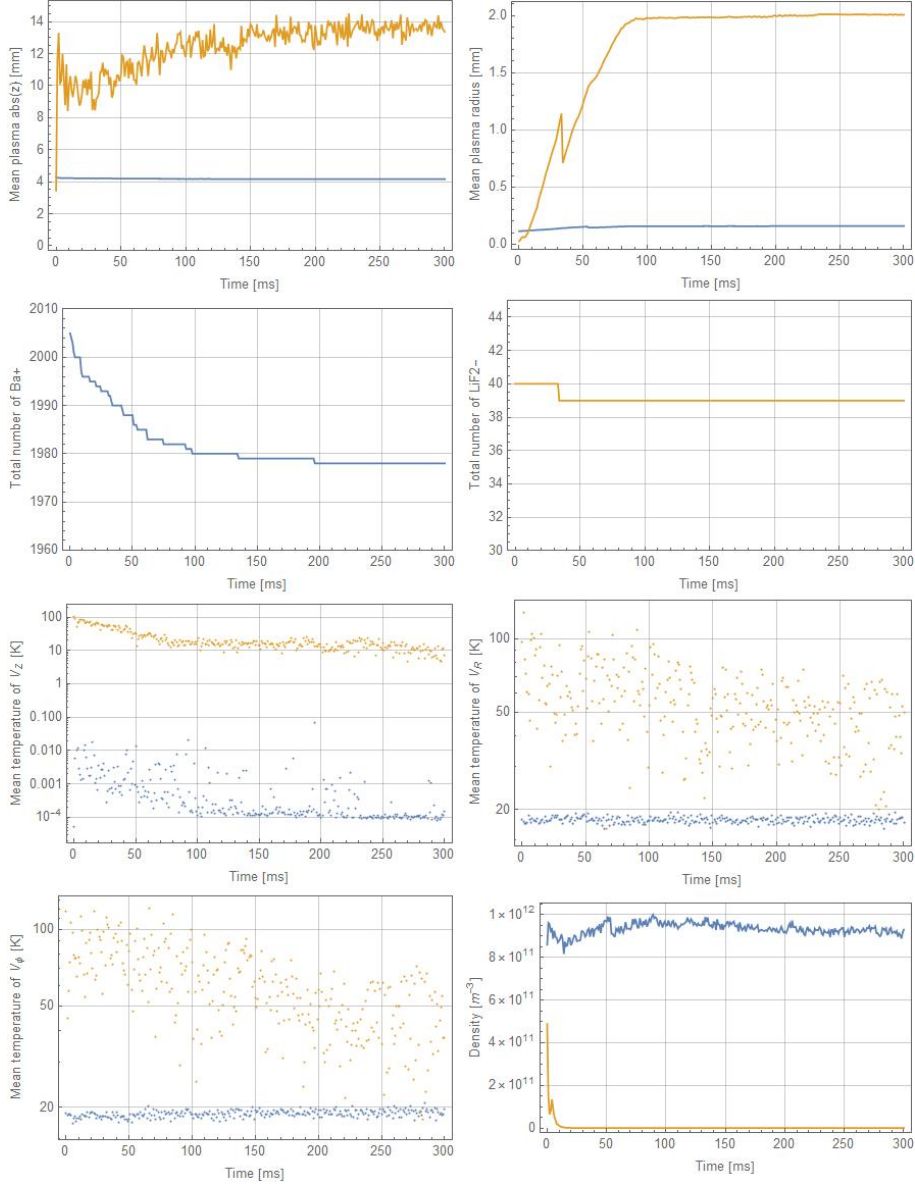


Figure 43: Plasma-temperature (without magnetron motion), -density, -radius, -axial distance from trap-center and -number, Ba^+ (blue) and LiF_2^- (orange).

The widening of the the mean plasma-radius of the LiF_2^- -ions from 0.05 mm to 2 mm in the first 100 ms, can be explained again by pair formation between the two species. The Ba^+ -mean plasma radius is naturally not as much increasing since the ratio of the species was set to 1:50.

Another detail worth noticing is that, 24 Ba^+ -cations leave the trap axially during this simulation and two particles hit the electrode wall (leave the trap radially) - one LiF_2^- - Ba^+ -pair.

7.5.2 Positions and Frequencies of the LiF_2^-

To learn more about the behaviour of the charged particles and their interaction some analysis was done which is presented in the following. Figure 44 and 45 analyse the spatial positions of the individual LiF_2^- . In figure 45 the mean position of the Ba^+ -cloud is further indicated in blue. What can be seen in these figures is that the LiF_2^- falls back into the potential sidebags after the initialization at the trap-center. Besides, there is no significant change in the axial direction on average. Thus, most LiF_2^- ions sit in the potential-sidebags, while interacting with the Barium-cations. Only a few ions are crossing the cloud. And also the radial widening can be clearly observed in these to figures.

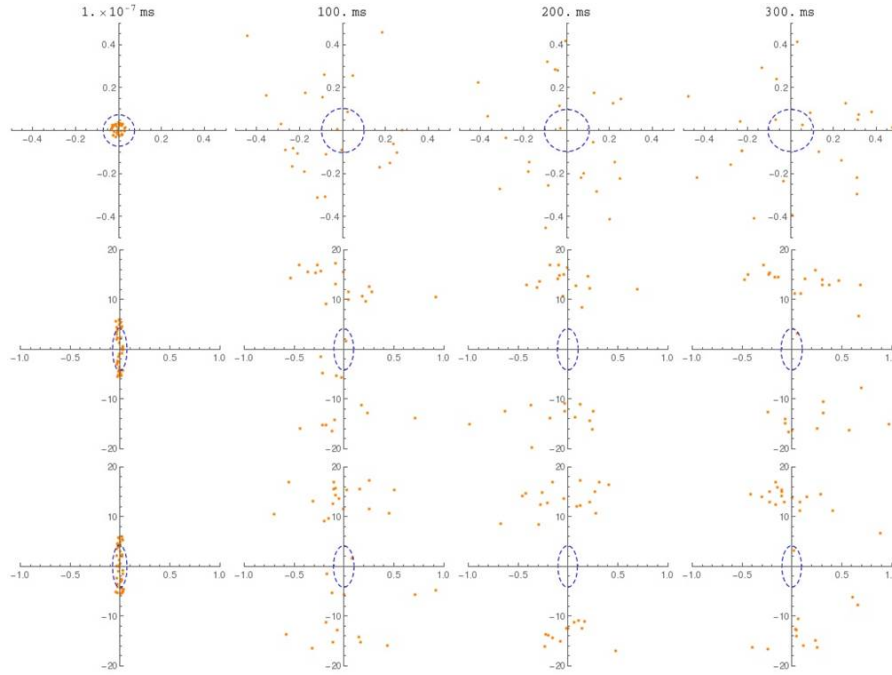


Figure 44: LiF_2^- spatial-shape (yellow) and Ba^+ absolute mean position (blue).

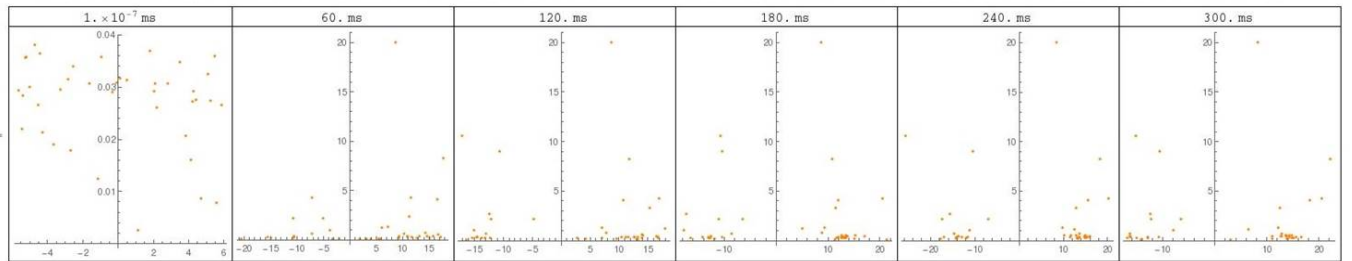


Figure 45: LiF_2^- positions only: radial position (y -axis) against the axial position (x -axis).

The next analysis done focuses on the particle frequencies ω_z (axial frequency), ω_+ (reduced cyclotron frequency), ω_- (magnetron frequency) and ω_c (cyclotron frequency), see also section 4. The frequencies were estimated by looking at the trajectory of an individual LiF_2^- in the respective direction:

To get an idea in which time-range the respective oscillations should be resolved, the frequencies were calculated in a first step for a harmonic potential, with the given trap-parameters.

ω_-	8 Hz
ω_c	6.6 MHz
ω_+	6.4 Hz
ω_z	10.1 kHz

Table: Calculated frequencies for a harmonic trap potential.

As can be seen in figure 46, the magnetron frequency is very difficult to estimate, since the radii of the individual LiF_2^- vary too severely. The range of the magnetron frequency is about from ~ 5 to 15 Hz.

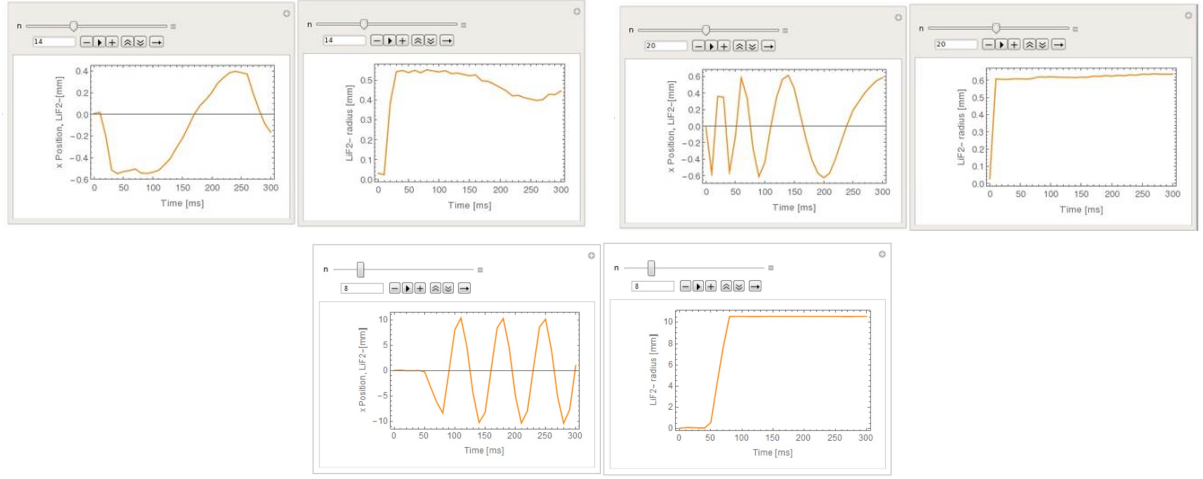


Figure 46: Magnetron motion estimated by looking at individual LiF_2^- : x -coordinate of the LiF_2^- , in addition, the anion-radius is shown.

The axial frequency can be estimated to be around ~ 1 to 2.5 kHz. In figure 47, the axial trajectories are shown for two individual anions. One of them crossing the cold Barium-cloud axially during the simulation and one of them is caught in a potential sidebag.

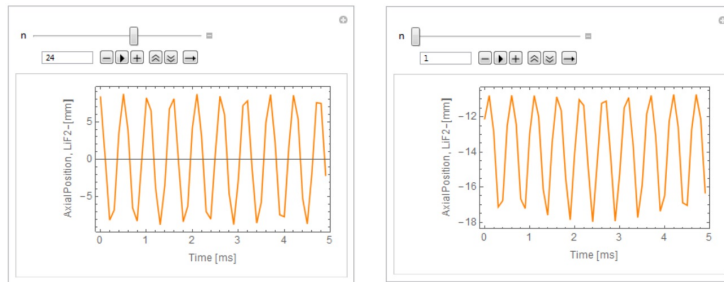


Figure 47: Axial frequency estimated by looking at individual LiF_2^- : x -coordinate of the LiF_2^- , in addition, the anion-radius is shown.

For the estimation of the comparatively very high cyclotron frequency the trajectory in x -direction was observed with a higher resolution for 0.01 ms. The frequency could be estimated to lie around ~ 1 MHz, as can be seen in figure 48.

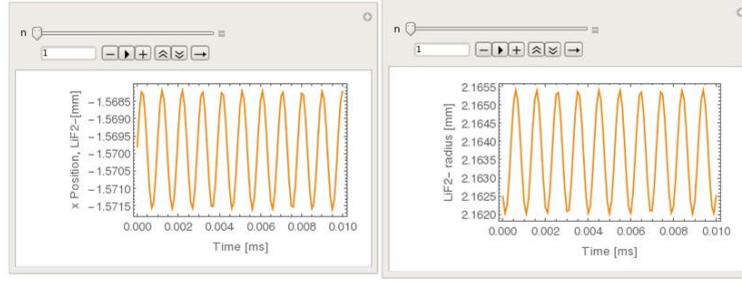


Figure 48: Cyclotron frequency: Axial position and radial distance from the trap-center of an individual LiF_2^- .

These values should be kept in mind for the following detailed analysis of individual LiF_2^- ions, to be able to interpret oscillations occurring in the analysis-plots correctly.

7.5.3 Detailed analysis of individual LiF_2^-

To study the behaviour of the LiF_2^- even further and its interaction with the Ba^+ , a detailed analysis of the 300 ms simulation shown in 43 is done for individual LiF_2^- in this section. The quoted examples are analysed in the following and labelled as **anion-xx**, where **xx** represents a number and corresponds to the respective particle number outputted by Simbuca.

Included in this analysis is also the number of collisions between the two species. By implementing the respective Code in Simbuca, the number of collisions was outputted for individual LiF_2^- . A collision was chosen to take place if the distance between a LiF_2^- and a Ba^+ (d_{LB}) is smaller or equals $10 \mu\text{m}$. Besides, to save simulation-time, only the first 30 ms were outputted since the collision-code was implemented in the CPU-code.

Li-index2044,collisions	67553	←
Li-index2043,collisions	22706	
Li-index2042,collisions	30639	
Li-index2041,collisions	43032	
Li-index2040,collisions	36747	
Li-index2039,collisions	32745	
Li-index2038,collisions	28599	
Li-index2037,collisions	35610	
Li-index2036,collisions	50965	←
Li-index2035,collisions	11316	
Li-index2034,collisions	51622	
Li-index2033,collisions	29092	
Li-index2032,collisions	40737	
Li-index2031,collisions	59157	
Li-index2030,collisions	36597	
Li-index2029,collisions	43222	
Li-index2028,collisions	35763	
Li-index2027,collisions	30795	
Li-index2026,collisions	49504	
Li-index2025,collisions	65132	←
Li-index2024,collisions	31046	
Li-index2023,collisions	39874	
Li-index2022,collisions	41235	
Li-index2021,collisions	54282	
Li-index2020,collisions	14331	
Li-index2019,collisions	44705	
Li-index2018,collisions	31551	
Li-index2017,collisions	89968	←
Li-index2016,collisions	42671	
Li-index2015,collisions	30999	
Li-index2014,collisions	20089	
Li-index2013,collisions	41111	
Li-index2012,collisions	46330	
Li-index2011,collisions	45274	
Li-index2010,collisions	45120	
Li-index2009,collisions	67860	
Li-index2008,collisions	53893	
Li-index2007,collisions	9779	←
Li-index2006,collisions	25156	
Li-index2005,collisions	22239	

Figure 49: Number of collisions of individual LiF_2^- after 30 ms. The arrows indicate high and low rates.

In the first example, a LiF_2^- is observed, which forms a bound state with a Ba^+ cation and leaves the trap radially after around 30 ms and hits the electrode walls with a radius of 2 cm.

In figure 50 it can be seen that the radial position of the particle increases sharply after ~ 5 ms. Besides, the axial position oscillates in the first 5 ms, what means that the particle crosses the Barium cloud several times before it gets caught by the Coulomb-field of a single Barium at 5 ms. Before the anion gets caught a (sympathetic) cooling process is visible in axial direction.

Figure 51 shows on the left side the collision-rate of the LiF_2^- of **anion-3**. The rate stays constant at ~ 9700 collisions at the time the distance d_{LB} reaches its minimum, respectively the bound state is formed. This can be explained by having a closer look at the distance between the couple which is oscillating around $30 \mu\text{m}$, the maximal distance to output a collision was set to $10 \mu\text{m}$, therefore the bound state is not seen as a collision. Besides, it is clearly observable that the interparticle distance is varying in the first 5 ms since the LiF_2^- is axially crossing the Barium cloud repeatedly (see figure 50).

In the next example (Anion-8), the full 300 ms simulation of a single LiF_2^- is analysed. This example should show that the anion leaves the bound state and is afterwards caught by a potential sidebag without any further cooling observation.

In figure 52 it can be seen that the anion crosses the cold Barium cloud in the first 50 ms multiple times, then from the 50th to 80th ms a drifting-pairs formed and the radius of the LiF_2^- widens to around 10.5 mm. After the 80th ms the anion leaves the bound state again and gains kinetic energy through the electrostatic potential-sidebag, in which the particles oscillates without any further observable interaction with the Barium cloud.

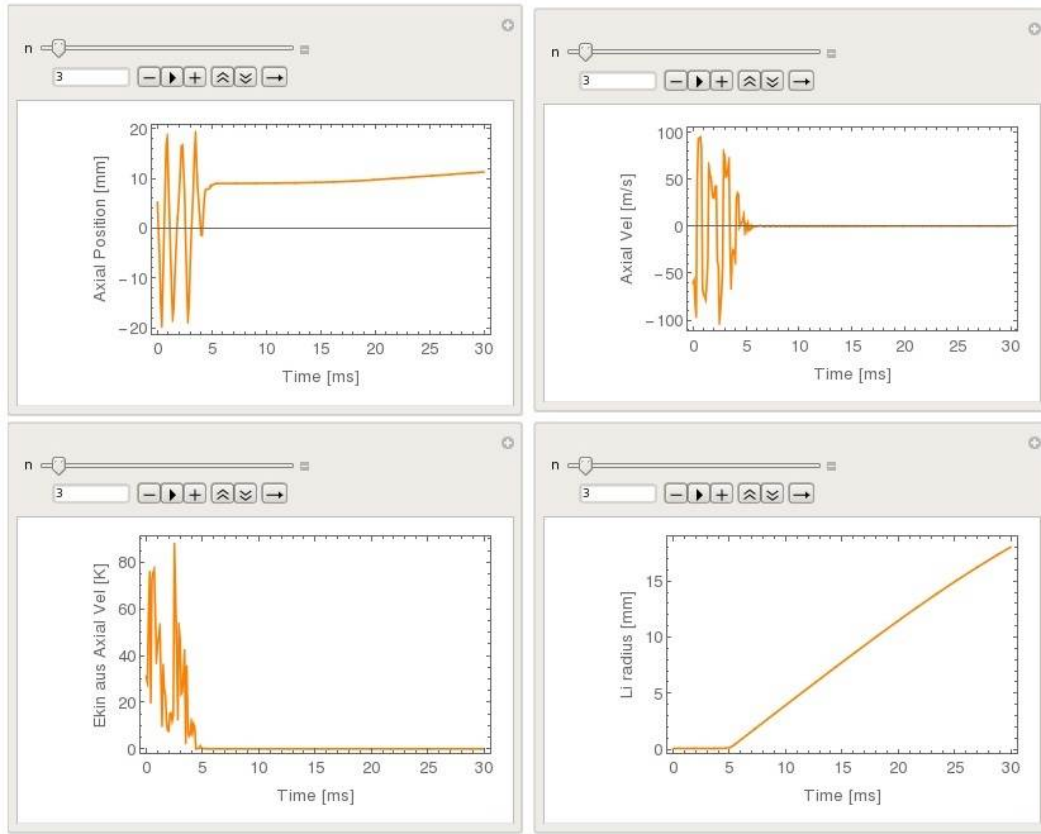
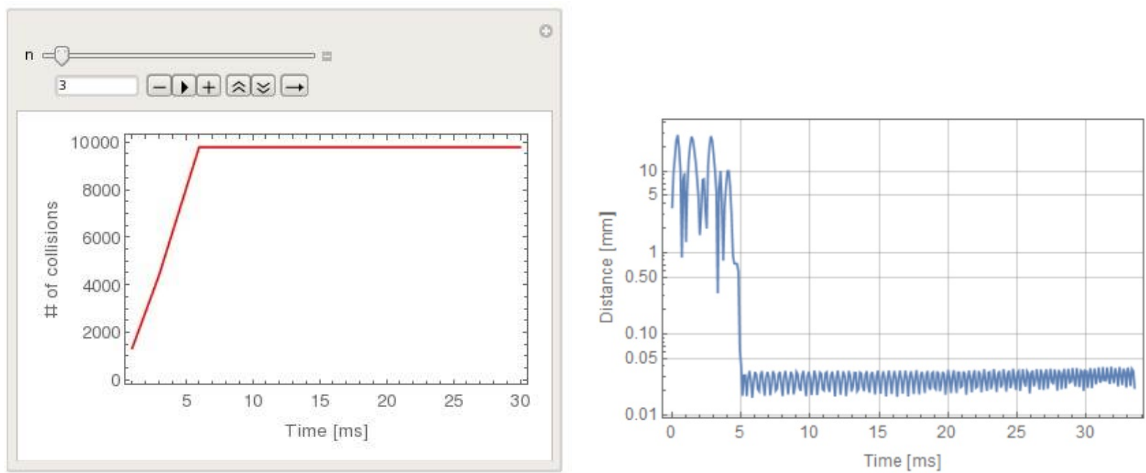


Figure 50: **Anion-3: Pair-Formation:** Axial Position, Axial Velocity, Axial Temperature, Radial Position of LiF_2^- leaving the trap after 30 ms.



(a) LiF_2^- -collision-rate

(b) Absolute distance of the couple in logarithmic scaling

Figure 51: **Anion-3:** Analysis the LiF_2^- of the formed neutral bound state.

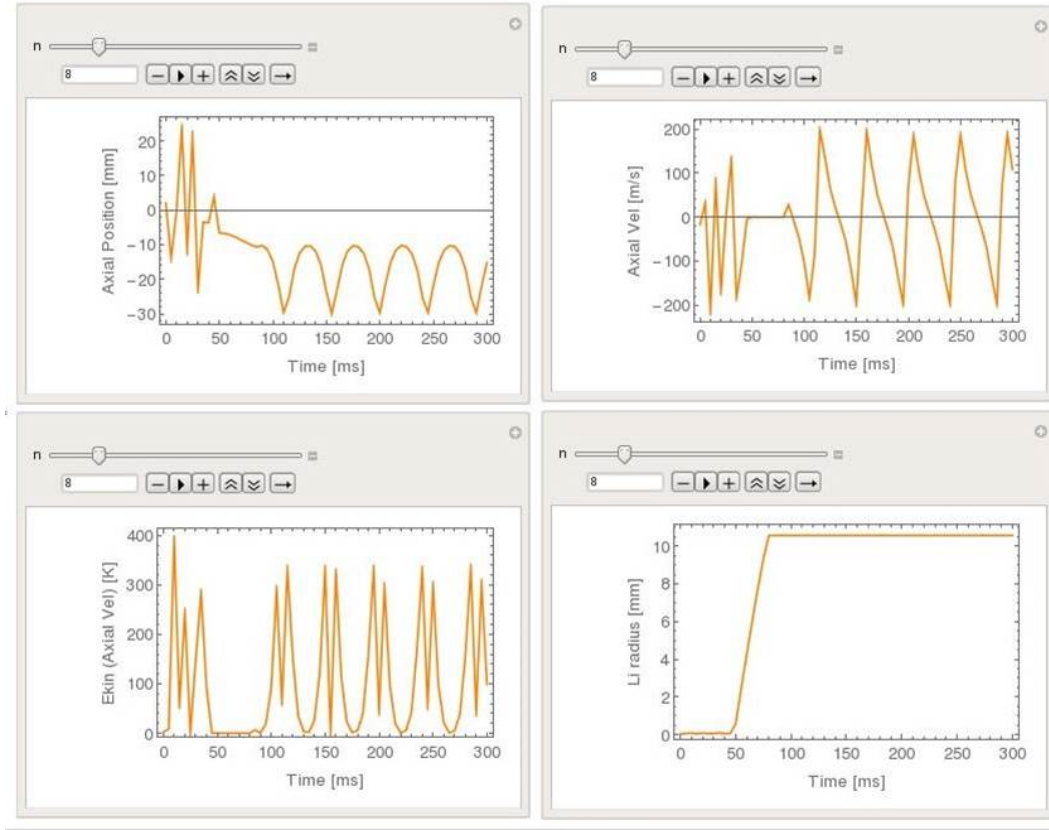
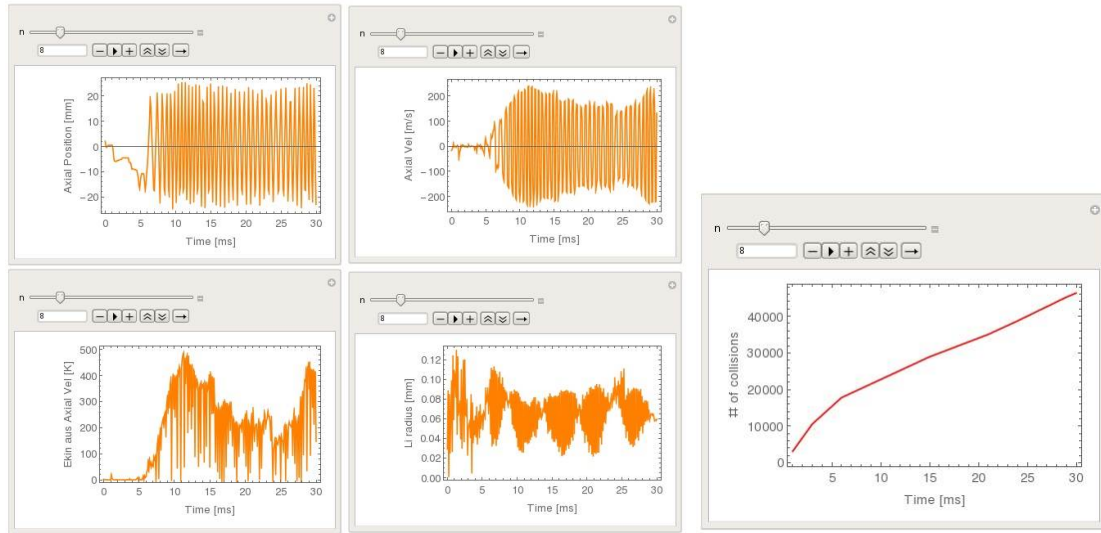


Figure 52: **Anion-8: Pair-formation and break up:** Axial Position, Axial Velocity, Axial Temperature, Radial Position of a single LiF_2^- for 300 ms.



(a) Axial Position, Axial Velocity, Axial Temperature, Radial Position of a single LiF_2^- .

(b) LiF_2^- -collision-rate.

Figure 53: **Anion-8:** High-resolution-analysis of the behaviour of a single LiF_2^- during the first 30 ms.

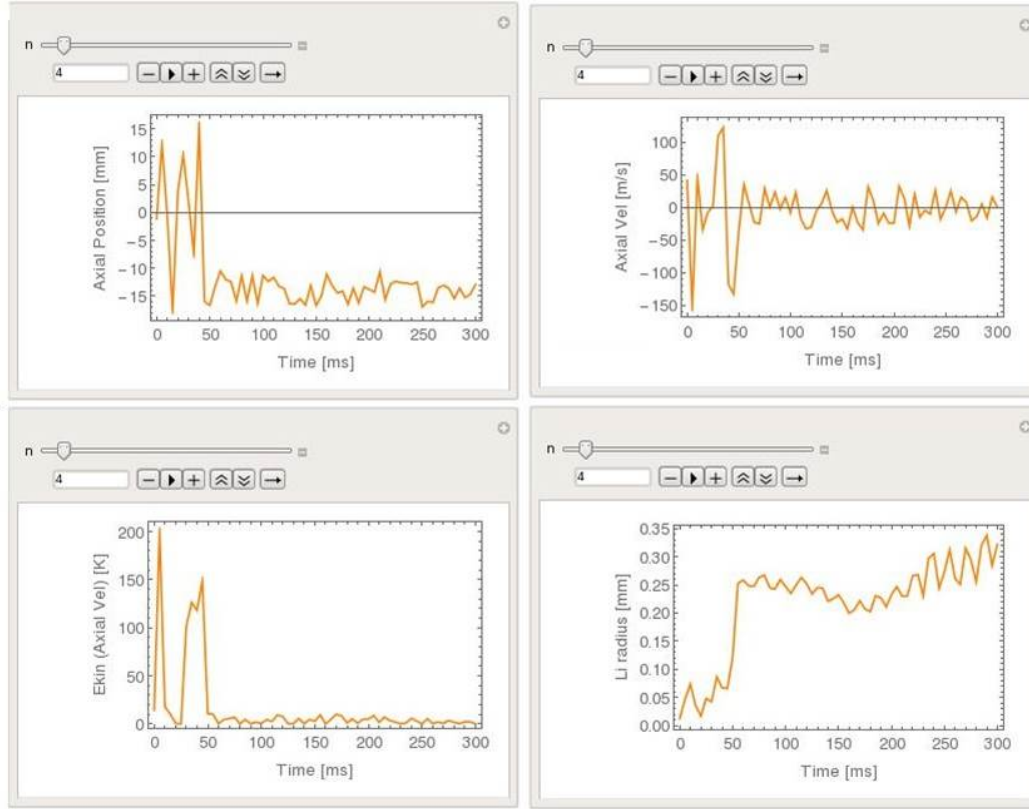


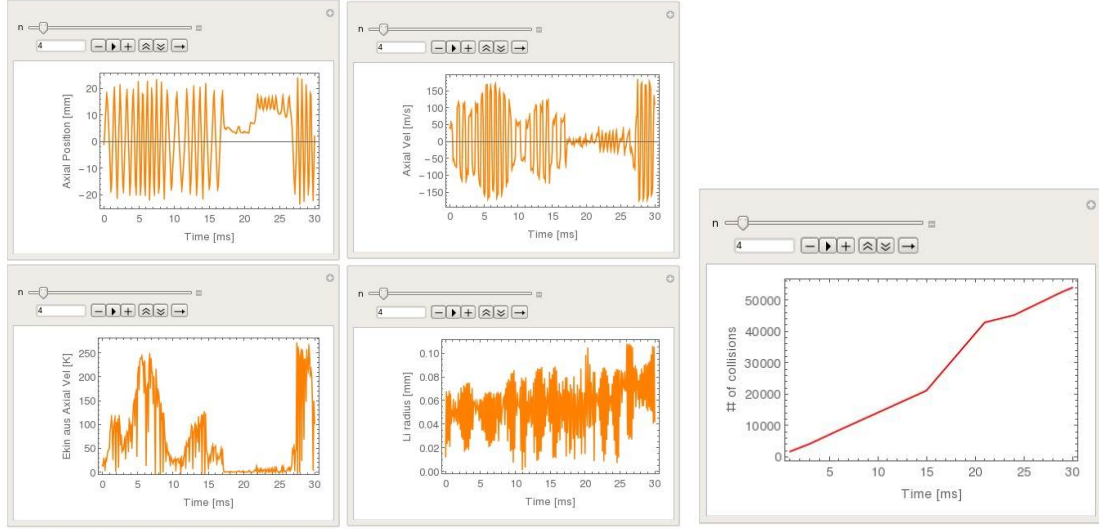
Figure 54: **Anion-4: LiF_2^- is crossing the Barium cloud and gets caught in the lower potential bag:** Axial Position, Axial Velocity, Axial Temperature, Radial Position of a single LiF_2^- for 300 ms.

Figure 53 shows the first 30 ms of the 300 ms simulation (of **anion-8**) with a higher resolution to resolve the axial motion of the anion and to relate the behaviour of the particle with the collision-rate. The axial frequency can be estimated from the axial-position plot in figure 53 to be around 2 kHz, see also subsection 7.5.2. Furthermore, it should be noticed that the LiF_2^- is at the beginning relatively cold with a temperature of around 2 K, then it seems to collide with many cations inside the cold Barium cloud in the first few milliseconds. This can be concluded by looking at the radial and axial position of the anion and additionally at the high collision-rate in the first milliseconds. After leaving the Barium cloud axially, the LiF_2^- gains kinetic energy through the potential respectively collisions and starts crossing the Barium cloud. No sign of couple formation is shown in the first 30 ms.

The next example (**anion-4**) follows a LiF_2^- which is crossing the Barium cloud axially multiple times and then gets caught in the lower potential-bag, with low kinetic energy of a few Kelvin.

In figure 54 one can observe that the LiF_2^- -anion is crossing the cold Barium cations multiple times axially and is caught subsequently in one of the potential sidebags at 50 ms with comparatively low kinetic energy of a few Kelvin. Besides around the 50th millisecond a bound-state is formed according to the sharp increase of the anions radial position.

Interesting to see in the high resolved plots 55 is that the number of collisions in-



(a) Axial Position, Axial Velocity, Axial Temperature, Radial Position of a single LiF_2^-

(b) LiF_2^- -collision-rate.

Figure 55: **Anion-4:** High-resolution-analysis of the behaviour of a single LiF_2^- during the first 30 ms.

creases sharply in the interval from 17 to 22 ms. During the whole 30 ms the LiF_2^- is radially within the Barium cloud and the high collision rate starts at very low kinetic energies of the anion. Around the 26th ms the anion gains kinetic energy and starts crossing the cation cloud again.

Anion-31 is again caught in one of the potential-sidebags after around the 11th ms. Besides, the sharp increase of radius indicates a short pair-formation around the 6th ms.

In figure 56 an efficient cooling phase is visible in the first few ms. After the short pair-formation the anion is caught inside the sidebag-potential. There are irregularities in the oscillation of the axial position respectively velocity and radius observable (in comparison to e.g. **anion-8**) which could be an indication that still interaction with the cations occurs.

Figure 57 shows a comparatively low collision rate, which can be explained by the fact that the anion leaves the Barium cloud around the 7th ms radially.

The next Example (**anion-11**) shows an axial cooling process of the anion in the first 200 ms while crossing the Barium cloud. The anion is sympathetically cooling down from around 720 to a few Kelvin.

Like shown in figure 58 the LiF_2^- stays radially within the Barium cloud for the first 200 ms. Afterwards, the cold anion is again caught in one of the sidebag potentials.

The collision rate is relatively low with ~ 31000 collisions after 30 ms, as can be seen in figure 59. The reason is probably the high kinetic energy of the particle during this time. Since the anion is too fast to get caught in any coulomb-potential it just randomly gets close enough to individual cations to trigger a collision.

The next example shows a LiF_2^- which gets caught again in one of the potential sidebags, where it oscillates axially. Thus, the axial temperature oscillates as well around 20 K. The radius of this anion is again already around 4 mm, due to a previous

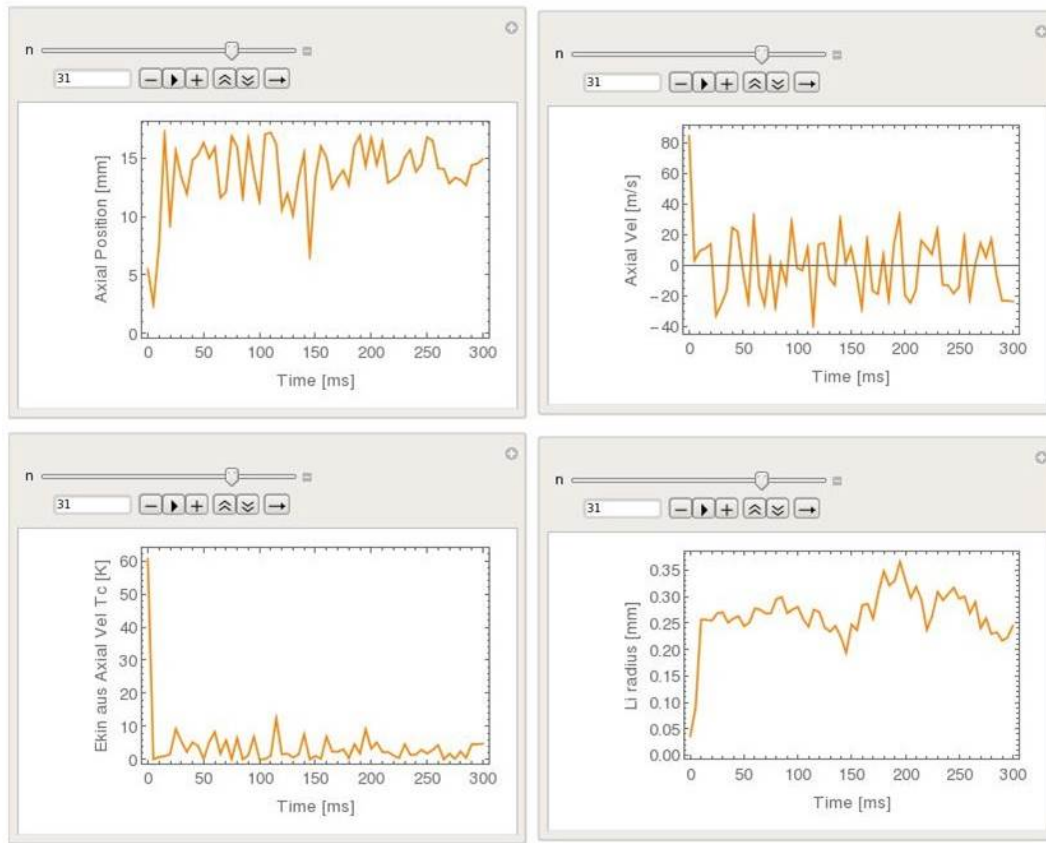
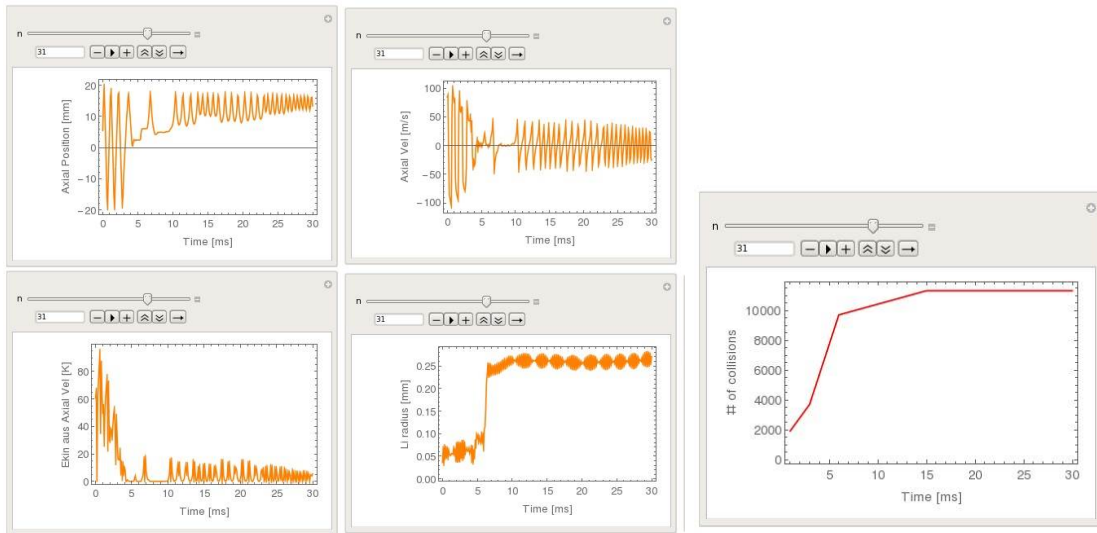


Figure 56: **Anion-31** LiF_2^- is caught in upper potential-bag: Axial Position, Axial Velocity, Axial Temperature, Radial Position of a single LiF_2^- for 300 ms.



(a) Axial Position, Axial Velocity, Axial Temperature, Radial Position of a single LiF_2^- .

(b) LiF_2^- -collision-rate.

Figure 57: **Anion-31**: High-resolution-analysis of the behaviour of a single LiF_2^- during the first 30 ms.

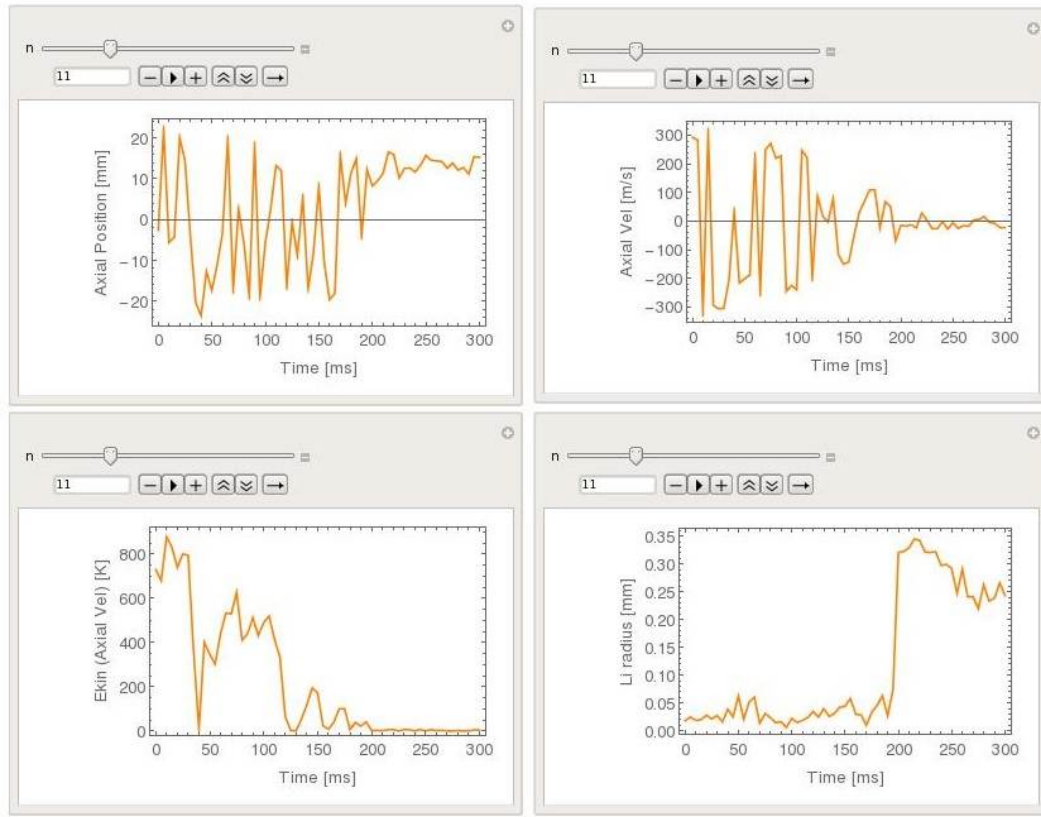
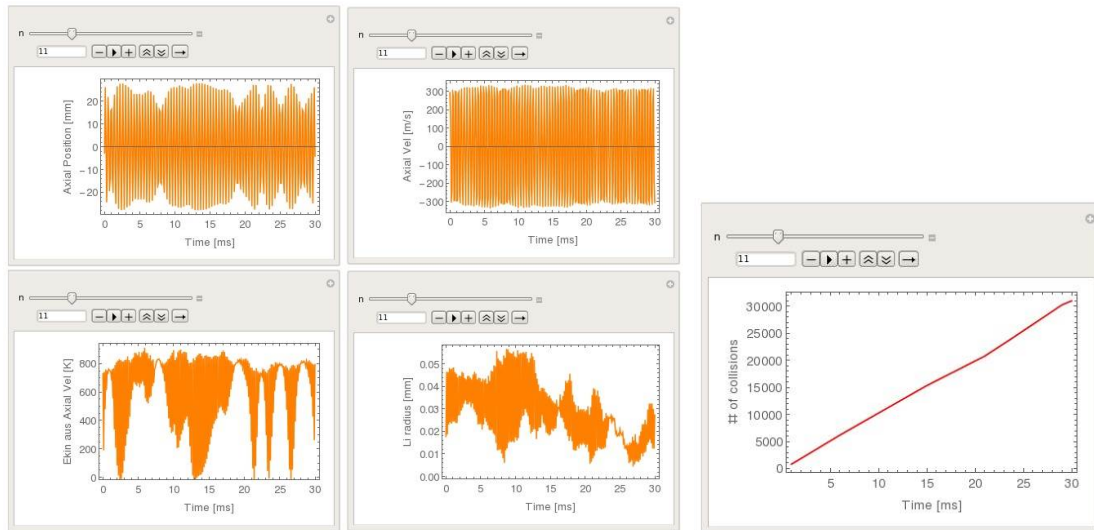


Figure 58: **Anion-11: The LiF_2^- is crossing the Barium cloud and cooling down to a few K:** Axial Position, Axial Velocity, Axial Temperature, Radial Position of a single LiF_2^- for 300 ms.



(a) Axial Position, Axial Velocity, Axial Temperature, Radial Position of a single LiF_2^- .

(b) LiF_2^- -collision-rate.

Figure 59: **Anion-11: High-resolution-analysis of the behaviour of a single LiF_2^- during the first 30 ms.**

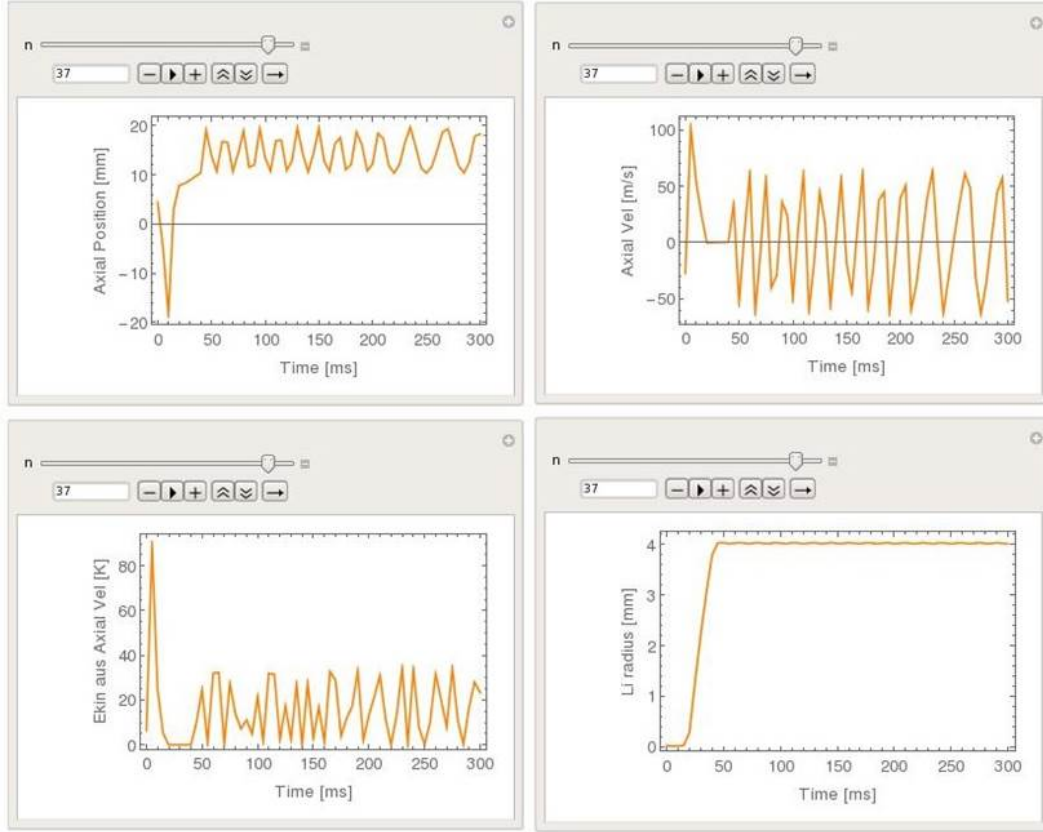


Figure 60: **Anion-37: The LiF_2^- is caught in one of the potential sidebags without a sufficient cooling effect visible:** Axial Position, Axial Velocity, Axial Temperature, Radial Position of a single LiF_2^- for 300 ms.

pair-formation after 18 ms.

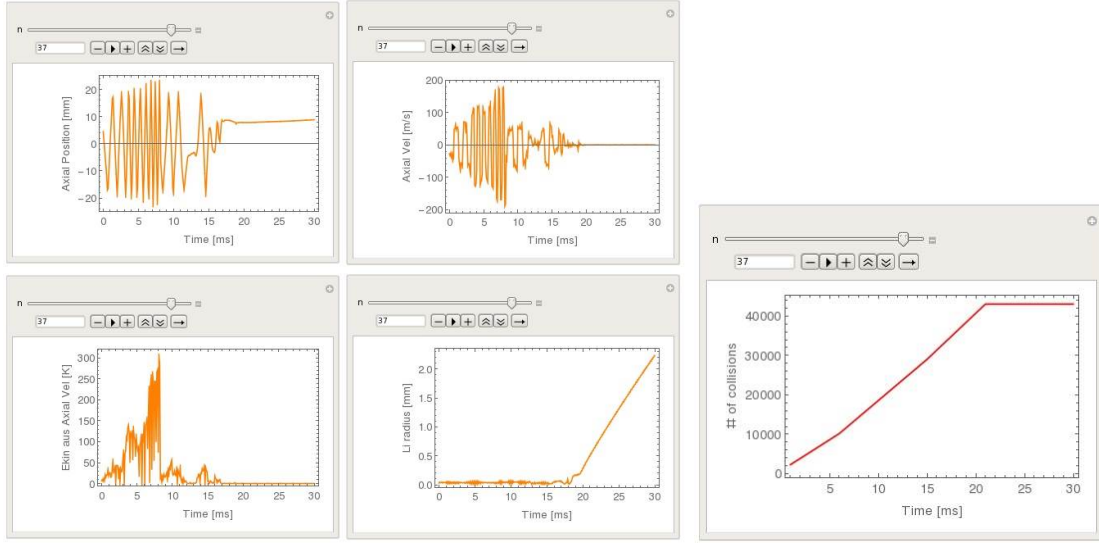
Like shown in figure 60 the LiF_2^- oscillates inside the sidebag potential with no cooling effect visible, since the size of the radius of the anion makes any interaction unlikely.

In the first 30 ms of 61 **anion-37** crosses the Barium cloud multiple times until it pairs with a cation around the 17th ms. At the time of pair-formation, the LiF_2^- is again relatively cold with a temperature of a few Kelvin. The irregularities in the axial oscillations between the 8th and the 17th ms can be attributed to the coulomb-interaction between the species. The collisions stop again immediately after the bound-state was formed.

In the next example (**anion-21**), especially the high resolution plots are of interest with respect to the collision rate.

The 300 ms simulation in figure 62 shows a evident cooling effect during the first ~ 50 ms, then the cold anion is again caught in one of the potential sidebags.

In figure 63 it can be clearly observed that the number of collisions increase during the time-intervals where the axial oscillations show irregularities. More precisely, the intervals from 3 to 7 ms and 24 to 29 ms. The kinetic energy of the charged particle is during this intervals in the range of a few Kelvin. Therefore it is straight forward to argue that at low energies, the LiF_2^- is slow enough to be caught by the coulomb-fields of the cations for a short timespan. If the kinetic energy of the anion is low enough a



(a) Axial Position, Axial Velocity, Axial Temperature, Radial Position of a single LiF_2^-

(b) LiF_2^- -collision-rate

Figure 61: **Anion-37:** High-resolution-analysis of the behaviour of a single LiF_2^- during the first 30 ms.

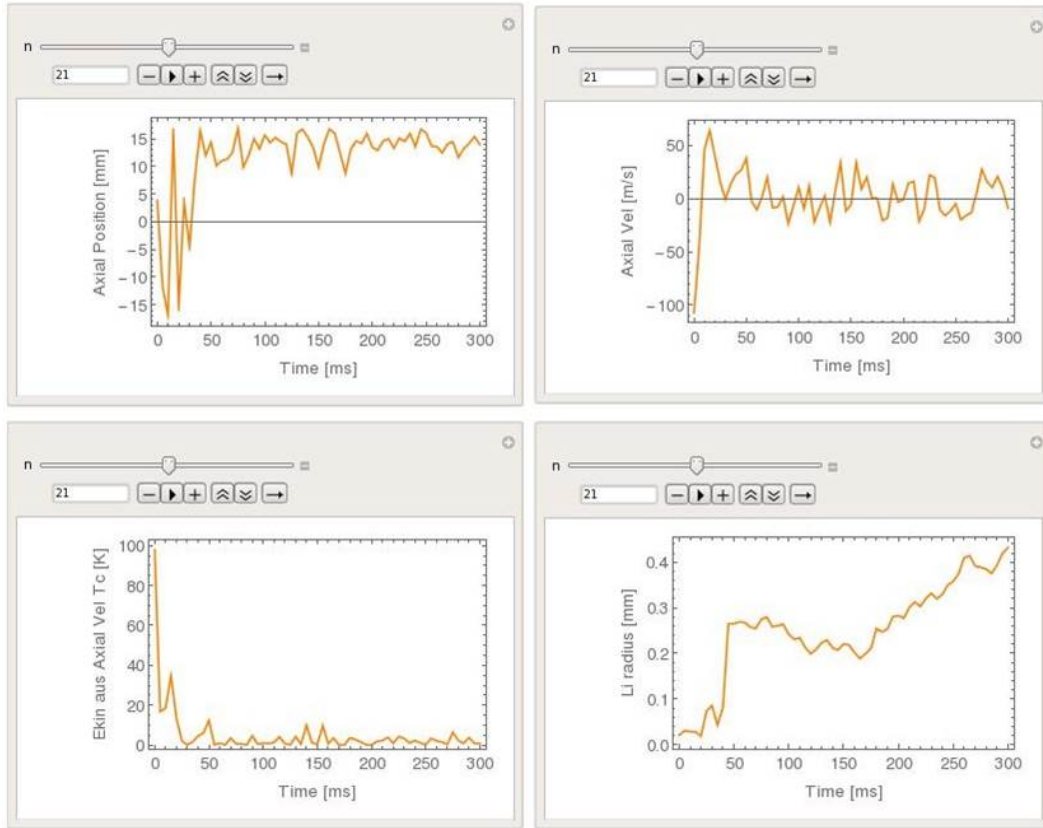
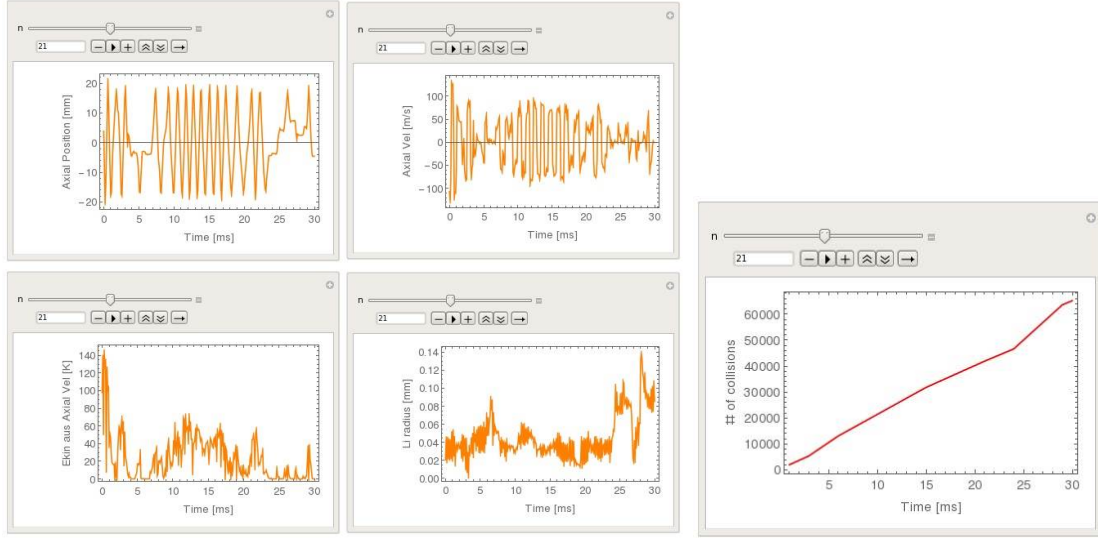


Figure 62: **Anion-21:** The LiF_2^- is crossing the Barium cloud and then caught in one of the potential sidebags: Axial Position, Axial Velocity, Axial Temperature, Radial Position of a single LiF_2^- for 300 ms



(a) Axial Position, Axial Velocity, Axial Temperature, Radial Position of a single LiF_2^-

(b) LiF_2^- -collision-rate

Figure 63: **Anion-21:** High-resolution-analysis of the behaviour of a single LiF_2^- during the first 30 ms.

pair-formation is possible.

The next example (**anion-24**) tracks a LiF_2^- which is initialized with a comparatively high temperature of ~ 800 K.

A clear sympathetic cooling process is visible in figure 64 especially during the first 50 ms.

The high resolution plots in figure 65 show a decrease in (axial) temperature from around 800 to 250 K. The anion is oscillating axially without any irregularities and the variation of the radius is comparatively small. The collision-rate is nearly constant during the whole timespan. At this velocities no sign of pair-formation is shown.

The next example (**anion-13**) shows a LiF_2^- which is initialized at lower temperature (around 13 K) compared to the last example. Interesting to see is that even though the particle was caught in the potential sidebag a cooling effect is still observable. Besides the collision rate in this example is the highest outputted.

The anion is caught again by a cation around the 20th ms as can be seen in figure 66. But although the anion is oscillating after leaving the bound-state inside the potential bag, irregularities are visible. The anions is still interacting with the barium cloud and the radius stays of course comparatively constant.

Between the 17th and 28th ms a high number of collisions can be observed, as can be seen in figure 67. The collisions stop again immediately at the time the pair-formation takes place. The collisions in this example count around 90000, which is the highest number of collisions of all individual LiF_2^- during the first 30 ms. After the 28th ms the anion binds again to a cation, the radius is increasing and the axial position stays comparatively constant.

The LiF_2^- in the next example (**anion-40**) is crossing the cold Barium and gets then caught in the sidebag potential, interesting here is that no cooling effect is visible.

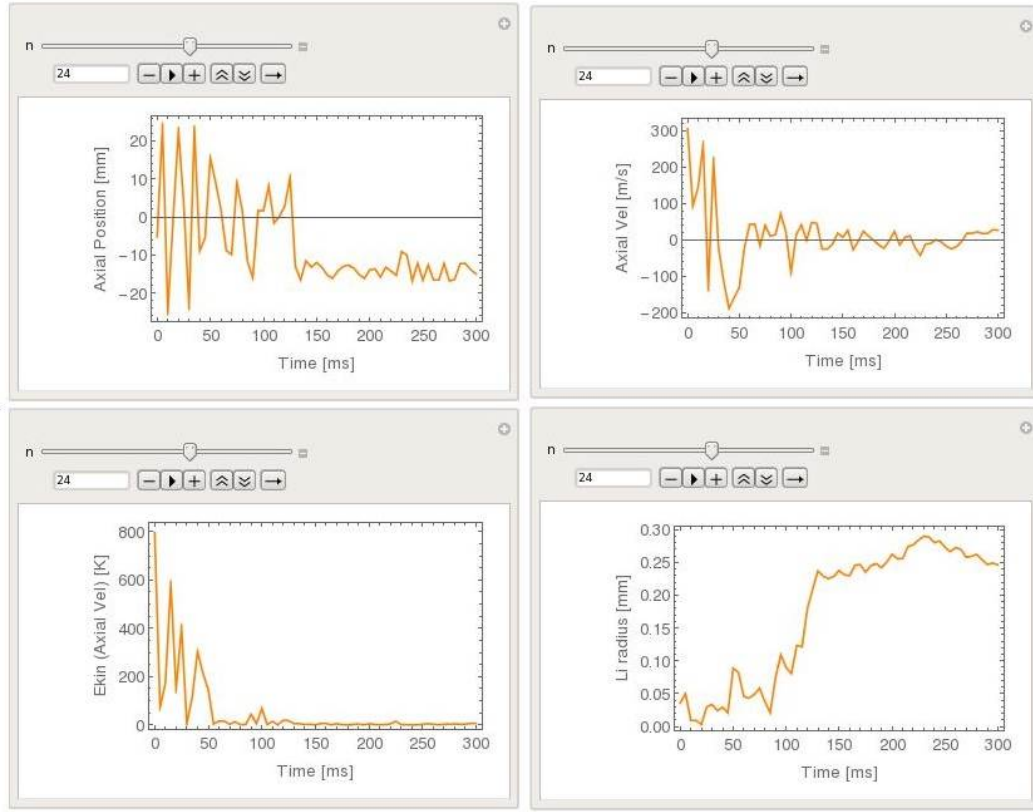
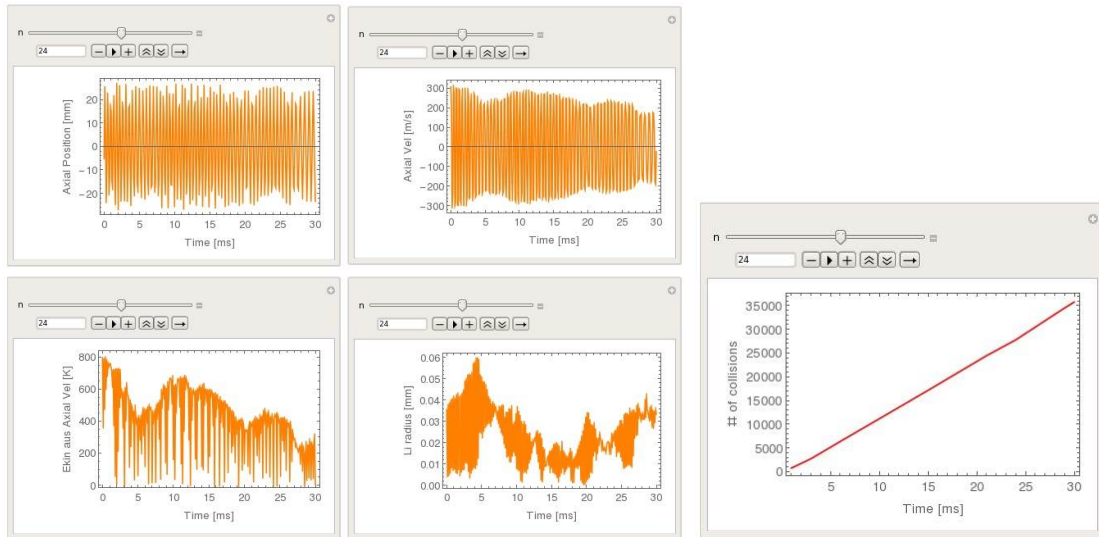


Figure 64: **Anion-24:** The LiF_2^- is initialized at high temperature and a sympathetic cooling effect is visible: Axial Position, Axial Velocity, Axial Temperature, Radial Position of a single LiF_2^- for 300 ms.



(a) Axial Position, Axial Velocity, Axial Temperature, Radial Position of a single LiF_2^-

(b) LiF_2^- -collision-rate.

Figure 65: **Anion-24:** High-resolution-analysis of the behaviour of a single LiF_2^- during the first 30 ms.

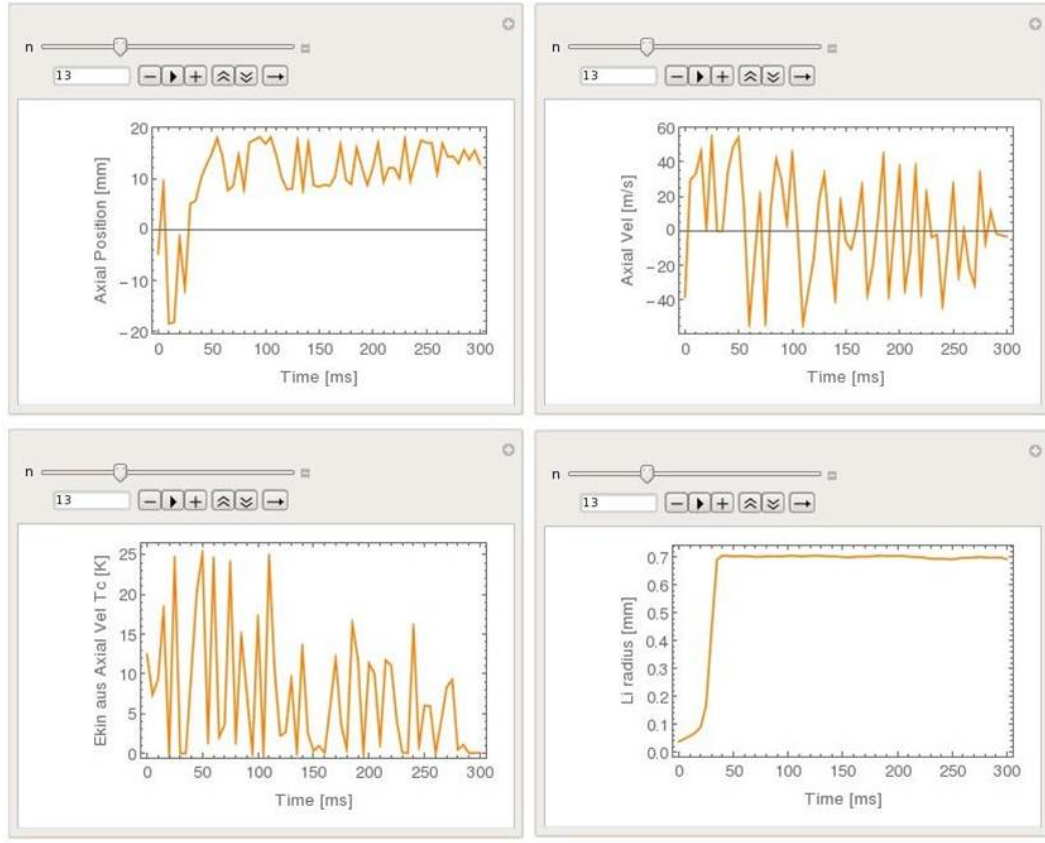
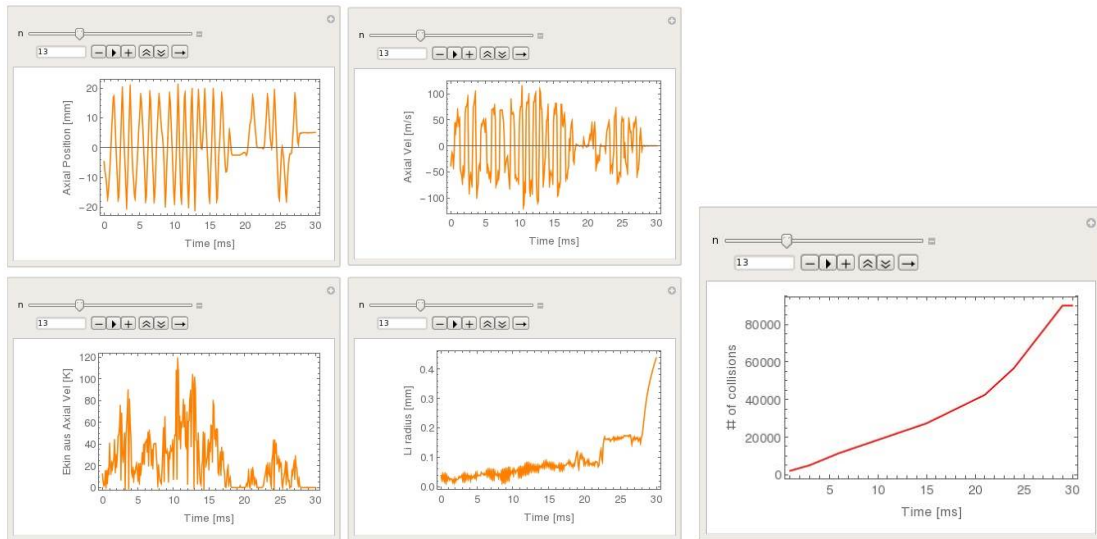


Figure 66: **Anion-13:** The LiF_2^- is initialized at a temperature around 13 K and a sympathetic cooling effect is visible: Axial Position, Axial Velocity, Axial Temperature, Radial Position of a single LiF_2^- for 300 ms.



(a) Axial Position, Axial Velocity, Axial Temperature, Radial Position of a single LiF_2^-

(b) LiF_2^- -collision-rate

Figure 67: **Anion-13:** High-resolution-analysis of the behaviour of a single LiF_2^- during the first 30 ms.

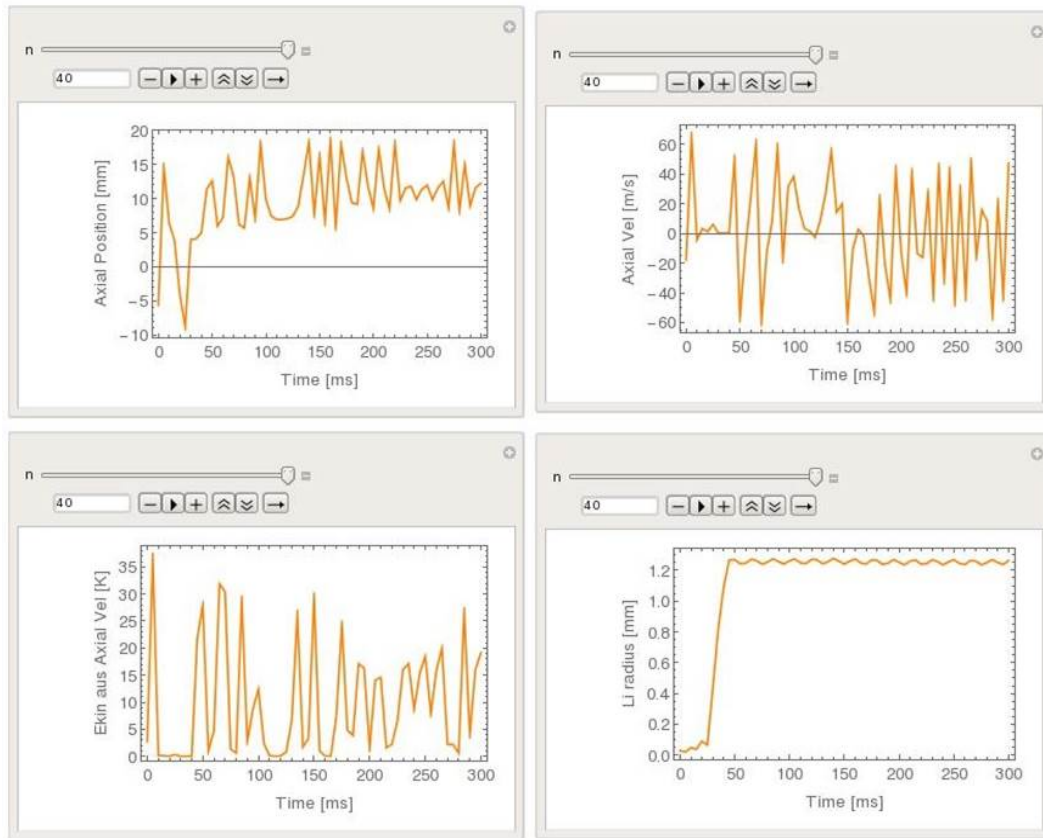
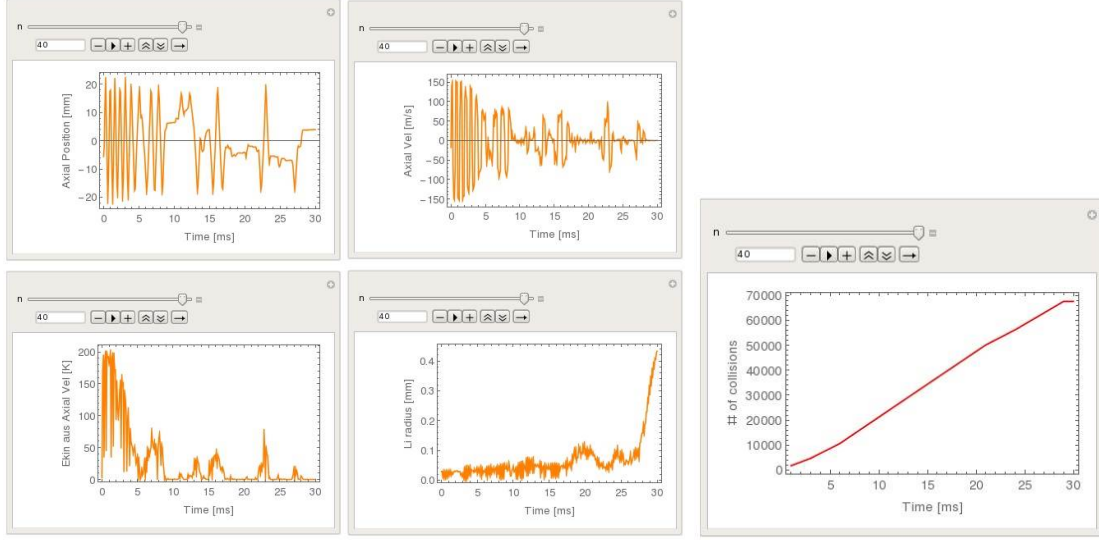


Figure 68: **Anion-40: The LiF_2^- is caught in the sidebag potential and no cooling effect is visible:** Axial Position, Axial Velocity, Axial Temperature, Radial Position of a single LiF_2^- for 300 ms.



(a) Axial Position, Axial Velocity, Axial Temperature, Radial Position of a single LiF_2^-

(b) LiF_2^- -collision-rate.

Figure 69: **Anion-40**: High-resolution-analysis of the behaviour of a single LiF_2^- during the first 30 ms.

This LiF_2^- should be still in the interaction-range of the Barium cloud since there are again irregularities in the axial oscillations (compared to **anion-37**). The anion starts with a relatively small temperature of around 5 K. Radial the anion leaves the Barium cloud after around 30 ms due to pair formation.

In figure 69 it can be observed that the anion is for a long timespan, starting around the 9th ms, mostly inside the Barium cloud colliding with particles, see also the high collision rate. Besides, the axial temperature cools down to the mK-range. Since the collisions stop abrupt around the 29th ms and the radius increases, a bound state formation is probable, which can be further pursued in the 300 ms simulation.

The last example shows a comparatively hot LiF_2^- which gets effectively cooled and is then caught in one of the potential sidebags.

The anion is cooled down from ~ 500 K to a few K in the first 100 ms and is then caught in the potential sidebag without any pair-formation, as can be observed in figure 70.

The collision rate of this example ranks in the middle range with around 41200 collisions. Besides, the LiF_2^- is crossing the cold Barium cloud in the first 30 ms and cooling down in axial temperature while doing so. The radius of the anion varies only slightly, as can be seen in 71.

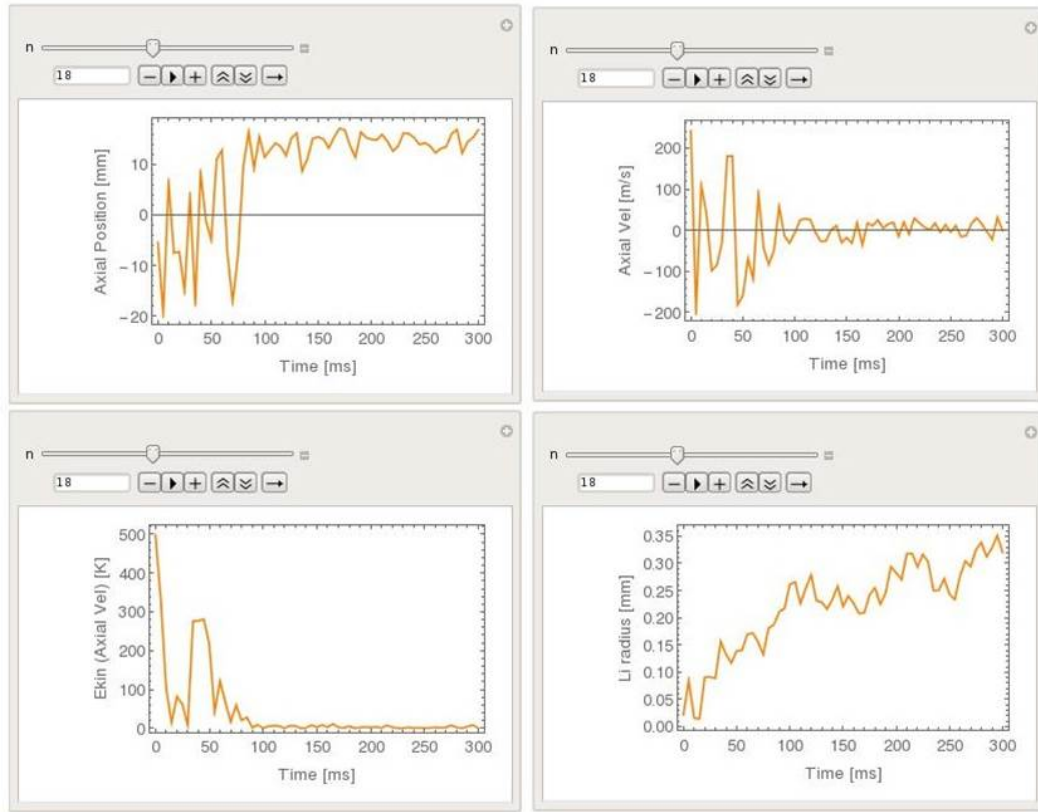
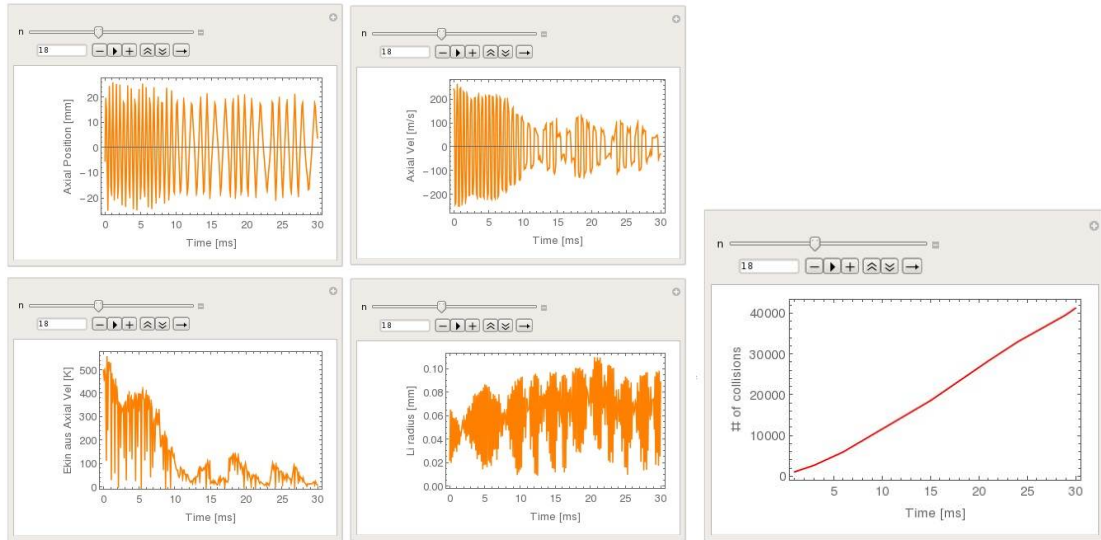


Figure 70: **Anion-18:** The LiF_2^- is caught in the sidebag potential and no cooling effect is visible: Axial Position, Axial Velocity, Axial Temperature, Radial Position of a single LiF_2^- for 300 ms.



(a) Axial Position, Axial Velocity, Axial Temperature, Radial Position of a single LiF_2^- .

(b) LiF_2^- -collision-rate.

Figure 71: **Anion-18:** High-resolution-analysis of the behaviour of a single LiF_2^- during the first 30 ms.

7.5.4 Summary and conclusion of the simulations with LiF_2^- and Ba^+

After observing and analysing the behaviour of individual LiF_2^- , I could draw the following conclusion:

The anions with high axial kinetic energies (100 K and above), cool down sympathetically while crossing the cold Barium plasma, without getting caught in the Coulomb-field of the cations. At lower energies (starting around 5 K) two processes can occur: Either the anions axial kinetic energy is too low to overcome the potential out of the potential sidebag. At even lower temperatures in the mK-range, the anion is caught by the coulomb-field of a single Barium cations forming a neutral bound-state. This exotic atom (drifting pair) leaves the trap always radially, while the axial position of the anion during a bound state changes only slightly. This behaviour is typical for drifting pairs, since these pairs move perpendicular to the magnetic field. Besides it should be pointed out that the Barium cation is axially cooled via lasers to the doppler-limit while the radial temperature is still relatively high around 20 K. The bound-state can last long enough that the exotic atom reaches the electrode walls with a radius of 2 mm (**anion-3**), more frequently, the bound-state decompose again after a few ms. This decomposition of the bound state could occur due to the slightest displacement of the particles. At the point, when bound state is seen as a dipole by the acting forces the state breaks up again. Additionally, the binding energies of these drifting pairs are comparatively low so a decomposition is rather likely to occur. Also interesting to observe is, that depending on the radial position of the bound state during decomposition, the LiF_2^- gains energy again through the acting forces. The further away from the trap-center the radial position of the particle is at the time of the break-up, the more kinetic energy the particle gains after the decomposition. As can be seen in the case of **anion-8** (figure 52) compared to **anion-31** (figure 57). This is probably the case because the particle is closer to the electrodes and therefore the particle sees the potential sidebags more sharply, so even higher energetic anions can be caught in the sidebag potential (see figure 39). Besides, as mentioned in the example of **anion-3** a bound state can be clearly identified by observing a sharp increase of the radius and an abrupt stop of collisions happening. This can be explained since the euclidean distance between the couple is oscillating around $30\text{ }\mu\text{m}$, the maximal distance to output a collision was set to $10\text{ }\mu\text{m}$, what means that due to the interparticle distance the bound state is not seen as a collision. It also should be noticed that the sudden widening of the anion's radius (which indicates a formation of a bound-state) can not be interpreted as a collision in radial direction with a cation, since the widening clearly just occurs at a point of very low kinetic energies. This pattern makes it rather unlikely that collisions in radial direction are the reason for this effect.

Another interesting effect observable is, that the collision rate of the LiF_2^- increases with decreasing kinetic energy of the anion. This can be explained by the fact that at high (axial) kinetic energies (100 K or higher) the anion crosses the cold Barium cloud in axial direction without getting caught in a Coulomb-potential of a cation. It just randomly gets close enough ($d_{\text{LB}} \leq 10\text{ }\mu\text{m}$) to another particle, which triggers a collision (see also **anion-24**). Has the anion reached lower axial energies (40 K or less), the collision rate increases significantly (see the examples with a very high collision rate (**anion-13** and **anion-40**)). In this state the anion slips from one coulomb-field to another and stays for a longer period inside the Barium cloud until the axial energy is

low enough that the anion finally gets caught by a cations coulomb field. But as can be seen in the case of **anion-21** even though the collision-rate is relatively high in the first 30 ms and the anion cooled down to low temperatures no binding state occurs.

Another fact which has to be pointed out is that anions which are stuck in one of the sidebags of the potential at high radial distances (see **anion-8**) are lost for all further sympathetic cooling processes. Although the coulomb-interaction is a long-range force there is no evidence for further sympathetic cooling at high radial distances. A reason for this could be that the electrode potential, due to its strength close to the electrodes overshadows the coulomb-interaction. Obviously, anions which are confined inside the sidebag-potential with radial distance that allows the particles to interact with the cations are still coolable (see **anion-31**).

7.5.5 Initialization of antiprotons

The last step of my simulations was to initialize antiprotons around the 5th ms of the 300 ms simulation shown in figure 42 and 43. This was done by overwriting 10 LiF_2^- as antiprotons.

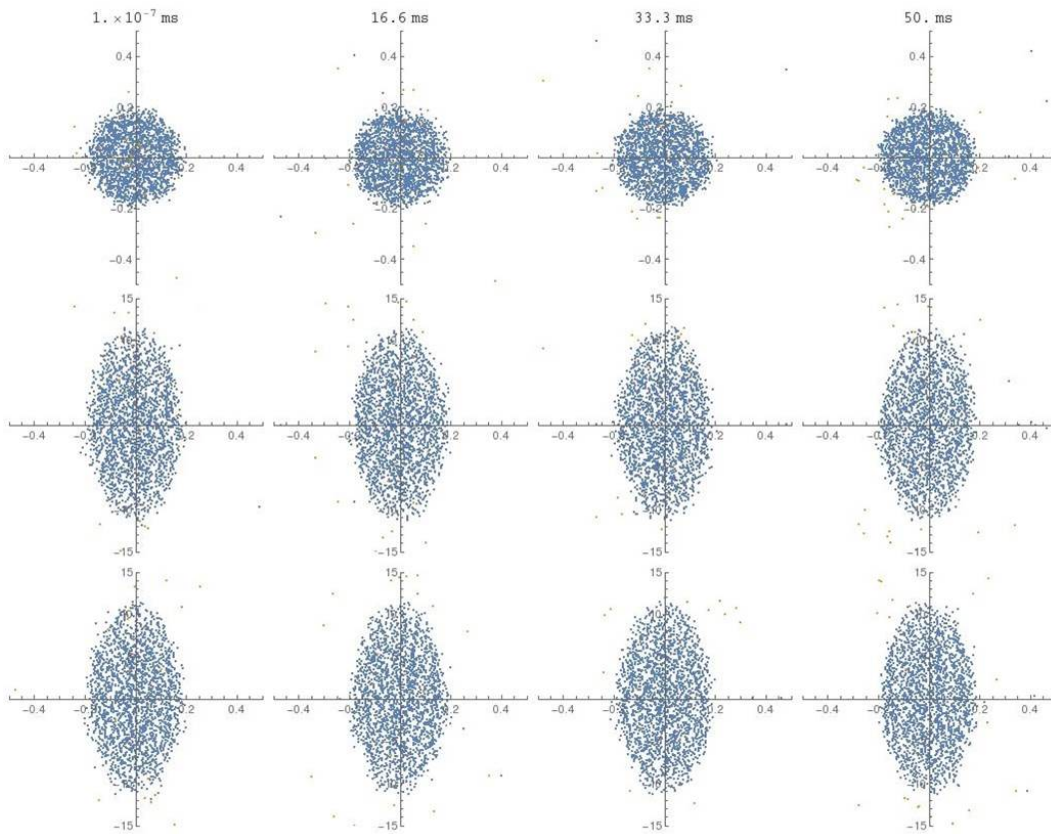


Figure 72: **Spatial shape: 10 LiF_2^- -anions are replaced by antiprotons.**

As can be seen in figure 72 the antiprotons, anion and cations are simulated for 50 ms simultaneously confined in a penningtrap.

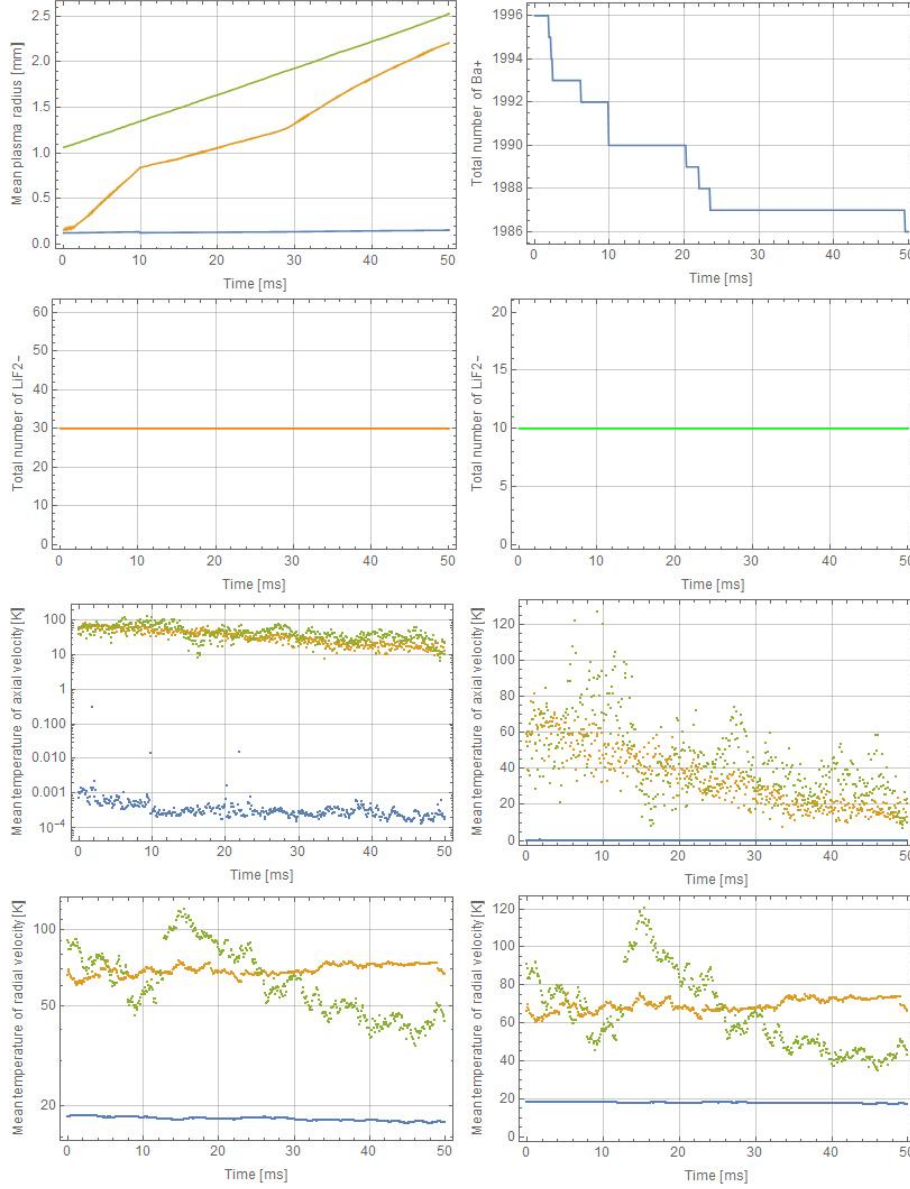


Figure 73: Plasma-temperature in axial and radial direction (calculated through mean-velocities in linear and logarithmic scale), -radius, -number, Ba^+ (blue), LiF_2^- (orange) and antiproton (green).

In figure 73 the analysis of the simulation involving all 3 species is shown. The pbars are initialized with a mean plasma radius of 1 mm, because 10 LiF_2^- were randomly overwritten and one of them was an 'outlier' at 8 mm. Besides we see again the increase of radii for the antiprotons and the LiF_2^- . Only a few Barium cations were lost axially and no pbars or LiF_2^- during 50 ms. Axially the pbars were cooled from 60 to 10 K and radially from 91 to 43 K. The peak in the radial temperature of the pbars is probably due to collisions with an anion or a cation.

The conclusion and outlook for the simulation involving antiprotons can be found in the next section 8.

8 Conclusion and Outlook

This section gives a conclusion and an overview over my efforts and achievements gathered, while testing a doubly sympathetic cooling scheme for antiprotons. For this scheme three species (antiprotons, LiF_2^- and Ba^+) are simultaneously confined in a penning trap, sympathetically cooling each other. Furthermore, the Ba^+ -cations are laser-cooled and the LiF_2^- was introduced to act as a buffer-species to prevent annihilations between the antiprotons and the cations. Since the charged particles with different masses obtain a certain q/m hierarchy, which ensures a radial shell formation of the species, with the heavies species (Ba^+) outermost and the lightes species innermost (antiprotons), the anionic species is included with a mass of 45 u, while $m_{\text{Ba}^+} = 137$ u. This separation-effect occurs due to the rotationally induced centrifugal migration.

To test this scheme, the penning-trap-simulation-program Simbuca was used. Working with Simbuca was very instructive and interesting since the program is very powerful, even though it took me a while to get an overview over the 32 *.cpp*-files. After getting familiar with Simbuca and how to work with it, I started to implement adjustments to the code, i.e. for the laserforce, or the potential-ramping and the collision-rate calculation. Then, several tests were done involving only two species (LiF_2^- and Ba^+) trying to find suitable plasma parameters (shape, density, number, initial temperature, etc.) and trap-parameters (B -field, form and strength of the electrostatic-potential, ramping-velocity of the potential, etc.), to eventually find an indication of a sympathetic cooling effect respectively radial shell formation. The potential-shape was soon chosen to be a double well potential, with the cationic species axially centered and the anionic species confined inside the potential sidebags. The interaction-strength respectively the distance between the species could be controlled by varying the electrode-potential.

Several tests showed that a stable concentric shell formation is hard to implement. On the one side, since uncontrolled plasma-rotations occurred, most probably due to the opposing magnetron and cyclotron motion of the species. These rotations could finally be controlled by enhancing the magnetic field and flattenting the shape of the cationic species in axial direction. But, in addition, the particle losses of the Ba^+ were significant during the 'mixing-phase' of the species and the cationic density decreasing until no further interaction between the species was observable.

Furthermore, the Simbuca-simulations showed that some single LiF_2^- are caught by the coulomb-field of a single Barium cation forming a neutral bound-state. This exotic atom (drifting pair) leaves the trap always radially, while the axial position of the anion during a bound state changes only slightly. This behaviour is typical for drifting pairs, since these pairs move perpendicular to the magnetic field.

Also interesting to see was that a cooling-effect for the LiF_2^- -ions in axial direction was observable which could be related to the variation respectively decreasing of the absolute value of the potential U_0 . This adiabatic cooling effect arises, since the density of the charged particle cloud decreases while ramping down the potential.

Finally, after a vast number of tests, varying the plasma- and trap-parameters, a set of parameters could be found which allowed a clearly visible sympathetic cooling effect between the two species. Therefore, antiprotons were included in the simulation, as a next step.

Thus, 10 antiprotons were initialized, to see if they cool down in temperature, along with the LiF_2^- . This cooling process could clearly be observed and the pbars cooled down from 60 to 10 K in axial direction and radially from 91 to 43 K in 50ms, while the Ba^+ was lasercooled in axial direction to $54\,\mu\text{K}$, a temperature close to the doppler-limit ($40.37\,\mu\text{K}$).

Since previous tests showed that no concentric shell formation occurs, the LiF_2^- as a buffer species is somehow obsolete. To analyse the possibility of annihilations between the Barium-cation and the antiprotons, the euclidean distance between a LiF_2^- - Ba^+ -bound states was determined and found to be around $30\,\mu\text{m}$. Since this distance is far away from fm scale, at which annihilations occur, the particles will not annihilate during a phase of a bound state. It should be noted, that the antiprotons and the Ba^+ certainly can annihilate while the antiprotons are crossing the Barium-cloud in axial direction.

Besides, cooling the antiprotons with this scheme down to the mK range or lower temperatures is probably unlikely, mostly because of the bound-state formation (drifting-pair), which displace the pbars in radial direction. Depending on the severity of this displacement, the antiprotons are lost for further cooling processes.

Besides, previous tests also indicate, that the probability of a drifting-pair-formation increases for decreasing temperatures of the LiF_2^- respectively antiprotons. Thus, antiprotons with temperatures in the mK-range most likely will form bound states with the cations and displace in radial direction. Obviously, this process can also lead to antiproton-losses, as soon as the drifting-pair hits the electrode walls. Furthermore, the antiprotons caught inside the potential sidebag should experience a decrease of the cooling efficiency, since their axial oscillations are damped (through sympathetic interaction), which causes an increase of the distance between the coolant and the anion in axial direction.

Nevertheless, it could be possible to gain control over the most severe obstacle preventing this scheme to reach the mK-region for the pbar temperatures, the pair-formation of the species. This could be achieved by implementing a torque laser pulse in i.e. x -direction close to the plasma edge. This torque-laser increases the rotation frequency of the Ba^+ , compresses the plasma radially and makes a bound state formation of the two species less likely to happen, see also [40].

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