

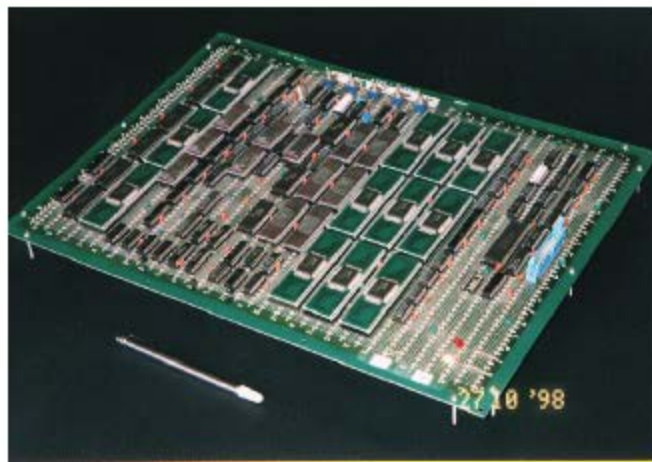
GPUによる反水素生成 --CUNBODYとSIMBUCA--

飯高敏晃(理研戎崎計算宇宙,iTHES)

Simon van Gorp(理研山崎原子物理)

(I) 演算加速器研究

初代GRAPEは20万円

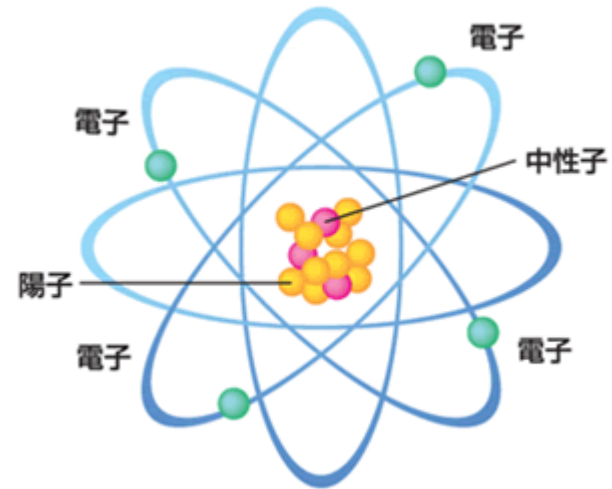


なぜ安かったか

秋葉原で市販品(量産品)の部品を買ってきて組み立てた。

http://www.iitaka.org/bookshelf_j.html#special_computer

宇宙 \leftrightarrow 原子 対称性



$$F_i = G \sum_j m_i m_j \frac{(\vec{r}_j - \vec{r}_i)}{|\vec{r}_j - \vec{r}_i|^3}$$

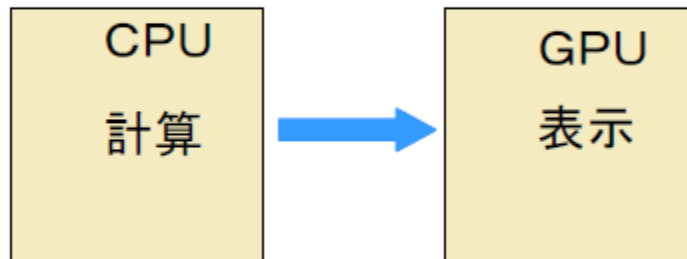
重力

$$F_i = -k \sum_j q_i q_j \frac{(\vec{r}_j - \vec{r}_i)}{|\vec{r}_j - \vec{r}_i|^3}$$

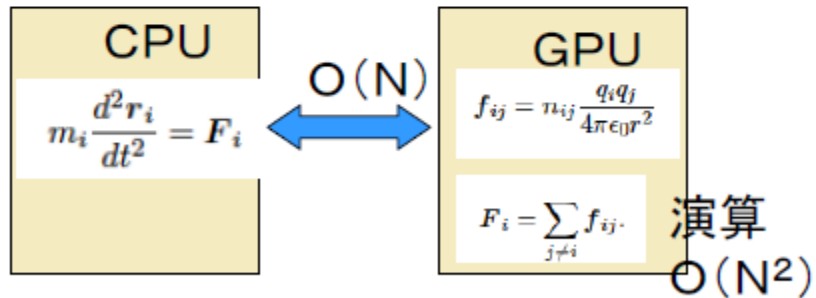
クーロン力

CPUとGPU

通常の利用



補助計算機
として



Cg言語 (GPU用C言語)

クーロン力の和の計算

$$f_{ij} = n_{ij} \frac{q_i q_j}{4\pi\epsilon_0 r^2}$$

```
struct Output {  
    float4 color : COLOR;  
};
```

```
Output main(  
    float2 i : TEXCOORD0,  
    uniform int mx,  
    uniform int my,  
    uniform samplerRECT texture):COLOR
```

```
{  
    Output OUT;  
    float r,rr,k,l;  
    float2 j;  
    float3 ri,rj,rij,force;  
    const float eps2=1e-6;  
    force=0;  
    ri = texRECT(texture,i);  
    for(l=0.5; l <my; ++l){  
        for(k=0.5; k <mx; ++k){  
            j=float2(k,l);  
            rj = texRECT(texture,j);  
            rij= rj-ri;  
            rr = eps2+dot(rij,rij);  
            r = sqrt(rr);  
            force += rij/(r*rr) ;  
        }  
    }  
    OUT.color.xyz=force;  
    return OUT;  
}
```

GPUでの数値表現

✦ 各色が単精度浮動小数点(32bit)に対応

✦ 画素の構成



✦ 例: 128x128粒子の座標



MD-GRAPEとの比較

Data	GF7800GTX	MDGRAPE-2[3]	MDGRAPE-3[4]
# of pipeline	32	4	20 20
clock (MHz)	400	100	460 250
peak (Gflops)	150	16.4	300 165
peak (Gpair/sec)	6	0.4	9 5
sustained (Gflops)	15	3.75	NA (165)
sustained (Gpair/sec)	0.6	0.09	NA (5)

✧ [3] R. Susukita et al., Phys. Commun. 155, 115 (2003).

✧ [4] M. Taiji et al., in Proceedings of SC'03, November 15-21, 2003, Phoenix Arizona, USA.

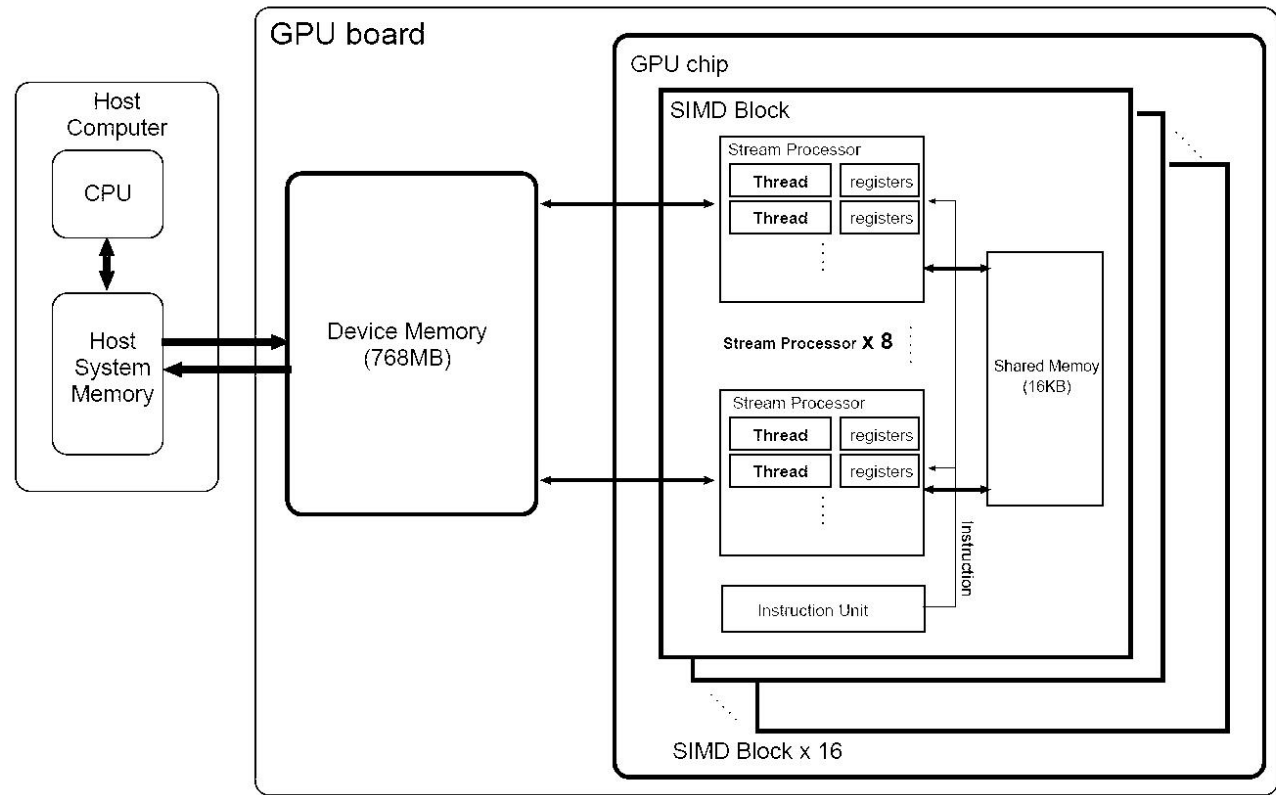
http://mdgrape.gsc.riken.jp/?easiestml_lang=xlang:ja

Why a GPU?

GPU

- high parallelism (pipelining!)
- very fast floating point calculations
- CUDA programming language for GPU's

Geforce 8800 GTX



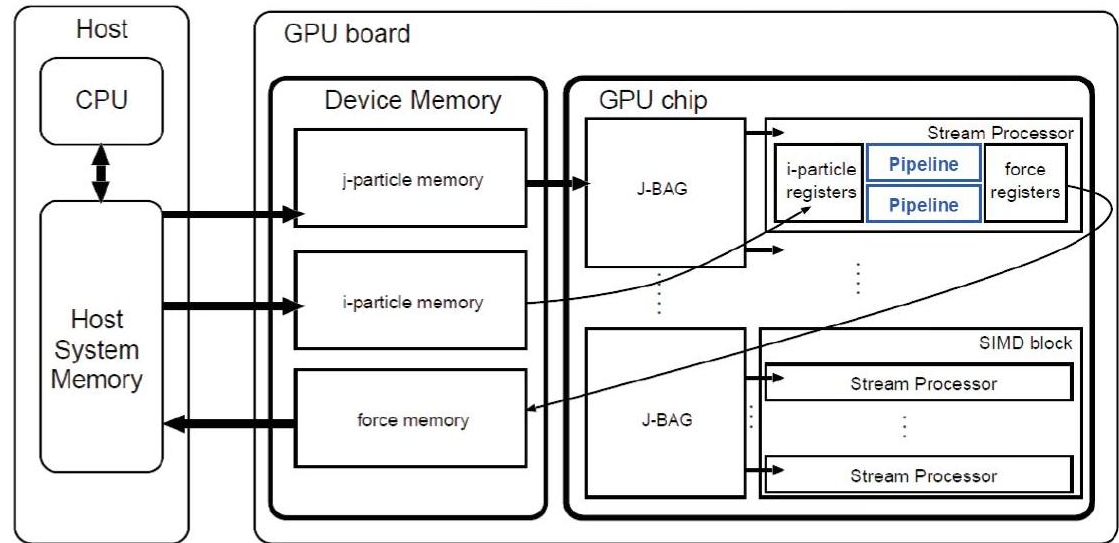
Stream processor

≈ CPU

= Comparable with a factory assembly line with threads being the workers

Chamomile scheme

- Calculating gravitational interactions on a **Graphics Card** via the **Chamomile** scheme from Hamada and litaka (in 2007).



i-particles piece available for each 'assembly line'

j-particles piece presents itself sequentially to each line

force is the output of each line

[7]: T. Hamada and T. litaka, *arXiv.org:astro-ph/0703100*, 2007
<http://arxiv.org/pdf/astro-ph/0703100v1.pdf>

Chamomile scheme: practical usage

- Function provided by Hamada and Itaka:

`cunbody1_force(xj, mj, xi, eps, ai, nmax, nmax)`

- Gravitational force \approx Coulomb Force

$$\mathbf{F}_{grav} = G \frac{Mm}{|\mathbf{r}|^2} \hat{\mathbf{r}} \qquad \mathbf{F}_{coulomb} = k_e \frac{Qq}{|\mathbf{r}|^2} \hat{\mathbf{r}}$$

- Conversion coefficient:

$$a_{Coulomb} = -\frac{q^2 k_e}{m} ai;$$

- Needed:
- 64 bit linux
 - NVIDIA Graphics Card that supports CUDA
 - CUDA environment v2.3 - 5.0

Not needed: -CUDA knowledge

-...

反水素

背景

- 宇宙誕生時は通常の物質と同量あったはずの反物質は、現在の宇宙には同量ない。理由を解明すれば、宇宙誕生の謎に迫れる。

CPT対称性

- パリティ(P)変換

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} \xrightarrow{P} \begin{pmatrix} -x \\ -y \\ -z \end{pmatrix}$$

- 電荷(C)変換

$$Q \rightarrow -Q$$

- 時間(T)変換

$$T \rightarrow -T$$

- 普通の古典力学、量子力学、場の理論はC、P、Tそれぞれについて対称(不変)

- 例:

$$m_1 \frac{d^2 r_1}{dt^2} = \frac{Q_1 Q_2}{4\pi\epsilon_0} \frac{r_1 - r_2}{|r_1 - r_2|^{3/2}}$$

古典水素原子 \leftrightarrow 古典反水素原子

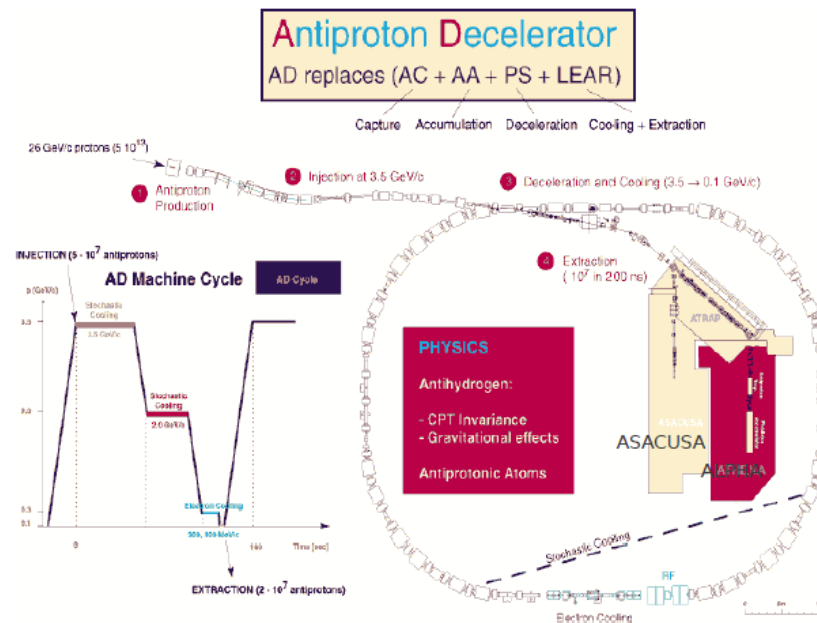
$$m_2 \frac{d^2 r_2}{dt^2} = \frac{Q_2 Q_1}{4\pi\epsilon_0} \frac{r_2 - r_1}{|r_2 - r_1|^{3/2}}$$

CPT対称性の破れ

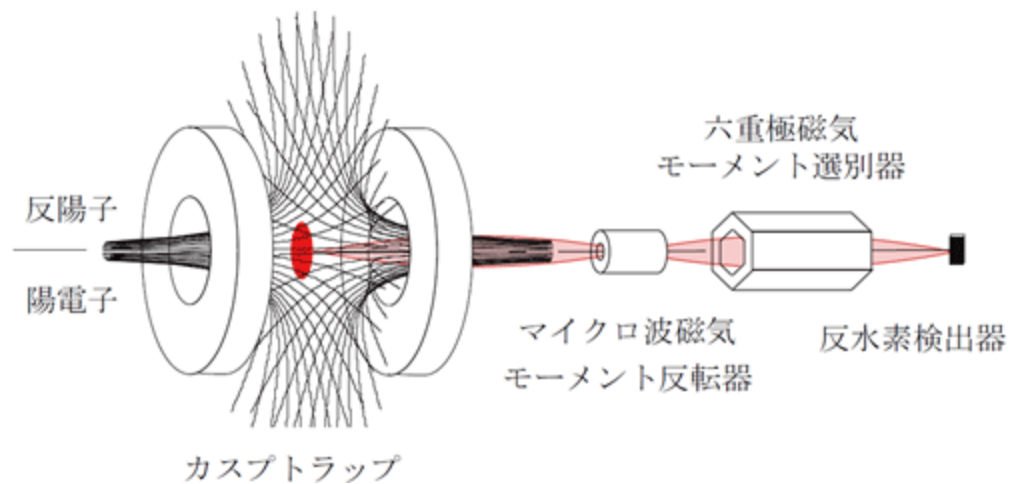
- C,P,CP対称性の破れは見つかった。
- CPT対称性の破れは見つかっていない。
- 普通の「場の量子論」では破られない
(証明済)
- ほんとうにそうか。実際はどうか。
水素と反水素のエネルギーレベルを比較
- 低エネルギー反水素を生成する必要

Ion Trap

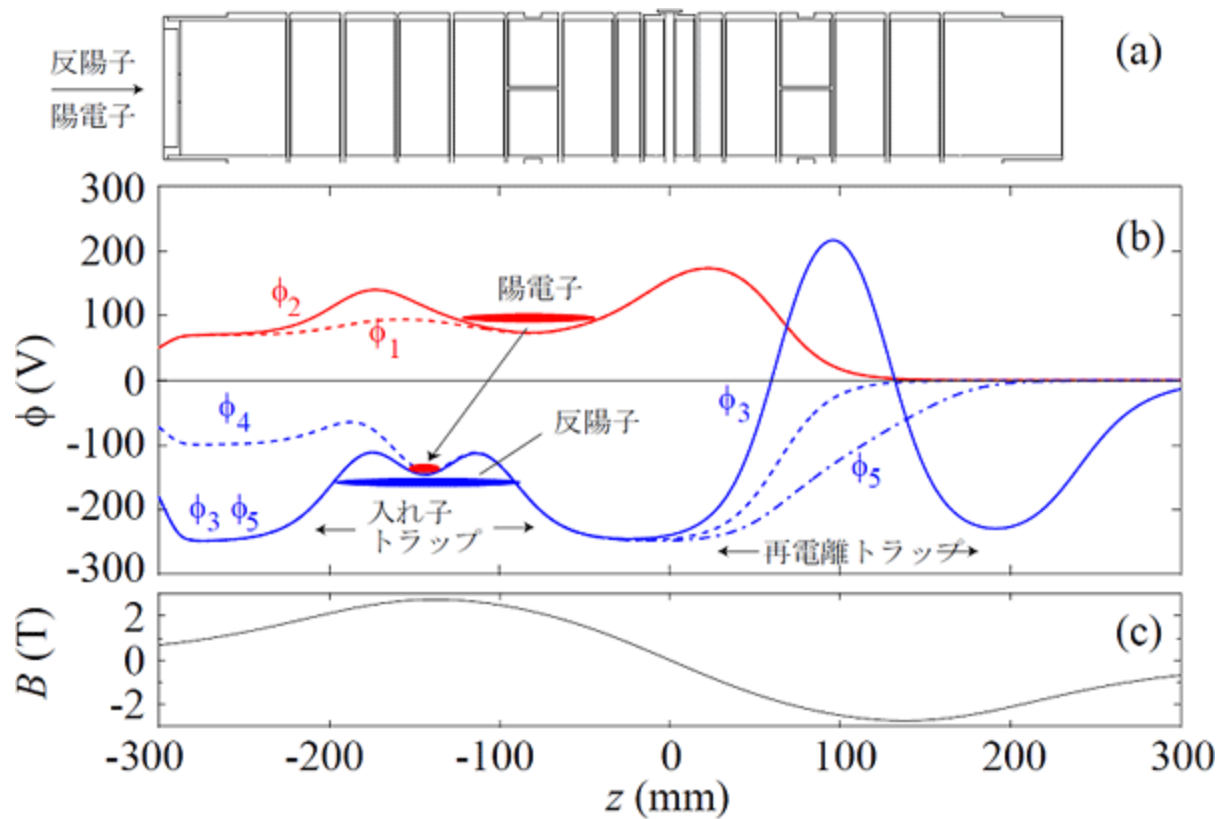
- 反陽子は、真空から対生成によって作られる。
 ~GeVのエネルギー→冷却する必要がある。



http://athena-positrons.web.cern.ch/ATHENA-positrons/wwwathena/graphics/AD_OVERVIEW.gif



反陽子とポジトロンをIon Trap に捕まえて反水素を合成、測定
http://www.riken.go.jp/pr/press/2010/20101206_2/digest/
http://www.riken.go.jp/en/pr/press/2010/20101206_2/



反水素合成には**クーロン相互作用をする**反陽子とポジトロンの雲の運動をうまく制御する必要
 \Rightarrow Ion Trap Simulation

http://www.riken.go.jp/en/pr/press/2010/20101206_2/

SIMBUCA:



Simon van Gorp

Ion Trap Simulation

Simbuca overview

Simbuca is a modular Penning trap simulation package.

Reading external fieldmaps

Comsol

SIMION

....

Trap excitations

3 different integrators

3 buffer gas routines

Can run on CPU and GPU

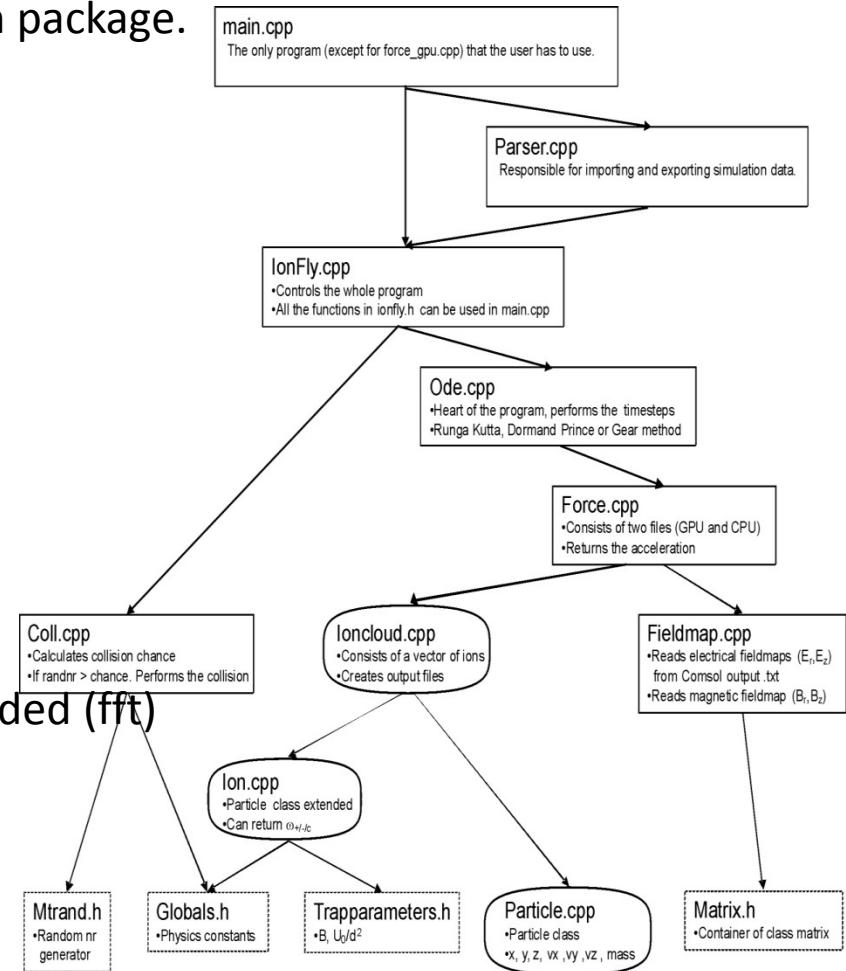
Compile with g++ or icpc

Several analysis tools are provided (fft)

A Makefile is provided

Support by me 😊

<http://sourceforge.net/p/simbuca/wiki/>



[5]: T. Hamada and T. Itaka (2007), [arXiv.org:astro-ph/0703100](https://arxiv.org/astro-ph/0703100)

<http://arxiv.org/pdf/astro-ph/0703100v1.pdf>

Why ?

Understanding the effect of **Coulomb interaction** where calculations are not possible
Initially created for the WITCH experiment (Energy and position of the ion cloud or $^{35}\text{Ar}^{1+}$).

How ?

Using a timestep **integrator** (f.e. Runge Kutta adaptive 4th or Gear or Dormand-Price 5th order) to calculate the particle tracks due to the presence of **Electric and Magnetic fields**. **Initially** written for **Penning traps** – now also used for Paul traps, RFQs, MR-TOFs, ...

Coulomb interaction is calculated on a Graphics card (GPU) which is much faster than the conventional CPU (see later).

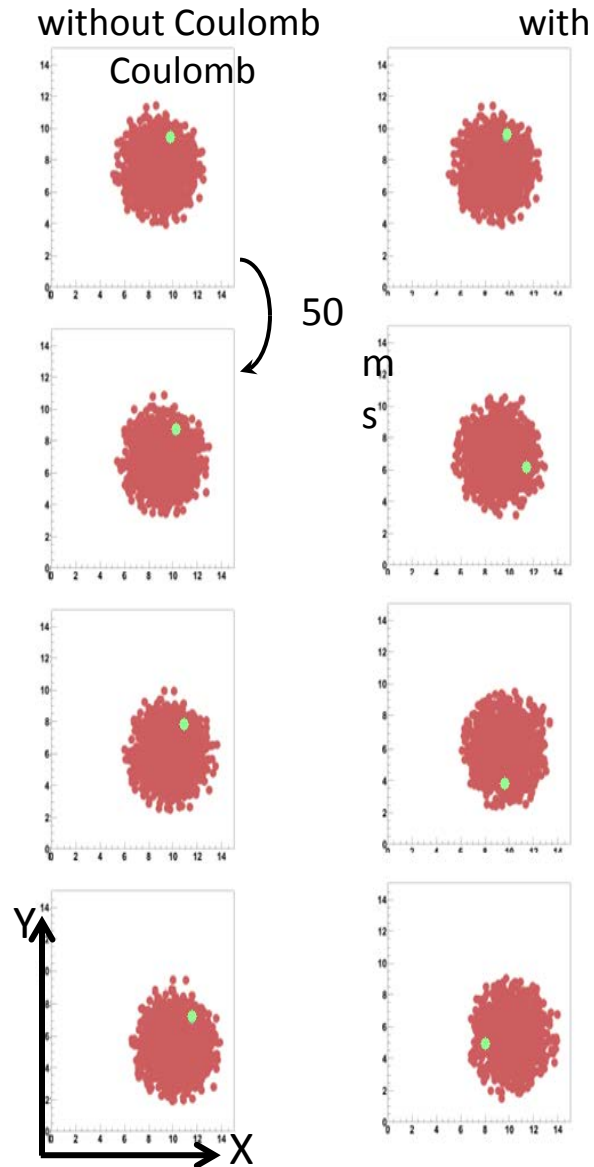
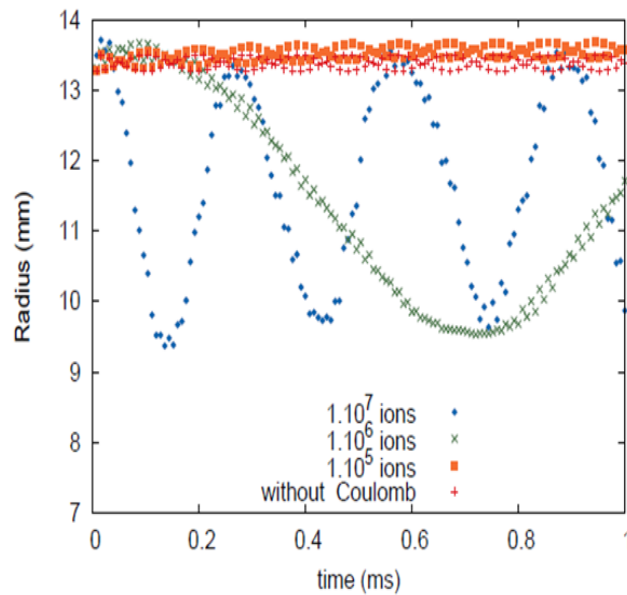
Example

Test of Simbuca by comparing it with the equations of motion of a **dipolar excitation** at the eigenfrequency . Perfect correspondence between Simulation and theory is found [1].

[1]: S. Van Gorp, et al. (2011), *Nuclear Instruments and Methods in Physics research A*, 638, 192-200

Other space charge effects examples:

When trapping a **large amount** of $^{133}\text{Cs}^+$, the cloud's own **electric field** will create an **$E \times B$ drift** force for the ions which scales with particle number



まとめ

- CPT対称性の破れと反水素
- クーロン相互作用をする反陽子・ポジトロンの雲の操作と反水素生成のシミュレーション
- SIMBUCAパッケージ (Ion Trap Simulation)
- CUNBODYライブラリ (クーロン相互作用)