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MD Simulations of Resistive Cooling in HITRAP Using GPUs

J. Steinmann^{*,†}, J. Groß[†], F. Herfurth^{*} and G. Zwicknagel^{**}

^{*}GSI Helmholtzzentrum für Schwerionenforschung GmbH, Planckstraße 1, D-64291 Darmstadt

[†]Fachbereich Mathematik und Naturwissenschaften, Hochschule Darmstadt, Haardtring 100, D-64295 Darmstadt

^{**}Institut für Theoretische Physik, Universität Erlangen-Nürnberg, Staudtstraße 7, D-91058 Erlangen

Abstract. In the HITRAP facility at GSI it is planned to store 10^5 highly charged ions up to U^{92+} in a cryogenic Penning trap and cool them down to 4 K via electron and resistive cooling. During the cooling process the ion density increases and the characteristics of the ion cloud are increasingly determined by Coulomb interactions. We present a parallel algorithm for the simulation of the resistive cooling for ion clouds in cylindrical Penning traps. For the simulation of the resistive cooling we run an OpenCL code on a single GPU device.

Keywords: numerical simulations, resistive cooling, ion clouds, gpgpu computing, parallel algorithms, ion cooling, ion trapping

PACS: 02.60.Cb, 37.10.Rs, 37.10.Ty

INTRODUCTION

The HITRAP (highly charged ions trap) facility at GSI was developed to provide slow, cold, highly charged ions up to U^{92+} . After production at 400 MeV/nucleon the highly charged ions are decelerated and cooled. The final cooling takes place in a cryogenic Penning trap, designed to store up to 10^5 Ions at a temperature of about 4 K. Ions are injected into the Penning trap with an energy of 6 keV/nucleon and cooled down to 10 eV with electron cooling. Then the ions are collected in the center of the trap, and the ion cloud is cooled resistively down to about 0.3 meV.

The simulation of ion clouds taking the full ion-ion interaction into account is associated with large computational effort. This applies especially for the simulation of cooling methods like the resistive cooling, where the cooling force has a complex structure. In [1] a simulation method for the resistive cooling was presented, using a particle in cell code. The ion-ion interaction was approximated with a mean-field approach. This leads to a loss of information of the dynamics and a loss of accuracy. In this paper we present a parallelized algorithm for the simulation of resistive cooling including full ion-ion interaction running on a single GPU device.

PRINCIPLE OF GPGPU COMPUTING

The architecture of a graphic board is an optimized device for parallel pixel calculation. The use of this property for non graphic generating applications is summarized by

the term GPGPU (General Purpose Computation on Graphics Processing Units). The computing power of a single device has increased from a few GFLOPS to about thousand GFLOPS in recent years, allowing to do simulations on a single device, which some years ago could only be done on small CPU clusters.

A graphic board consists of a fixed number of identical compute units and a global memory. The compute unit itself consists of a number of arithmetic logical units and a local memory. Each of these units can perform the same number of parallel tasks, the so called Threads. All Threads within one Block can address the local memory of the corresponding compute unit and all Threads can address the global memory. An addressing of the local memory is much faster than addressing the global memory and should therefore be preferred, if possible.

Figure 1 shows the working principle of a graphic board.

- (a) Threads are identified with integer numbers.
- (b) m Threads together build one Block. The number of Blocks is given by $n = N/m$.
- (c) The Blocks are arranged in k stacks, k corresponds to the number of compute units.
- (d) Blocks are processed iteratively in n/k steps.

FIGURE 1. Working principle of a graphic board.

Due to the parallel processing of Threads, only parallel algorithms can be implemented, which do not need to know the current iteration step. However, all explicit numerical single and multistep methods to solve the equation of motion can be implemented in parallel. The tests presented in this paper use an explicit fourth order Runge-Kutta method.

ION DYNAMICS IN PENNING TRAPS

The equations of motion for an ion cloud is:

$$\ddot{\vec{x}}_j = \frac{q_j}{m_j} \cdot \left(\dot{\vec{x}}_j \times \vec{B} - \vec{\nabla} V + \frac{1}{4\pi\epsilon_0} \cdot \sum_{\substack{k=1 \\ k \neq j}}^N \frac{q_k \cdot (\vec{x}_j - \vec{x}_k)}{|\vec{x}_j - \vec{x}_k|^3} \right) + \frac{\vec{F}_j}{m_j} \quad (1)$$

V represents the electrical potential, $\vec{B}$ the magnetic flux density, $\vec{x}_j$ the position of the j -th particle, q_j the charge of the j -th particle, m_j the mass of the j -th particle, N the number of particles and $\vec{F}_j$ all other forces applied on the j -th particle. In case of the HITRAP Pennig trap the electrical potential is used for the axial confinement and is defined by a stack of 25 cylindrical electrodes [2]. A homogeneous magnetic field of 6 T provides the radial confinement and the force $\vec{F}_j$ represents the cooling force.

Interaction Force Evaluation

Equation (1) splits into external forces effecting all particles and the term describing forces from particle-particle interaction. Using a fourth order Runge-Kutta integrator, the discretization leads to $6N$ equations, $3N$ each for position and velocity. The velocity time propagation for the j -th particle can be written as

$$\{\dot{\vec{r}}_j\}_{s+1} = \frac{\Delta t}{m_j} \left(\vec{F}_{ext}(\{\dot{\vec{r}}_j\}_s, \{\vec{r}_j\}_s) + \sum_{\substack{k=1 \\ k \neq j}}^N \vec{F}_{jk}(\{\vec{r}_j\}_s, \{\vec{r}_k\}_s) \right). \quad (2)$$

The computational effort for updating the velocity for a large number of particles is determined by the second, the interaction term. For a system of N particles without taking advantage of symmetry, $N \cdot (N - 1)$ Coulomb force evaluations must be calculated. The algorithm we use for our calculation is based on the algorithm presented in [3], but we avoid the softening parameter which was introduced in [3] to circumvent the zero division problem. In our code we take advantage of the memory structure of the data.

Each Thread is identified with one particle and processes the following program sequence.

- (1) Each Thread out of the same Block (1 Block = m Threads) copies one particle position value in parallel from the global to the local memory.
- (2) Parallel calculation of the Coulomb forces corresponding to all particle position values in the local memory.
- (3) Repeat step (1) and (2) until the end of the particle position vector is reached (n times).

Using this parallel algorithm the computational effort reduces to $O(N)$.

RESISTIVE COOLING

Charged particles moving between two conductive electrodes induces a surface charge Q on both of them and cause a potential imbalance u . Connecting the electrodes to an external RLC-circuit leads to an electrical current i , depending on the positions, velocities and charges of the ions. Due to energy dissipation in the resistor of the circuit the ions loose energy which vice versa causes changes in the induced charges on the electrodes and the related electric field. This leads to a non-trivial coupling between the

circuit and the ions motion. For testing the algorithm we use a parallel RLC-circuit, which is described by the equation

$$\frac{d^2u}{dt^2} + \frac{1}{RC} \frac{du}{dt} + \frac{1}{LC} u = \frac{1}{C} \frac{di}{dt}. \quad (3)$$

Where we used the circuit parameters:

$$\begin{aligned} R &:= \text{Electrical resistance} \\ L &:= \text{Inductance} \\ C &:= \text{Capacitance} \end{aligned}$$

FIGURE 2. Cross-section of the center electrodes of HITRAP. Voltage between trap and ring electrodes generate the trapping potential. The pick-up electrodes are additionally used as correction electrodes, to approximate a harmonic potential.

In case of symmetric coupling of the pick-up electrodes, see figure 2, the induced current is given through

$$i = \dot{Q}_L - \dot{Q}_R, \quad (4)$$

where $Q_{L/R}$ is the induced charge on the left/right electrode. The induced charged on the eletrodes can be calculated from the surface charge density σ

$$Q_{L/R} = \int_{A_{L/R}} \sigma dA, \quad (5)$$

where $A_{L/R}$ corresponds to the surface of the left/right electrode. The surface charge density for a cylindrical geometry can be calculated by the normal derivative of the ions potential at the trap radius R by

$$\sigma = \epsilon_0 \left. \frac{\partial V_{ions}}{\partial r} \right|_R. \quad (6)$$

The potential V_{ions} created by the ions is given by the solution of Poissons equation for a discrete charge density distribution

$$\Delta V_{ions} = \sum_{k=1}^N \frac{q_k}{\epsilon_0} \delta(\vec{r} - \vec{r}_k), \quad (7)$$

and the boundary conditions

$$\begin{aligned} V_{ions}(r = R, \phi, z) &= 0 \\ V_{ions}(r, \phi, z \rightarrow \pm\infty) &= 0 \\ V_{ions}(r, \phi, z) &= V_{ions}(r, \phi + 2\pi, z). \end{aligned}$$

Under the assumption that the cylinder is infinitely long and ignoring the separating slits between the electrodes, the solution of equation (7) is given by ¹

$$V_{ions} = \sum_{k=1}^N \frac{q_k}{2\pi\epsilon_0 R^2} \sum_{n=1}^{\infty} \sum_{m=0}^{\infty} (2 - \delta_m^0) \cdot e^{-\mu_{n;m}|z-z_k|} \frac{J_m(\mu_{n;m}r_k) \cdot J_m(\mu_{n;m}r)}{\mu_{n;m} \cdot J_{m+1}^2(\mu_{n;m}R)} \cos(m \cdot (\phi - \phi_k)), \quad (8)$$

with the following definitions:

$$\begin{aligned} (r_k, \phi_k, z_k) &:= \text{position of k-th particle} \\ q_k &:= \text{charge of k-th particle} \\ R &:= \text{trap radius} \\ J_m &:= \text{m-th Bessel function of first kind} \\ R \cdot \mu_{n;m} &:= \text{n-th positive zero of } J_m. \end{aligned}$$

Simulation of resistive cooling

In figure 3, the workflow of the resistive cooling algorithm is shown. The algorithm starts with an initial distribution of the ions position and velocity, while the electrical Potential V_{Img} caused by the image charge is neglected at first. Next equation (1) is solved numerically to calculate a new set of positions, velocities and accelerations from which the right hand side of equation (3) is evaluated. After solving equation (3), finally the electrical potential V_{Img} caused by the induced current, as obtained analytically from the set of equations (4), (5), (6), is calculated and it serves together with the new positions and velocities as a starting point for the subsequent cycle.

Here, the cooling force due to the additional induced potential V_{Img} , which enters the equations of motion (1), is derived from

$$\vec{F}_j = -\vec{\nabla} V_{Img}(\vec{x}_j). \quad (9)$$

SIMULATION RESULTS

Simulation time: CPU versus GPU

For all simulation results shown in this paper the graphic board ATI Fire Pro V8800 was used. Figure 4 shows a comparison of time when doing simulations on a ATI Fire

¹ $\delta_a^b = \begin{cases} 1, & a = b \\ 0, & \text{otherwise} \end{cases}$ i.e. the delta function.

FIGURE 3. Work flow resistive cooling algorithm. The white boxes mark numerical solvers; the gray shaded boxes mark analytically solved equations.

Pro V8800 and NVIDIA FX 880M (common notebook graphic board) and a single core of the Intel Core i7 CPU. We solved equation (1) using a RK 4 solver and choosing $\vec{F}_j = \vec{0}$, i.e. without cooling. We calculated 50 time steps in total, using single precision accuracy and a time-step size of 1 ns for a different number of particles. In the left graph the dashed and solid line represent the simulation result for the NVIDIA graphic board and the dotted and dashed-dotted line representing the result for the ATI graphic board. For the simulation results indicated by the dashed and dotted line no local memory was used. Both graphic boards need much less time for the simulation than the CPU, due to

FIGURE 4. Comparison of processing time for different GPU devices (left) and a CPU device (right). The graphs in the left figure show from top to bottom: 1. NVIDIA: local memory off, 2. NVIDIA: local memory on, 3. ATI: local memory off, 4. ATI: local memory on.

the high degree of parallelization of the Coulomb interaction. The expected cooling time for HITRAP are in the order of seconds. The simulation of 10^6 time steps (which covers only a time period of 1 ms) for $2 \cdot 10^4$ particles and otherwise identical configuration would take approximately 2 days for the ATI device and 450 days for the CPU.

Energy conservation

For the simulation of ion cooling, it is of great importance, that the ion cloud will not be heated or cooled due to numerical effects, i.e. the undamped system must be energy conserving. To ensure energy conservation, the time discretization must be chosen appropriately, in order to resolve the microscopic effects such as cyclotron motion and interparticle collisions sufficiently well. Figure 5 shows the total, kinetic, Coulomb and electrostatic energies of a simulation with a time discretisations of 20 ps in the left graph and 0.5 ns in the right. The left graph shows a conservation of the total energy with a maximum relative error of the order 10^{-3} , whereas a numerical heating is seen in the right.

FIGURE 5. Energy plot for a simulation of 768 $^{235}\text{U}^{92}$ with full ion-ion interaction and a time-step size of Left: 20 ps; Right: 0.5 ns. The lines mark from top to bottom, the total energy, the Coulomb energy, the electrostatic energy and the kinetic energy.

Coulomb interaction

To demonstrate the importance of the Coulomb interaction an ion ensemble of above ten thousand $^{235}\text{U}^{92+}$ has been cooled in the HITRAP cooler Penning trap. In this test case the standard deviation of the axial ion position was calculated. Initially the ions are distributed axially taking the full length of the trap of about 0.5 m. Along the trap axis a magnetic field of 6 T was applied to provide the radial confinement. For the electrical potential the complete stack of 25 electrodes is used. The trap is on a potential of 11 kV. The outer trapping electrodes are set to 18 kV. The three electrodes in the center are used to generate approximately a harmonic potential well of 100 V. In addition an artificial frictional force $\vec{F} = \eta \vec{\dot{x}}$ was applied for damping.

The simulation was done twice: once with Coulomb interaction (solid line) and once without (dotted line). Due to the energy loss because of the damping force the ions collect in the potential well in the trap center. The ion density increases and the repulsive Coulomb interaction becomes more important. Figure 6 shows the standard deviation for both simulation. After about 7 ms the standard deviation splits up, because the Coulomb interaction prevents further axial shrinking of the ion cloud. For simulations of electron cooling [4] in the HITRAP Penning trap which takes place after ion injection, where the ions are distributed over the full length of the trap, the ion-ion Coulomb interaction can be neglected so that the simulation times reduce significantly. But for the simulations of the resistive cooling in HITRAP, the ion-ion interaction must be taken into account.

FIGURE 6. Standard deviation of the axial ion position. Dotted line represents the simulation result without Coulomb interaction and the solid line with interaction.

Resistive Cooling of a single particle in the trap center

As another test case we investigated resistive cooling on a single ion moving along the trap axis with the initial values

$$\begin{aligned}\vec{r}(t=0) &= (0, 0, z_0) \\ \dot{\vec{r}}(t=0) &= (0, 0, v_0),\end{aligned}$$

where equation (1) together with equation (9) simplifies to

$$\ddot{z} = -\frac{q}{m} \left(\frac{\partial}{\partial z} V(z) + \frac{\partial}{\partial z} V_{\text{Img}}(z) \right). \quad (10)$$

For the symmetric coupling of the pick-up electrodes the potential V_{Img} on trap axis is given by

$$V_{\text{Img}} = \frac{u}{R} \cdot \sum_{k=1}^{\infty} \frac{e^{-\mu_k \cdot z_{R1}} - e^{-\mu_k \cdot z_{R2}}}{J_1(\mu_k \cdot R) \cdot \mu_k} \cdot \sinh(\mu_k \cdot z). \quad (11)$$

$$\begin{aligned}z_{R1/2} &:= z \text{ coordinates of the right electrode, } z_{R1} < z_{R2} \\ R \cdot \mu_k &:= k\text{-th positive zero of } J_0 \\ u &:= \text{solution of equation (3)}\end{aligned}$$

Assuming small amplitudes in z , equation (11) can be approximated as

$$V_{\text{Img}} \approx \frac{u \cdot z}{R} \cdot \sum_{k=1}^{\infty} \frac{e^{-\mu_k \cdot z_{R1}} - e^{-\mu_k \cdot z_{R2}}}{J_1(\mu_k \cdot R)} = u \cdot z \cdot A. \quad (12)$$

The parameter A resulting from the given fast converging series contains all geometric information of the trap. For the HITRAP design $A \approx 18.39$. Using equation (5), (6) and (8), the difference of the induced charges is

$$Q_L - Q_R = \frac{2q}{R} \cdot \sum_{k=1}^{\infty} \frac{e^{-\mu_k \cdot z_{R1}} - e^{-\mu_k \cdot z_{R2}}}{J_1(\mu_k \cdot R) \cdot \mu_k} \cdot \sinh(\mu_k \cdot z) \quad (13)$$

and the derivative of the induced current (see equation (4)) can be expressed as

$$\frac{di}{dt} = \frac{d^2}{dt^2}(Q_L - Q_R) = \frac{2q}{R} \cdot \sum_{k=1}^{\infty} \frac{e^{-\mu_k \cdot z_{R1}} - e^{-\mu_k \cdot z_{R2}}}{J_1(\mu_k \cdot R)} \cdot (\mu_k \cdot \dot{z}^2 \cdot \sinh(\mu_k \cdot z) + \ddot{z} \cdot \cosh(\mu_k \cdot z)) \quad (14)$$

For small amplitudes of z (keeping only first order terms in $z, \dot{z}, \ddot{z}$), equation (14) can be again approximated as

$$\frac{di}{dt} \approx \frac{2 \cdot \ddot{z} \cdot q}{R} \cdot \sum_{k=1}^{\infty} \frac{e^{-\mu_k \cdot z_{R1}} - e^{-\mu_k \cdot z_{R2}}}{J_1(\mu_k \cdot R)} = 2 \cdot q \cdot A \cdot \ddot{z} \quad (15)$$

Assuming a harmonic trap potential on axis $V(z) = \frac{V_0}{2} \cdot z^2$ and regarding equations (15), (12), (10) and (3), the resistive cooling of a single particle is described approximately by two coupled differential equations:

$$\begin{aligned} \ddot{z} + \frac{q}{m} \cdot V_0 \cdot z &= -\frac{q}{m} \cdot u \cdot A \\ \ddot{u} + \frac{1}{R \cdot C} \cdot \dot{u} + \frac{1}{L \cdot C} \cdot u &= \frac{2 \cdot q \cdot A}{C} \cdot \ddot{z} \end{aligned} \quad (16)$$

A numerical solution of equation (16) for a single $^{235}\text{U}^{92+}$ ion using the HITRAP geometry is shown in figure 7. The input parameters of the RLC circuit has been chosen as $(R, L, C) = (10 \text{ M}\Omega, 4.03 \text{ kH}, 0.1 \text{ fF})$. The simulation covers a period of 5 ms, where a time step of 0.5 ns has been used. The left graph shows the axial position of the ion. The amplitude as well as the total energy decrease exponentially with time, as expected.

SUMMARY

We are developing a numerical code for MD simulations of the dynamics of ion clouds in Penning traps which is capable to perform full 3D simulations of ion clouds with large particle numbers and multiple species on a single GPU device including the ion-ion Coulomb interaction as well as static and time-dependent external fields and cooling forces.

The current state of our code allows to perform 3D simulations on ion clouds with about 10^4 particles including full ion-ion interaction and static and time dependent field

FIGURE 7. Left graph shows the simulation results of the axial ion position and the right graph the corresponding energy.

forces and keeping energy conservation over long time periods for isolated systems. Currently we are implementing the algorithm for the resistive cooling of ion clouds and different RLC circuits. Work on a comparison of our simulation results with experimental data is in progress.

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