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Simulation of a large number of interacting charged particles trapped in a Penning trap on the BioDynaMo platform

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Abstract

This project aims to simulate large numbers of interacting charged particles trapped in a Penning trap, ideally with different masses or charges, on the BioDynaMo simulation platform for AEgIS experiment, AD-6 Anti hydrogen experiment gravity interferometry spectroscopy. If want to compare with other simulation platforms the BioDynaMo platform is an agent-based simulation, open-source, faster, cheap, easily understandable for complex systems, high-performance and modular simulation platform for agent-based simulations. It can be further developed and used in future studies.

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1 Introduction

The focus of this report is on simulating multiple plasma species in the same Penning trap, understanding the behavior of cold-charged plasmas, as well as simulating the behavior of large numbers of these in a planar geometry, and discovering their potential as qubits. For now, the **AEgIS experiment** at the Antimatter Factory, where I am a part, will determine what can be done with **BioDynaMo** simulation program and how it can be improved, and it will be understood both in my report and in future studies that it can be used in many areas of physics. Information about what has been done and will be done in the following sections of this report will be given.

1.1 AEgIS Experiment

The AEgIS experiment (**Antimatter Experiment: Gravity, Interferometry, Spectroscopy**) is an antimatter experiment conducted at CERN (European Organization for Nuclear Research) by the Antimatter Factory. The permanent objective of the experiment is to investigate the interaction of antimatter (typically antiprotons) with the Earth's gravitational field and determine how it behaves. In other words, it aims to measure with high precision the effects of Earth's gravitational force on antimatter. The experiment uses anti-hydrogen atoms to directly observe and measure the effects of gravitational acceleration on neutral anti-atoms.

To briefly summarize the objectives and activities of the AEgIS experiment:

1- Antimatter Production: This involves the production of antiparticles, which are produced in the CERN Antimatter Factory.

2- Antimatter Capture and Cooling: Antimatter is cooled to very low temperatures and captured.

3- Release and Observation of Gravitational Interaction: This involves the release of antimatter particles (usually antihydrogen) and the observation of their free fall under the influence of gravity. This allows for a precise measurement of how antimatter behaves.

4- Interferometry and Spectroscopy: Used to measure the interaction between antimatter and gravity, providing high-precision data on the gravitational interaction between

antimatter and Earth and enabling comparisons with normal matter.

5- Fundamental Physics Tests: Aims to answer questions about whether antimatter behaves the same way as normal matter in response to gravity, which has important implications for our understanding of the fundamental forces of the universe.

Regarding the content of the AEgIS experiment,

In the experimental setup, a pulsed beam of anti hydrogen atoms is initiated horizontally. The vertical displacement of neutral antimatter atoms induced by gravity is measured using a high-resolution detector and a gratings.

The formation of anti-hydrogen atoms is achieved through a charge-exchange reaction involving Rydberg-excited positronium atoms. Rydberg positronium atoms collide with antiprotons, resulting in the formation of Rydberg-excited anti-hydrogen and an electron. This reaction is initiated using positronium atoms sent into a trap of cooled antiprotons with an electromagnetic trap. The reaction is as follows as in the (Figure 1).

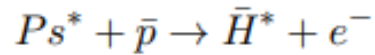


Figure 1: The resulting charge-exchange reaction

The emerging Rydberg anti-hydrogen atoms are subsequently accelerated horizontally by an electric field gradient (Stark effect). They are then passed through a Moiré Deflectometer. The vertical deflection caused by Earth's gravitational field is the first test of the Weak Equivalence Principle for anti-hydrogen. Detection is carried out through a position-sensitive detector. Approximately 10^3 anti-hydrogen atoms are needed to complete the gravitational measurement. The current situation is planned to be presented by paying attention to laser excitation to the $n=3$ state of positronium (Ps) and the production of positronium atoms in the transition geometry.

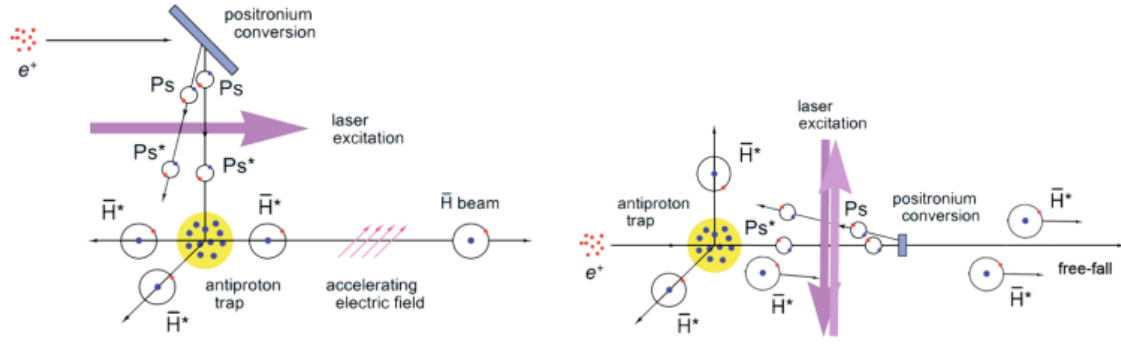


Figure 2: The one on the left is the first diagram in which the Ps fly orthogonally into the axial magnetic field. The one on the right is the upgraded collinear scheme implemented in the new anti hydrogen trap geometry.

The two important performance indicators for measurement are the number of atoms reaching the detector and the temperatures (Figure 2). The total number of hydrogen atoms and the efficiency of charge-changing reactions determine this. This efficiency is mostly determined by the principal quantum number, the number of atoms involved in the reaction, and the relative velocity between Rydberg-Ps atoms and antiprotons. The separation and temperature of the created beam depend on the initial temperature of the antiprotons and the efficiency of the beam production mechanism. In recent years, and currently, as changes are made to the experimental setup to improve efficiency, there is potential for significant achievements. To uncover the effects of gravity on antimatter, which is still an unknown field, complete understanding of the components used to form the neutral antiatoms with which gravity will be probed is needed, so as to optimize formation rates, minimize temperature, and study the effects of multiple charged particle species on each other.

2 BioDynaMo Simulation Platform

The BioDynaMo (Biological Dynamic Modeling) project was initiated to bridge the gap between highly specialized applications and large-scale systems, with the aim of understanding complex biological processes and providing access to rapidly growing computational resources. BioDynaMo is a software platform used to simulate and model biological systems at various scales, from cellular to tissue levels. It incorporates a high-performance simulation engine and can simulate the interactions of cellular components, genetic dynamics within cells, and 3D physical environments. The simulation model is dynamic, aiming to create computational models and enable multi-scale simulations, and it is an open-source platform. It aims to be run on hybrid cloud computing systems, effectively utilizing the latest computer technology.

The BioDynaMo platform has important fundamental features and capabilities such as Cellular Modeling, Tissue Simulation, Scalability, Open Source, Visualization and Analysis, High-performance Simulation Engine, Modular Software Architecture, Agent-based (meaning there is no central organizing unit regulating behavior), Large Scale, and Easily Programmable.

Furthermore, if you'd like to know more about the benefits, capabilities, and features of the BioDynaMo platform, the following can be explored:

- Simulations require high-performance computation, hence the use of the C++ language. It offers the right ecosystem for parallelization and optimization.
- It is designed to run on hybrid cloud computing systems.
- BioDynaMo primarily runs on multi-core CPUs and can transfer specific calculations to GPUs for acceleration, significantly improving simulation performance. Additionally, FPGA (Field-Programmable Gate Array) is employed as part of the hardware configuration.
- Runtime can be reduced through code modernization efforts.
- Parallelization is used for performance enhancement through OpenMP.
- BioDynaMo provides a consistent API and hides application details unrelated to computational modeling, such as parallelization strategies, synchronization, load balancing, or hardware optimizations.

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- It is capable of simulating up to 1 billion agents on a single server in a matter of hours.
 - Simulations that used to take days can now be executed in minutes.
 - Hardware utilization is optimized, reducing costs.
 - Currently, it is supported on Ubuntu 20.04/22.04, CentOS 7, MacOS 11.7/12.6 (Intel and ARM) platforms.
 - Third-party libraries like OpenMP, ROOT, and ParaView are used.

3 Methodology of Project

As can be understood from the information provided above about the BioDynaMo platform and the AEGIS project, this platform is intended to be used for large numbers of interacting charged particles. Depending on the results obtained, it aims to address the question of whether it should be used for this purpose and, in the future, in which other fields of physics it can be applied.

If you would like to compare and discuss the features of the COMSOL platform, which is used in many simulations, it is worth noting that deep and informative training materials for learning the COMSOL platform are not easily found, and a certain amount of money must be paid for training. It is costly, not open source, and not easily supported for development. Especially for solving large and complex problems, it may require long periods. High-performance devices may be needed. Due to these challenges, the BioDynaMo platform has the potential to replace some simulation platforms since it is accessible to everyone, can be developed, can model complex simulations, follows an agent-based approach, and is much faster than existing approaches. The information in the subheadings will be provided about the methodology.

3.1 The System to be Simulated

This project aims to simulate large numbers of interacting charged particles trapped in a Penning trap, ideally with different masses or charges, on the BioDynaMo simulation platform for AEGIS experiment. Briefly, it is simulating the behavior of large numbers of these in a planar geometry.

3.2 The Simulation Process and Results

To use the simulation, the CentOS 7 platform supported by the simulation was employed. The programming languages used were C++ and Python. One of the reasons for this choice is their ease of integration with each other. The writing and compilation of the code were done through Visual Studio Code. Customization of the simulation was achieved by using the necessary parameters. To facilitate the addition of extra parameters, a Param class was defined. It supports configuration files in the TOML or JSON merge patch format. The parameter value could be set through a TOML/JSON configu-

ration file, command-line arguments, or assignment in the source code. OpenMP, ROOT, and ParaView libraries were utilized. ROOT was used to implement automatic backup and restore functions. ParaView was used for visualizing the simulation. ParaView is a graphical user interface. JSON and C++ interpreter script were used for parameter configuration. The code was written within the established BioDynaMo package, specifically within the 'Src' directory, in files named 'flocking.cc', 'bdm.json', 'flocking.h' and 'sim.param.h'. Information regarding the content of these files can be accessed on the BioDynaMo platform's website. The simulation parameter values are provided in the "bdm.json" file. The data resulting from the simulation is stored in the "output/data.x" folders. To visualize this data, you can open a window using the "paraview" command and navigate to the "output/data.x" folder. You can find the commands to access the simulation on the BioDynaMo website.

From the demos and notebooks shown as examples on the BioDynaMo website, the "Flocking" demo was examined by considering the features required for simulating the desired particle. It was determined that it contained some of the features necessary for the simulation. To make the simulation model, which has a complex structure, more understandable, it was decided to add capabilities and extensions to the simulation later on. The behavior 'Flocking in Free Space: Simulation without extend cohesion term' and the behavior 'Flocking in Free Space: Avg neighbor distance' were added to obtain the desired flocking feature's visualization(Figure 3).

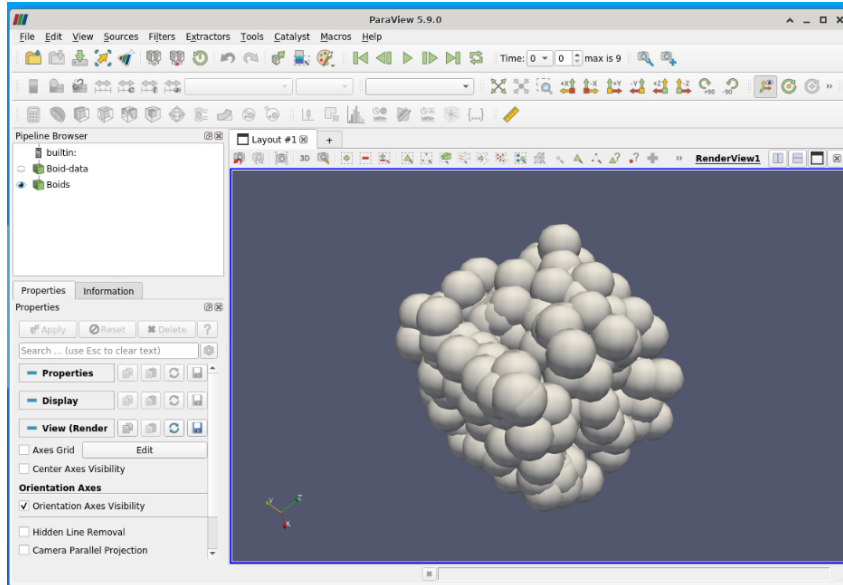


Figure 3: Simulation using 'Flocking' Simulation

3.3 Prospective Work and Anticipated Actions

In the subsequent phase of the project, as elucidated under the heading "Adding Functions to the Simulation" and "Travis CI Tool" the objective is to integrate these functions into the BioDynaMo project. This integration aims to simulate the forces governing the interactions of loaded particles and, through these forces, model the confinement of particles within the Penning Trap. In the project's long-term vision, the incorporation of laser cooling is envisaged. The advancement of the BioDynaMo platform's software, the creation and incorporation of various libraries, and its hardware enhancement are essential for achieving the objectives we desire and anticipate.

3.3.1 Travis CI Tool

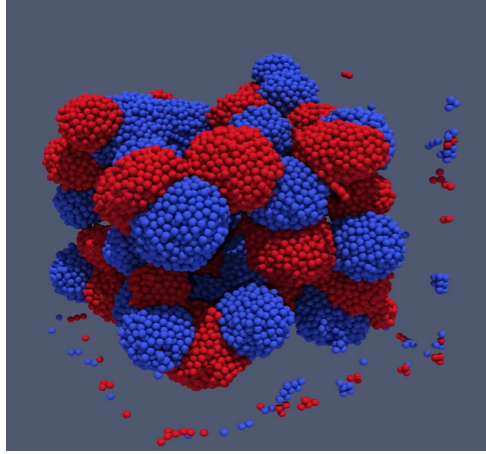
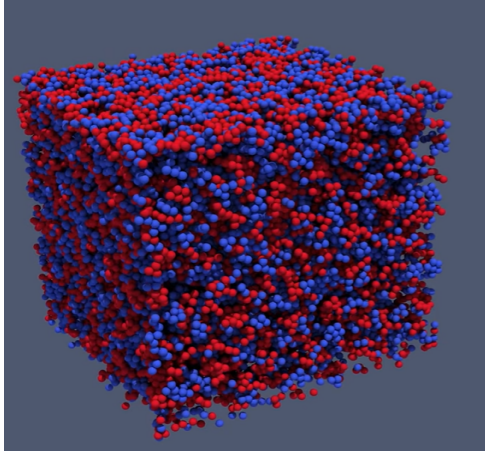
Travis CI is one of the Continuous Integration (CI) tools that facilitate the practice of continuously integrating small changes into an application during the development process, as opposed to making large-scale changes all at once. The objective is to effectively manage software development and testing by incrementally introducing small modifications. Travis CI serves as an automation tool for the continuous integration workflow, automating the build, test, and deploy processes. It not only supports your software development process but also provides feedback on the status of your project, automating various other facets of improvement. The utilization of this CI tool is essential in the development of the BioDynaMo platform to achieve the desired simulation model.

3.3.2 Adding Functions to the Simulation

"Soma Clustering Simulation"

The Soma clustering simulation involves two types of cells and two types of extracellular substances. Each cell secretes a substance and moves in the direction of the substance gradient. Cells are initially distributed randomly and form clusters during the simulation (a). At the end of the simulation, cell clusters emerge (b).

By utilizing this feature of the Soma clustering simulation, it will be easier to achieve the desired image result after cooling. This is because we can adjust the behavior of clusters, specifying where and how they should stop behaviorally, using a different library (it is anticipated that assigning different behavioral characteristics will be more effective)(Figure 4).



(a) Cells are initially distributed randomly and (b) Cell clusters emerge at the end of the simulation

Figure 4

”Hierarchical Model Support”

This aims to enable specific features of certain agents to be made available before others. First, operations are carried out for large agents, followed by small agents. Finally, a different set of operations is created and executed for both large and small agents. The behaviors of cold-charged plasmas within a Penning trap will be simulated using a hierarchical modeling approach.

”Multi-Scale Simulations”

The use of ’Multi-Simulation’ is aimed at running processes within simulations as separate and parallel processes on different time scales. This feature proves highly beneficial when simulations need to be repeated multiple times with varying temporal parameters. Instead of running simulations consecutively, this feature enables multiple instances to run simultaneously on one or more machines. BioDynaMo offers several default algorithms for exploring a parameter space (e.g., parameter sweeps, particle swarms). These algorithms leverage Multi-Simulation by running each iteration as a separate process. Using this model, it becomes possible to simulate the behavior of cold, charged plasmas in a Penning trap by adjusting the timing. Simultaneously, the behavior within the cold, charged plasma itself can also be simulated.

”Replace Mechanical Interaction”

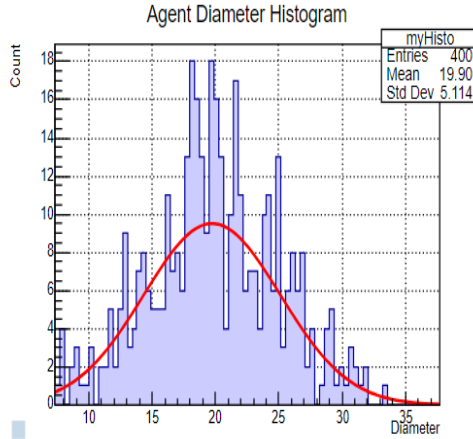
It provides the capability to replace the default interaction force with a user-defined force. The interaction force is used to calculate the forces between agent pairs that are in physical contact with each other. When creating a Penning trap, the forces that will be applied, as well as the forces involved in the interaction during the particle charging process, and the forces used for particle cooling, can be effectively demonstrated in the simulation through the mentioned model.

”Create agent attributes of a histogram”

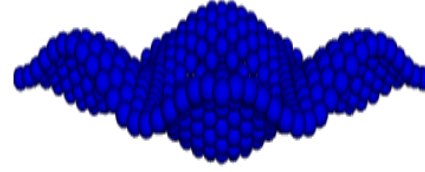
According to my research, applying reverse engineering and simulating agents while presenting them graphically has the potential to be a more effective method of comparison. This allows for easy integration of both analyses and the simulated figures or enables the asking of new questions by making comparisons.

Functions are defined that generate cells at specific positions with diameters drawn from a Gaussian distribution. A desired number of cells are then created. The histogram of all agent diameters in the simulation is generated, and the data is organized to fit the functions. A histogram object is created, and a function is defined to fill the histogram with the diameters of the given agents. The filling function is called for each agent, ensuring that all diameters are added to the histogram. Subsequently, the histogram is plotted. A TCanvas object is created, and the desired function is fitted to the data in the histogram. The expectation is for Gauss to fit the data.

If we apply this method in reverse, it becomes possible to create a simulation precisely from the values obtained from the data. Data is input into the system, and a histogram is generated. Cells are created from the histogram, and the simulation process is carried out.(Figure 5)



(a) The TCanvas object and the fitted versions of the data in the histogram

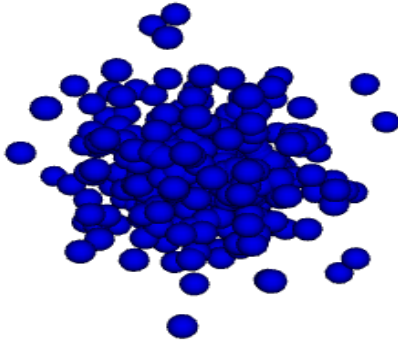


(b) Created cells on a plane

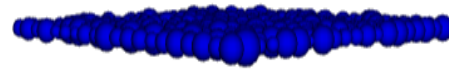
Figure 5: The goal is to transition from shape (a) to shape (b).

"Environment search"

The ability for an agent to execute a function for each of its neighbors is becoming configurable. Its function can be altered based on its surroundings, thereby allowing the assignment of trap behavior with this feature (Figure 6)



(a) Represented in a spherical shape



(b) Represented in a horizontal slice

Figure 6: The clustering and shape alteration of randomly distributed cells due to environmental influences

”Hybrid Model”

The hybrid model is based on visualizing the subdynamics generated by APM simulations. We can represent the simulation in a horizontal slice. Using different colors, simulating the cooled state of trapped particles becomes easier. Throughout the simulation, the total number of cells should be increased. It should be noted that simulating almost 8 million agents by filling the entire model represents a significant computational workload(Figure 7).

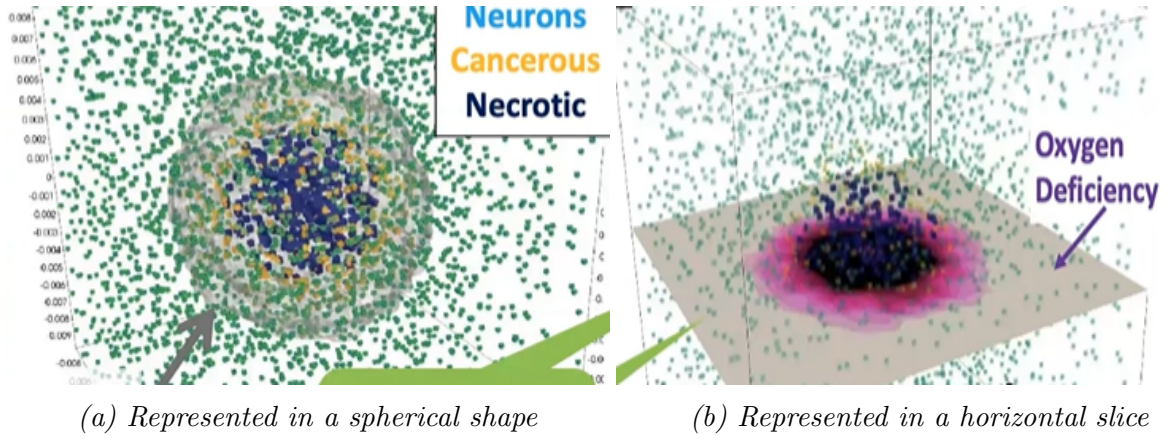


Figure 7: A simulation model related to oxygen deprivation

4 Discussion and Conclusion

This project aims to simulate multiple plasma types in a Penning trap, understand the behavior of cold charged plasmas, and simultaneously simulate the behavior of a large number of these plasmas in a planar geometry while exploring their potential as qubits. It has been observed that BioDynaMo can be used for these purposes.

With this project, it has become evident that BioDynaMo can be applied not only in the field of biology but also in various other domains. While similar simulations can be achieved with different platforms, the distinct capabilities of the BioDynaMo platform, such as its ability to develop modular models in various computational domains, rapidly obtain results with a parallelized execution engine, distribute the model to billions of agents on a single server, and enable scalability, lead to more effective outcomes. Continuing and advancing this project in the coming years will yield significant benefits in various fields.

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