PIC Method for Numerical Simulation

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NNP – Group

Contents

- Motivation
- Particle In Cell Method
- Projects
- Plasma and Ion Beam Simulations

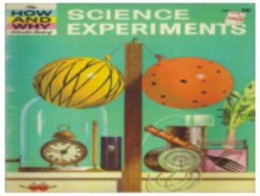
Motivation

Experiments with Computer

Science behind phenomena
that is not easily observed

Explain experimental
results that can not be
calculated by hand

Theory

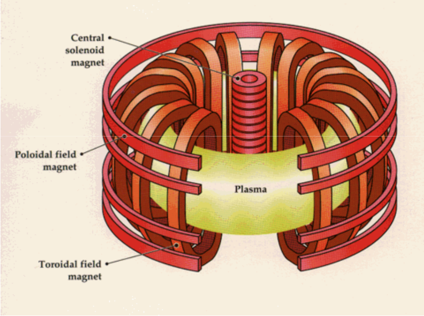


Experiments

Particle simulation

Ion beams and Plasmas

- Accelerators
    - Mostly single specie ions, different *A/q* ratio
    - Energy range from few *keV*
    - Main momentum component in forward direction
- Stellarators and Tokamaks
    - Thermal / Maxwellian distribution of momentum
    - Energy range from few *keV* till *MeV*
    - Magnetic confinement is the main issue
    - Neutral or non neutral
- Discharge plasmas
    - Pressure
    - Multi specie model: Ions, electrons, neutral atoms or molecules
    - Energy range upto few *keV*



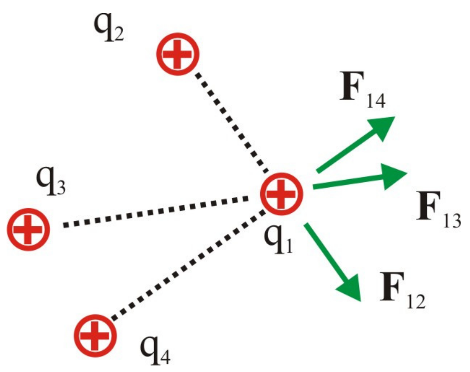
Particle in Cell : Philosophy

- Main Task
  - Calculate the force on charged particles through Lorentz Equation

$$\vec{F} = m\vec{a} = q(\vec{E} + \vec{v} \times \vec{B})$$

  - Simulate many particles

$$\vec{E}_i = \sum_{\substack{j=0 \\ j\neq i}}^{n} \frac{1}{4\pi\varepsilon_0} \frac{q_i q_j}{\left|\vec{r}_i - \vec{r}_j\right|^2} \left(\vec{r}_i - \vec{r}_j\right)$$



- Prof. Hartree and Phyllis Nicolson (1941-1944) used desk calculator 30 electrons in Magnetron, 1D, Space charge included

  - Computer with floating point operation 1µs

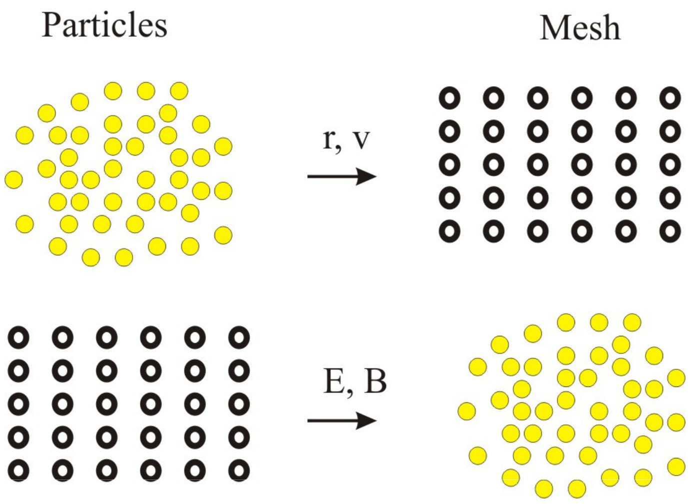
$$Operation \quad count = \alpha N_p + \beta(N_g)$$

$$\alpha = 20 \quad \beta = 5N^3 \log_2 N^3 \quad N = 32 \quad N_p = 10^5$$

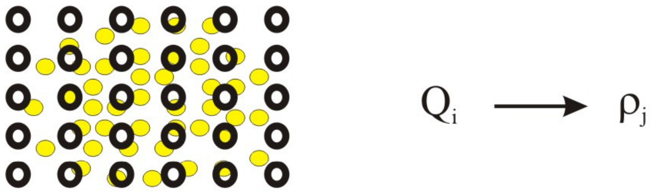
$$CPU \quad time \quad = \quad 1 \quad day \quad for \quad PP$$

$$= \quad 4.5 \quad \sec onds \quad for \quad PM$$

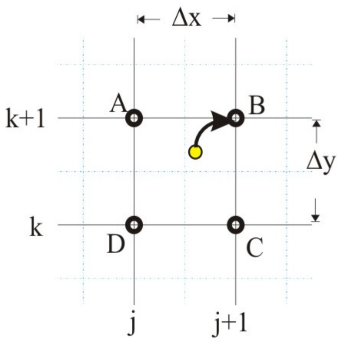
PIC model



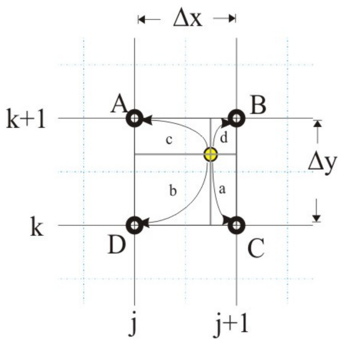
- Disordered data to the structured data form
- Periodicity, Symmetry



- Charge distribution on grid points and back interpolation
- Weighing schemes according to nessecity
  - \- Linear weighing
  - \- Functional form



Nearest Grid Point



Area weighing

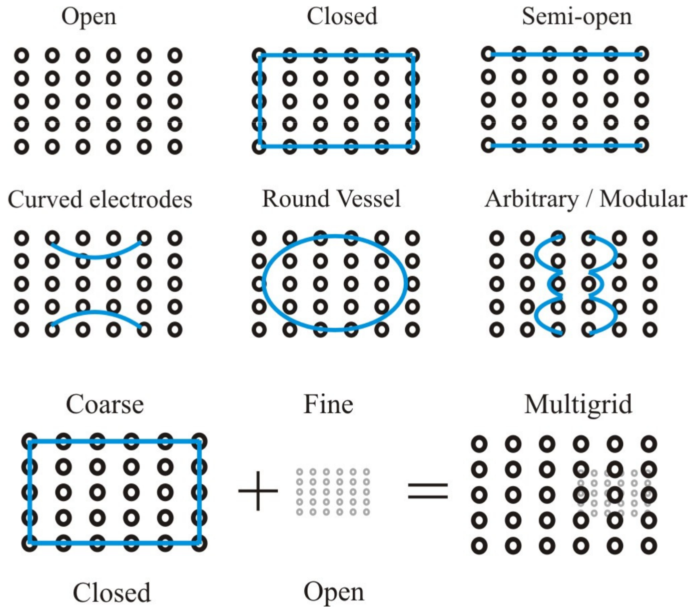
Poisson Equation

$$\nabla^2 \phi(\mathbf{r}) = -\frac{\rho(\mathbf{r})}{\varepsilon_0}$$

$$\begin{aligned}
\phi_{Ng} - 2\phi_1 + \phi_2 &= \rho_1 \\
\phi_1 - 2\phi_2 + \phi_3 &= \rho_2 \\
&\vdots \\
\phi_{Ng-2} - 2\phi_{Ng-1} + \phi_{Ng} &= \rho_{Ng-1} \\
\phi_{Ng-1} - 2\phi_{Ng} + \phi_1 &= \rho_{Ng}
\end{aligned}$$

$$\mathbf{A} \cdot \phi = -\frac{\rho}{\varepsilon_0}$$

Boundary conditions



1. Fourier Transform

$$\rho(\mathbf{x}) \rightarrow \rho(\mathbf{k}) \rightarrow \phi(\mathbf{k}) \rightarrow \phi(\mathbf{x}) \rightarrow \mathbf{E}(\mathbf{x})$$

2. Iterative methods

$$\rho(\mathbf{x}) \rightarrow \phi(\mathbf{x}) \rightarrow \mathbf{E}(\mathbf{x})$$

Applications

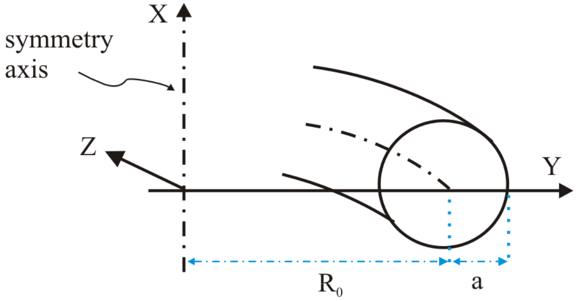
- Project MSR (Magnetostatic Storage Ring) at Frankfurt am Main
  - Ion Beam transport through toroidal segments
  - Confinement and guidance properties for ion storage
  - Injection scheme

- FRANZ facilty
  - Chopper System in LEBT setion

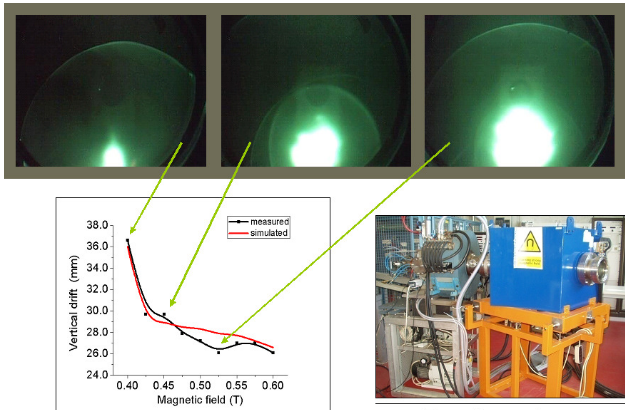
- SPIE-Program: Simulation code for Plasma and Ion Extraction
  - Dynamics of plasmas in small volume type ion source
  - Ion extraction
  - Production mechanism different species

Project MSR

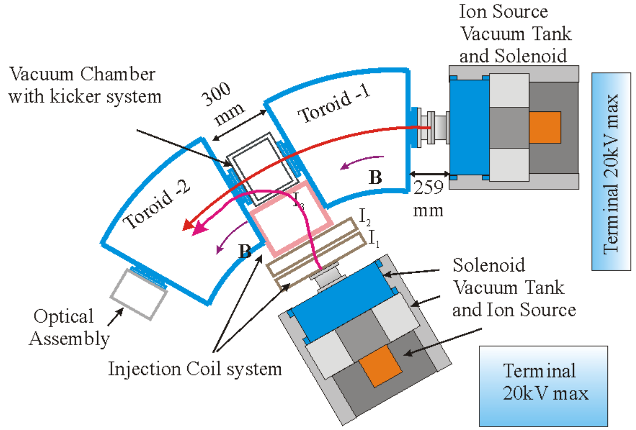
- High current beam storage in longitudinal magnetic field with closed magnetic field lines
  - Multi ampere proton beam with energy *150keV ~ few MeV*



- PIC simulation in toroidal coordinates
- Ion beam transport with electrons
- Direct comparison with experiments

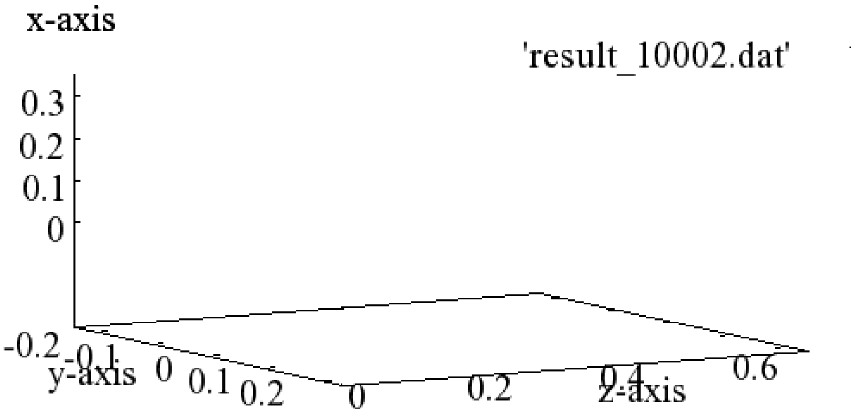


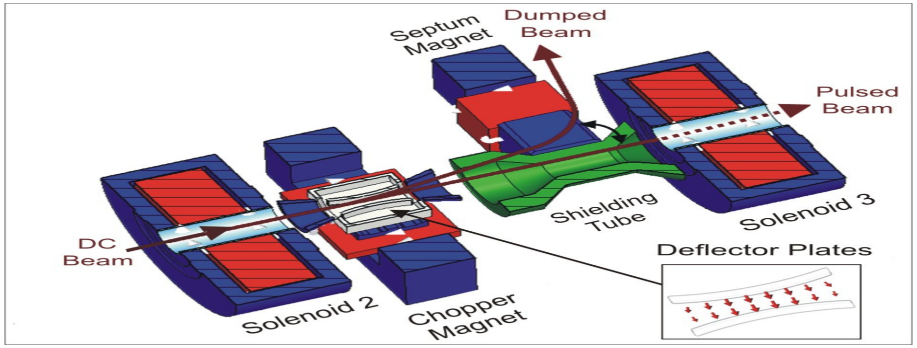
Experimental setup



FRANZ Facilty

- Chopper in Low Energy Beam Transport (LEBT) section
  - Input proton beam with current *200 mA* at the energy of *120 keV*

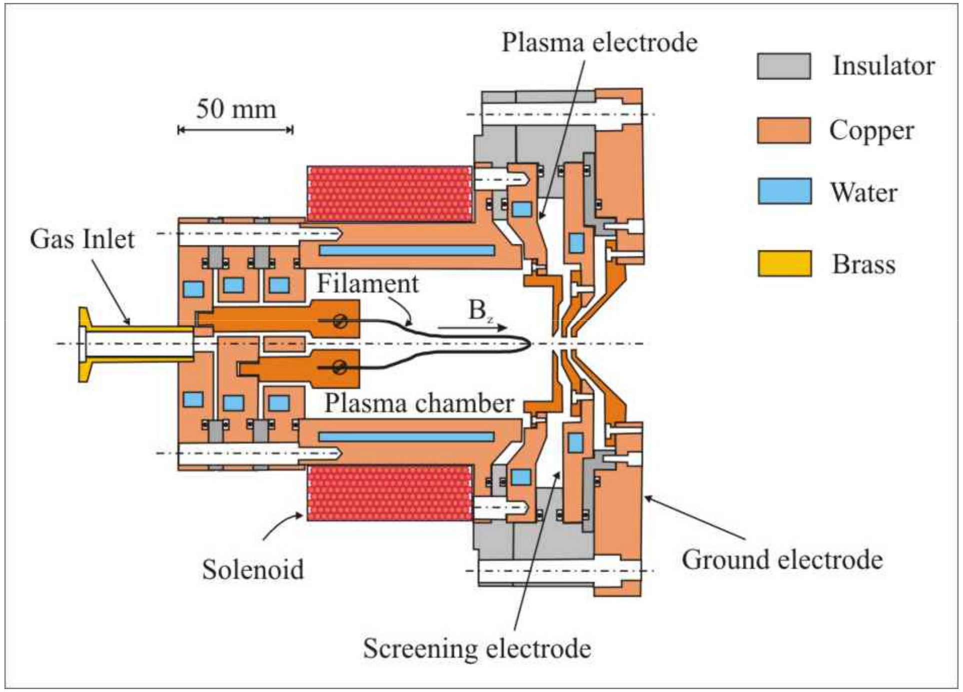




- Semi-open boundary conditions with definition of curved electrodes
- Continual generation of ions
- Space charge compensation due rest gas ionization and secondary electrons produced on wall
- Deflection due to electric field can be compared with experiments

SPIE : Ion source

Simulation code for Plasma and Ion Extraction - Program

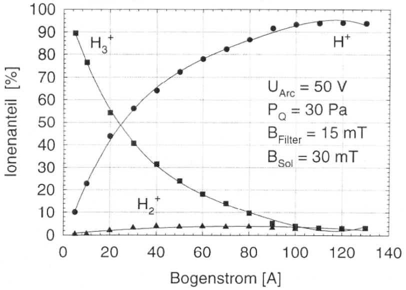


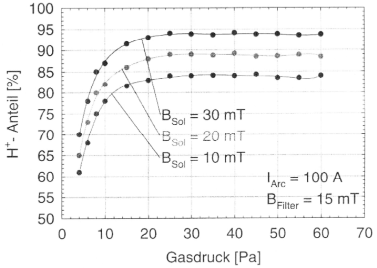
- Hot filament driven volume type ion source
- Originally constructed and developed by Peter Groß in 2000
- Triode extraction *20keV* max
- *He* ions as reference
- Proton beam for MSR experiments
- Ref: N. Joshi, doctoral thesis

Ion species

Ref: R. Hollinger, K. Volk, et.al., „Measurement of the beam emittance of the Frankfurt proton source“, RSI, 2002;
and doctoral thesis

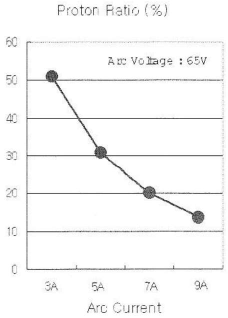
200 mA, ~93% p, @ 55 keV

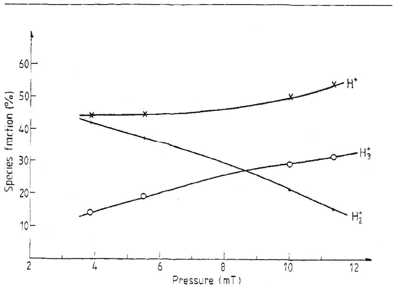




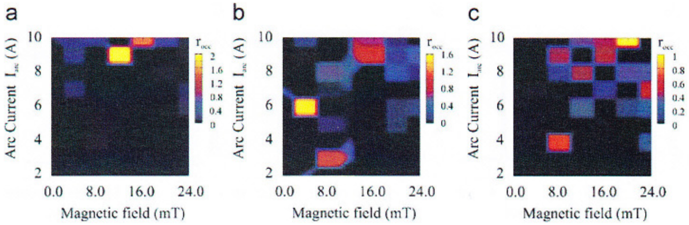
Ref: A. J. T. Holmes, et.al., „A compact ion source with high brightness“, J. Phy. E, 1980

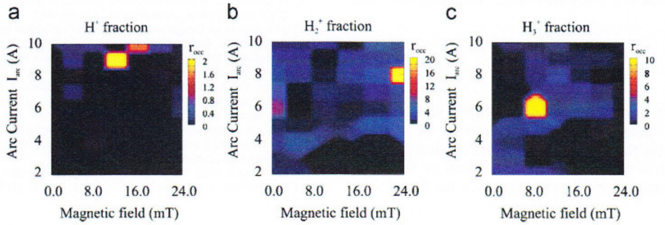
40 mA, ~60% p, @ 50 keV





Ref: N. Joshi, O. Meusel, et.al., NIM A, 2009, *5.0 mA, ~58% p, @ 10 keV*





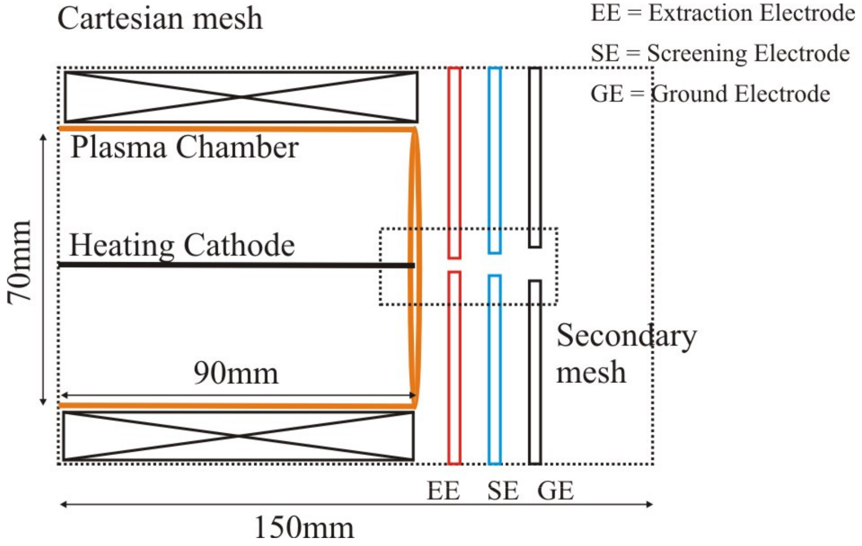
Questions

- Can we find theoretical limits of a given ion source by developing a simulation code ?
- How do the external components and fields influence the plasma properties and the production mechanism of different species in this type of source?
- Along with existing tools can we advance our code to investigate the hot filament driven ion source and find „science“ behind experimental results?

Recent compititors

- Existing codes IGUN , KOBRA, OOPIC
- China: Simulation code for description in complete 3D, with 3D graphics
- France: Simulation code to describe H^- production in negative ion source, ITER, (1D)

Simulation parameter



- Multiple Grids
- Cartesian mesh with definition of circular plasma chamber and electrodes
- Magnetic field from coils
- Continual generation of electrons at cathode

Typical potentials: HV= extraction voltage

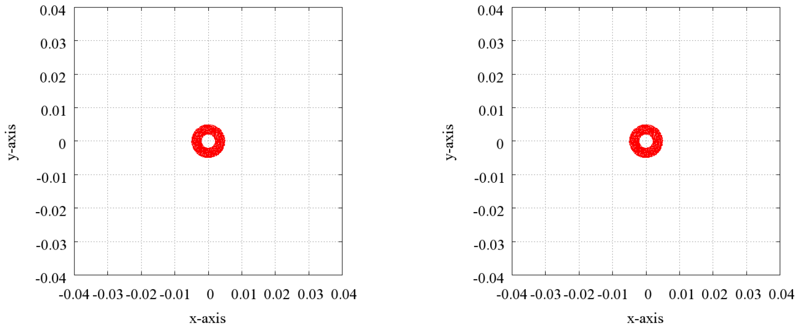
U-cathode = 0 +HV ; U-arc = 100 + HV

U-extraction = 90+ HV;

U-screening = 10% of HV

U-ground = 0.0 !!

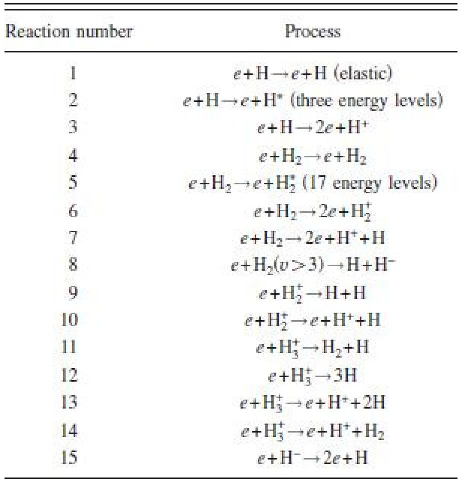
Electron simulation in plasma chamber (vertical plane), filament at the center



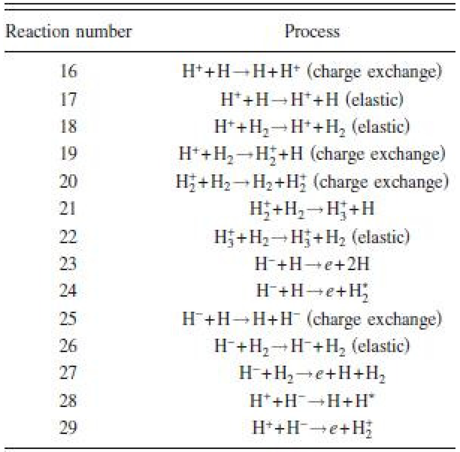
Without **B**

With **B**

Hydrogen Plasma



Reaction number	Process
1	$e+H \rightarrow e+H$ (elastic)
2	$e+H \rightarrow e+H^*$ (three energy levels)
3	$e+H \rightarrow 2e+H^+$
4	$e+H_2 \rightarrow e+H_2$
5	$e+H_2 \rightarrow e+H_2^*$ (17 energy levels)
6	$e+H_2 \rightarrow 2e+H_2^+$
7	$e+H_2 \rightarrow 2e+H^++H$
8	$e+H_2(v>3) \rightarrow H+H^-$
9	$e+H_2^+ \rightarrow H+H$
10	$e+H_2^+ \rightarrow e+H^++H$
11	$e+H_3^+ \rightarrow H_2+H$
12	$e+H_3^+ \rightarrow 3H$
13	$e+H_3^+ \rightarrow e+H^++2H$
14	$e+H_3^+ \rightarrow e+H^++H_2$
15	$e+H^- \rightarrow 2e+H$

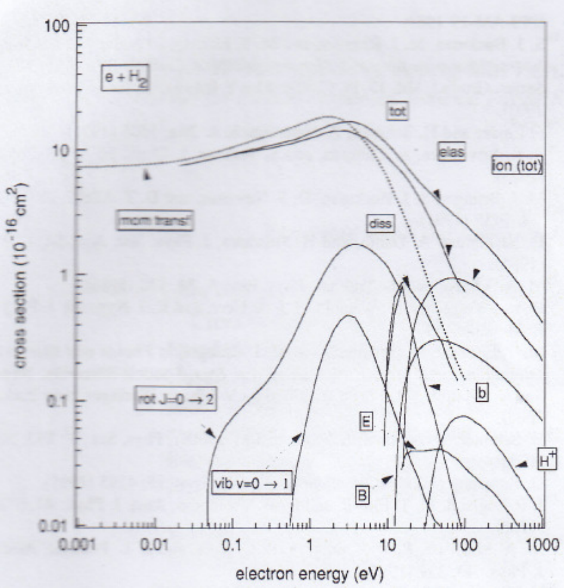


Reaction number	Process
16	$H^++H \rightarrow H+H^+$ (charge exchange)
17	$H^++H \rightarrow H^++H$ (elastic)
18	$H^++H_2 \rightarrow H^++H_2$ (elastic)
19	$H^++H_2 \rightarrow H_2^++H$ (charge exchange)
20	$H_2^++H_2 \rightarrow H_2+H_2^+$ (charge exchange)
21	$H_2^++H_2 \rightarrow H_3^++H$
22	$H_3^++H_2 \rightarrow H_3^++H_2$ (elastic)
23	$H^-+H \rightarrow e+2H$
24	$H^-+H \rightarrow e+H_2^*$
25	$H^-+H \rightarrow H+H^-$ (charge exchange)
26	$H^-+H_2 \rightarrow H^-+H_2$ (elastic)
27	$H^-+H_2 \rightarrow e+H+H_2$
28	$H^++H^- \rightarrow H+H^*$
29	$H^++H^- \rightarrow e+H_2^+$

Species => H_2 H_2^* H H^* H^+ H_2^+ H_3^+ H^- e^-

=> Total = 9

	Creation	Annihilation
H^+	5	3
H_2^+	3	3
H_3^+	1	4
H^-	1	6



Ref: „Cross Sections for Electron Collisions with Hydrogen Molecules“, Jung-Sik Yoon et.al., J. Phys Chem.

„Electron Collisions with Atoms and Molecules“, Atomic data and Nuclear data tables

PIC with Monte Carlo Collision

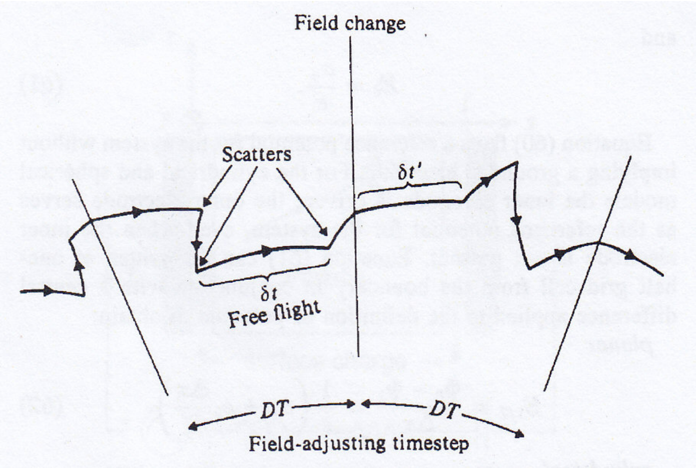
PIC

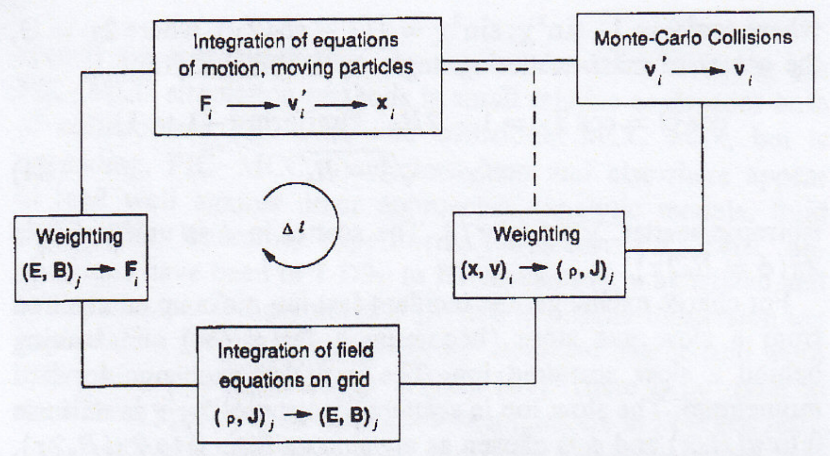
- Deterministic classical mechnics
- Moving particles in small time step
- Collective effect through self and applied fields

MC

- Probablistic
- Collisional effects in relatively weak electric fields

$$\sigma(E) \quad n(x) \quad \Delta s \rightarrow \nu_{coll} \quad P$$





MCC model

Kinetic Energy for ***i*** th particle of specie ***s***

$$E_i = \frac{1}{2} m_s v_i^2$$

Total collisional cross section is sum of where ***j*** is type of cross section

$$\sigma_T(E_i) = \sum \sigma_j(E_i)$$

Collisional probability for ***i*** th particle

$$P_i = 1 - \exp(-\Delta t v_i \sigma_T(E_i) n_t(\mathbf{x}_i))$$

Random numbers R_1, R_2 => [0,1]

Random numbers R_3, R_4 => [0,1]

$$R_1 < P_i \quad \Rightarrow \quad collision$$
$$R_2 \quad \Rightarrow \quad type \quad of \quad collison$$
$$R_3, R_4 \Rightarrow \quad Scattering$$

Error missed collision in Δt

$r<0.01$ => $P_i<0.095$

$$r \sim \sum_{k=2}^{\infty} P_i^k = \frac{P_i^2}{1-P_i}$$

Example He- ions

Single specie plasma from Helium

$$e^{-} + He \rightarrow He^{+} + 2e^{-}$$

Plasma chamber
length *0.1m*
radius r=*0.035m*

Filament *90mm*

Green : Electrons

Red : He - ions

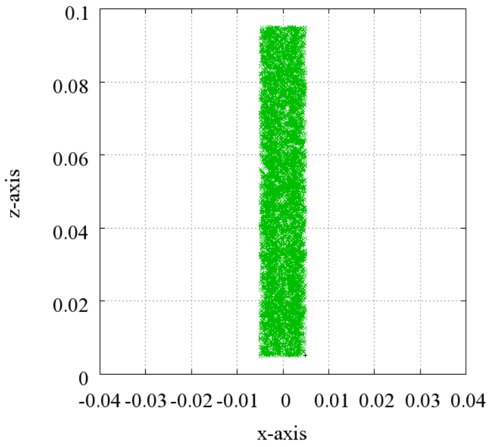
Horizontal plane

Simulation time

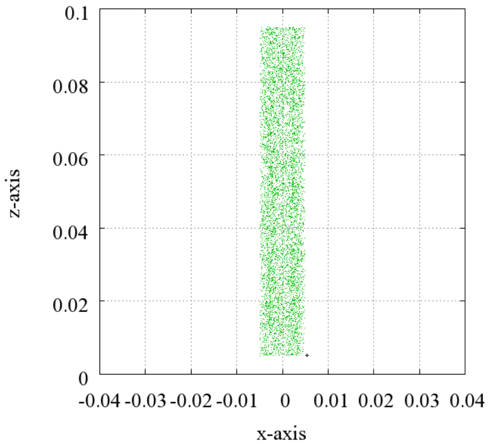
Each step ~ ns

Total time max 0.5 µs

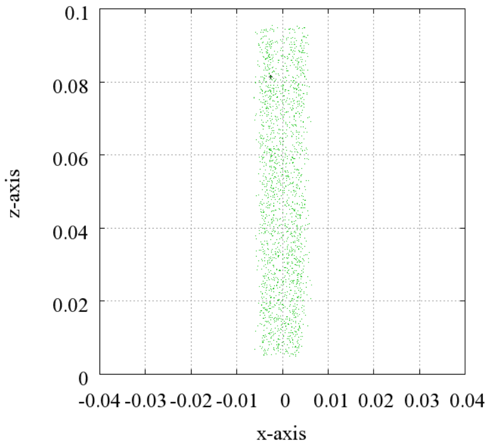
B ~ *0* Gauss



B~*few* Gauss

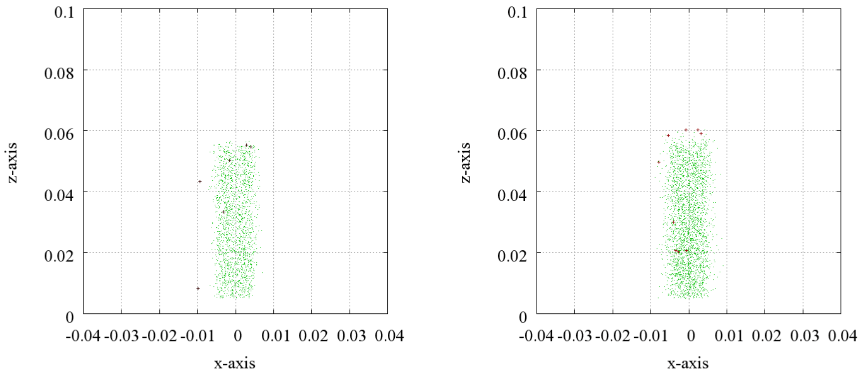


Potential Plasma electrode changed

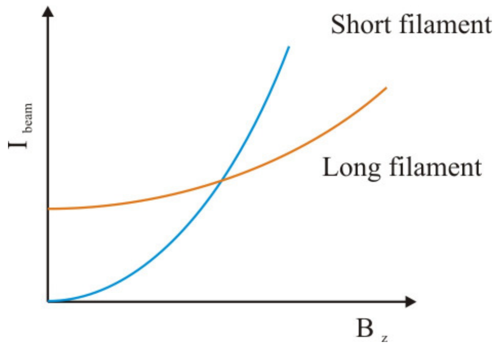


Influence on plasma

Shorter filament length *55 mm*



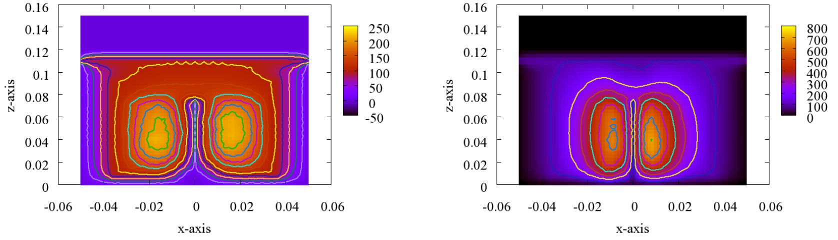
w/o **B** with **B**



Estimated beam current behaviour

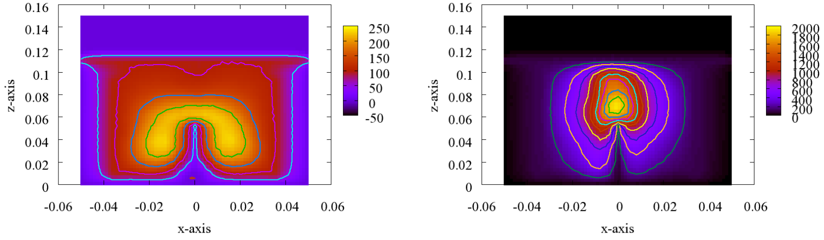
Potential distribution (Horizontal plane)

Long filament



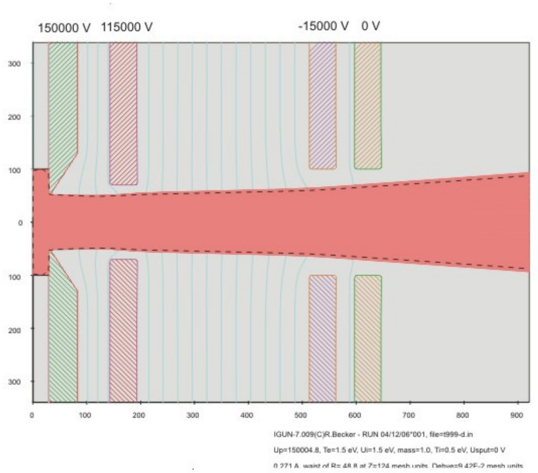
w/o **B** with **B**

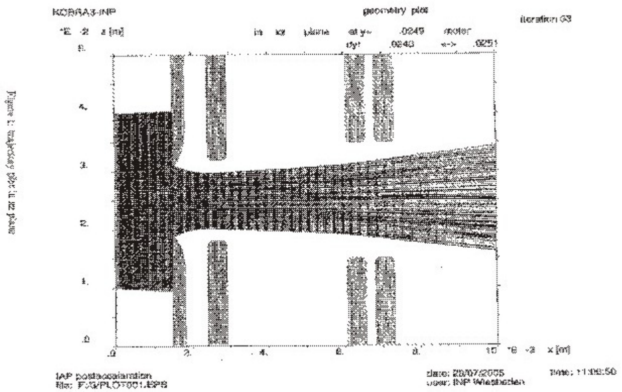
Short filament



w/o **B** with **B**

Comparison


150000 V
115000 V
-15000 V
0 V
300
200
100
0
100
200
300
0
100
200
300
400
500
600
700
800
900
IGUN-7.009(C)R.Becker - RUN 04/12/06*001, file=t999-d.in
Up=150004.8, Te=1.5 eV, Ui=1.5 eV, mass=1.0, Ti=0.5 eV, Usput=0 V
0.271 A, waist of R= 48.8 at Z=124 mesh units, Debye=9.42E-2 mesh units


KOBRA3-INP
geometry plot
iteration 63
*E -2 z [m]
in xz plane at y= .0249 meter
dy* .0248 <-> .0251
5.
4.
3.
2.
1.
.0
.0
2.
4.
6.
8.
10 *E -2 x [m]
Figure 1: trajectory plot in xz plane
IAP postacceleration
file: F:\G\PLOT001.EPS
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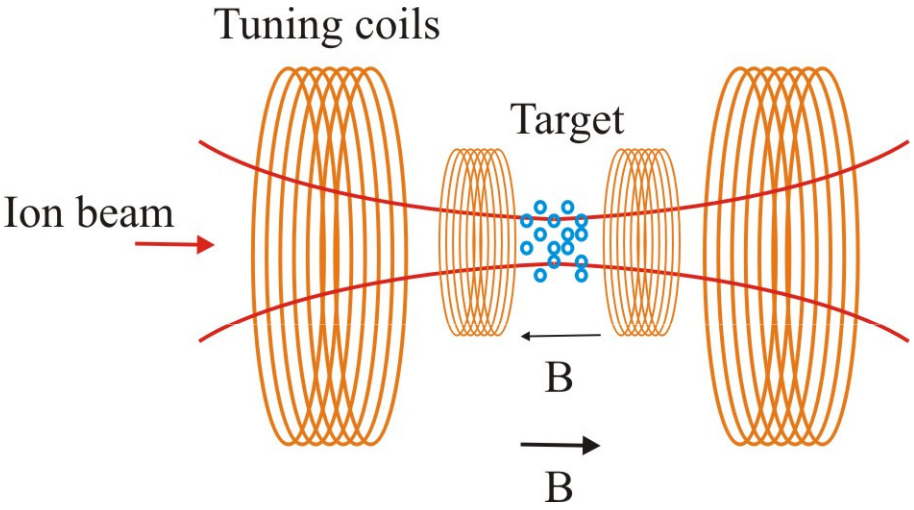
user: INP Wiesbaden
time: 11:08:50

Application to MSR

- Designing the target chamber for collision experiments



- Different Larmor gyration for ions and electrons in strong magnetic fields
- Configuration of tuning coil can be investigated for optimized particle density and scattering cross sections

References

- Computer simulation using particles
  - R. W. Hockney and J. W. Eastwood
- Plasma-based ion beam sources
  - Loeb, Plasma Phys. Control. fusion, (47), 2005
- Charged particle beams
  - S. Humphries, Jr.
- Particle-in-Cell Charged-Particle Simulations, Plus Monte Carlo Collisions With Neutral Atoms, PIC-MCC
  - C. K. Birdsall, IEEE Transactions on Plasma science, vol. 19 (2), 1991
- A Monte Carlo collision model for the particle-in-cell method: applications to argon and oxygen discharge
  - V. Vahedi, et.al., Comp. Phys. Commun., 87,1995
- Particle-in-cell with Monte Carlo collision modelling of the electron and negative hydrogen ion transport across a localized transverse magnetic field
  - St. Kolev, et.al., Phys. Plasmas, (16), 2009

- For more informaton see:
  http://www.uni-frankfurt.de/~joshi

Conclusions and Outlook

- Particle-in-cell model has been investigated and successfully applied for different problems
- The code is being upgraded Monte Carlo subroutine for simulation of collision
- The results can be directly compared with experiments
- New approaches required to study the target designing in magnetic field

Acknowledgements

- Prof. U. Ratzinger
- NNP – Group

Thank you ...!!