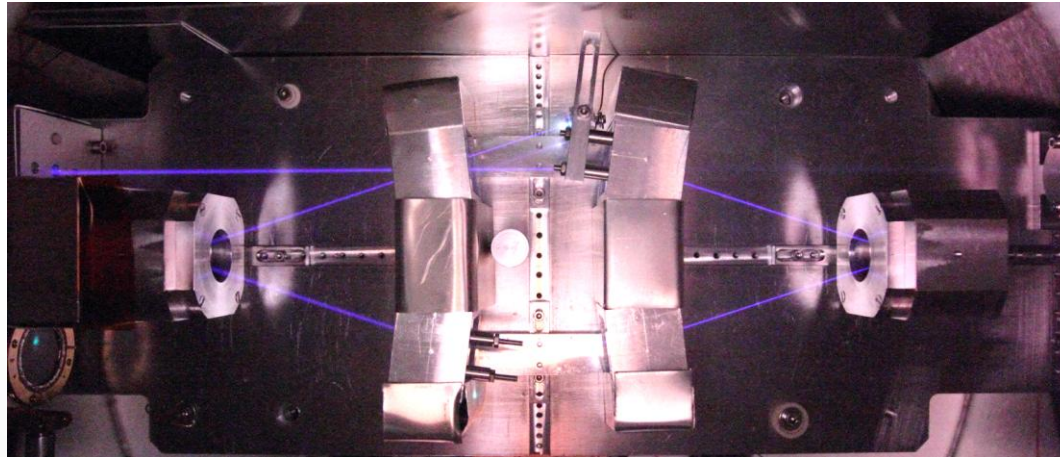# Ion trajectory simulations for the design of a compact electrostatic ion storage ring: the Mini-Ring

Jérôme BERNARD

M. Ji, C. Ortéga, G. Montagne, R. Brédy, L. Chen, S. Martin,

Institut Lumière Matière

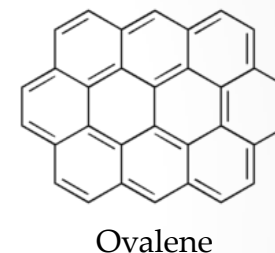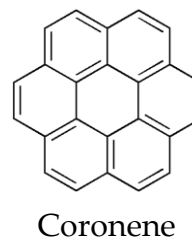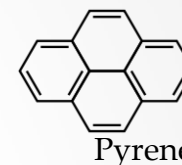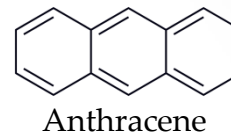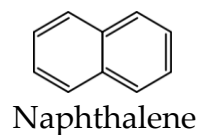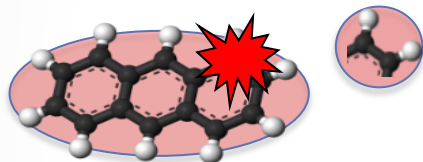

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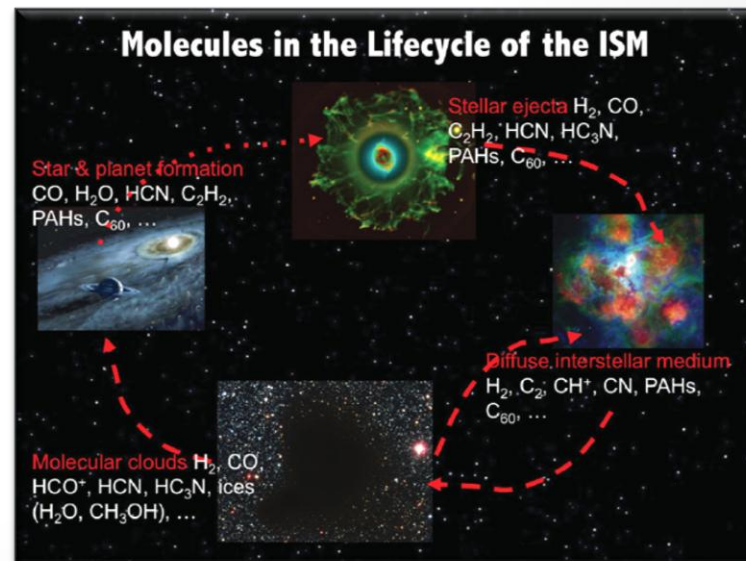Ion Technology and Spectroscopy at Low Energy Ion Beam Facilities

Current studies with the Mini-Ring

- Fragmentation and Radiative cooling of PAHs ions

Dissociation C_2H_2
                H

Naphthalene   Anthracene   Pyrene

Coronene   Ovalene

Mid-IR : vibration transitions
Red or near-IR : Poincaré Fluorescence

Molecules in the Lifecycle of the ISM

Stellar ejecta H_2, CO, C_2H_2, HCN, HC_3N, PAHs, C_{60}, ...

Star & planet formation CO, H_2O, HCN, C_2H_2, PAHs, C_{60}, ...

Diffuse interstellar medium H_2, C_2, CH^+, CN, PAHs, C_{60}, ...

Molecular clouds H_2, CO, HCO^+, HCN, HC_3N, ices (H_2O, CH_3OH), ...

A.G.G.M. Tielens, Rev. Mod. Phys.2013
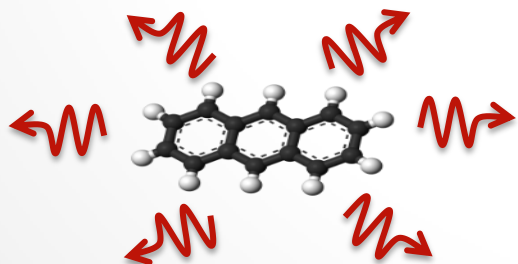
General overview of the Mini-Ring

400 mm

Ion optics

neutrals

IONS

LASER

neutrals
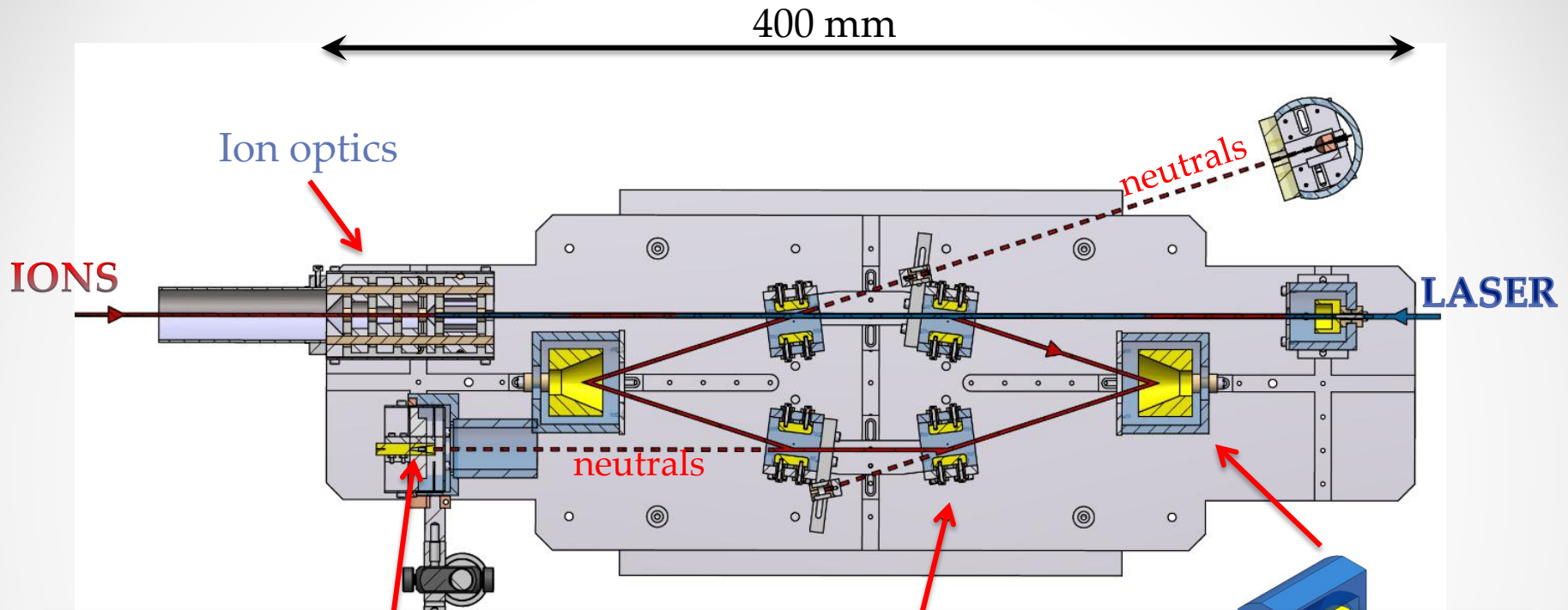
- All electrostatic (No magnetic field)
- Mass independant storage conditions
- Storage conditions (electrode voltages) only depend on kinetic energy

2 Conical mirrors
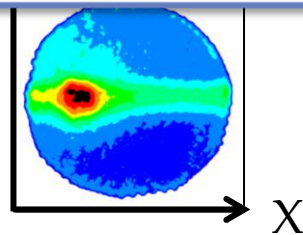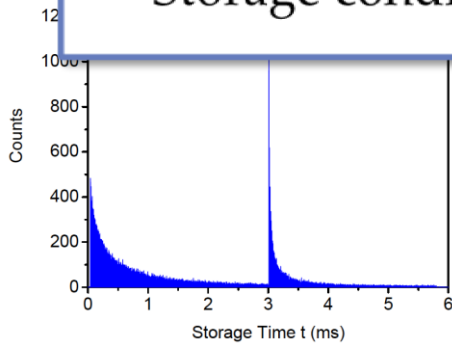
4 Parallel plate deflectors
tilted 7°

X

Low Energy Beam Line in Lyon

ECR ion source

Selection magnet

optics + chopper

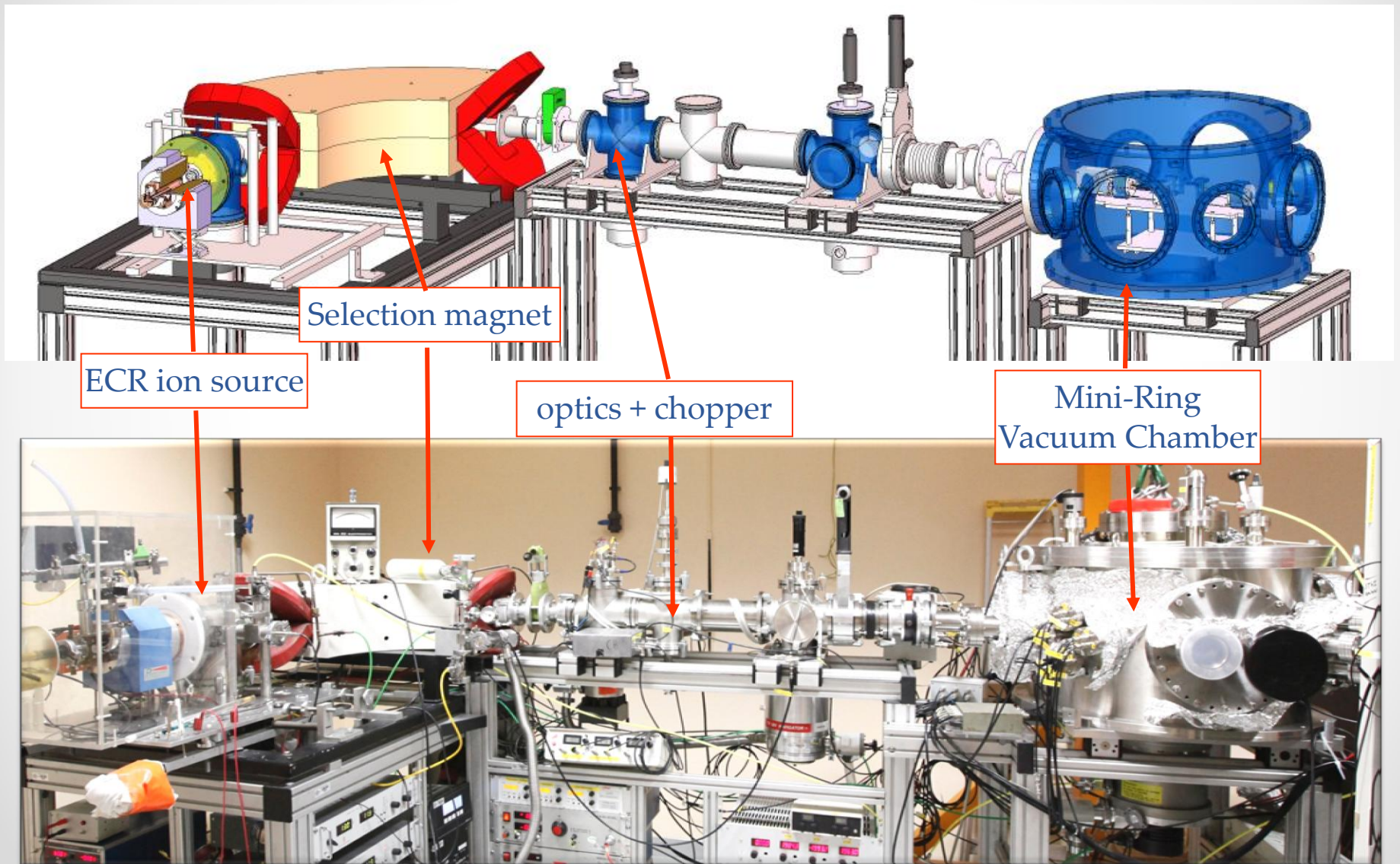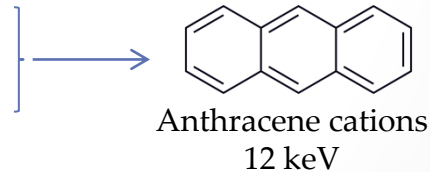Mini-Ring
Vacuum Chamber

Questions before starting the simulation of such a storage device

- ## PA design and RAM
    - Single big PA vs multiple PA assembled in IOB ?
    - Choice of grid size ?

- ## Long computation time
    - How do you know when a trajectory is a stable orbit ?
    - Computation time depends on quality factor Q
    - Q=103 seems a minimum in SIMION when velocity reversal is important

- ## Kinetic energy error?
    - It accumulates with the length of the trajectory
        1 turn -> 5 µs -> 0.7 m
        2000 turns -> 10 ms -> 1.4 km
    - It accumulates with velocity reversals

Anthracene cations
12 keV

- ## Coulomb repulsion?
    - Better ignore (neglect) it at first

The Mini-Ring – In Simion
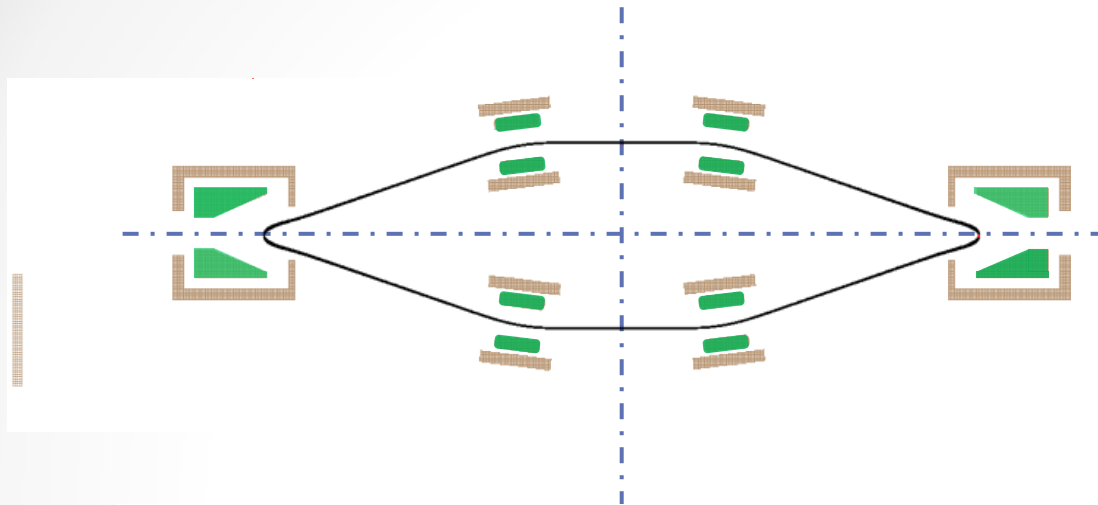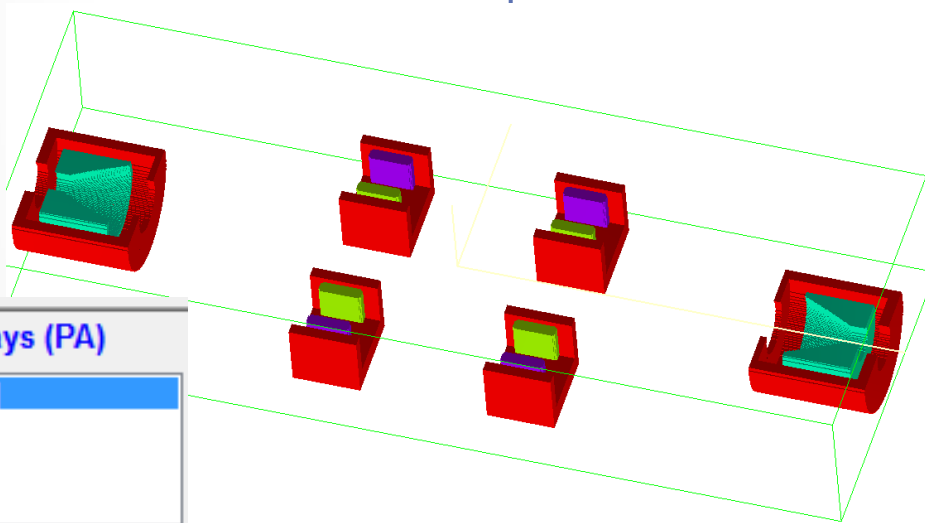

Draw 1/8th of theRing

Use 3 planar symmetries X,Y,Z

405×151×70 points
43 Mbytes PA
1 gu → 0.5 mm

My work (2006)

M. Ji's work (2011-15)

Draw 1/2 of the Ring

Uses 1 planar symmetry Z

810×241×70 points
137 Mbytes PA
1 gu → 0.5 mm

Potential Arrays (PA)

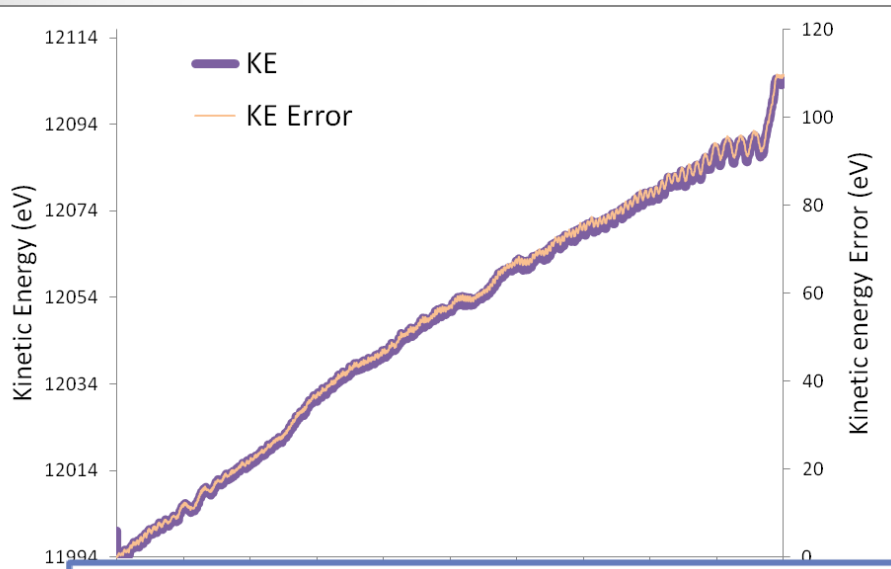MR-2012.PA0 [!]
MCP.PA0
--Empty PA--
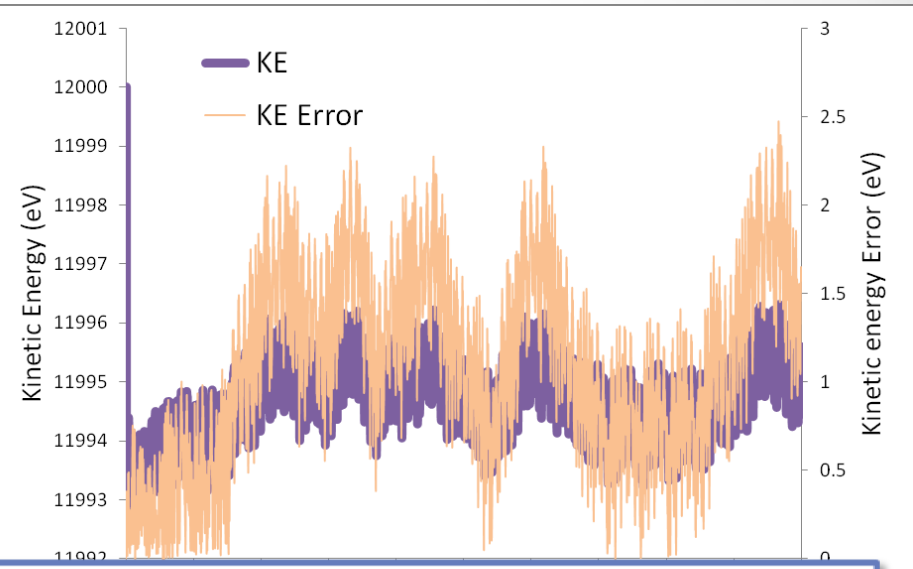
| New | Load | Save |

Remove All PAs from RAM
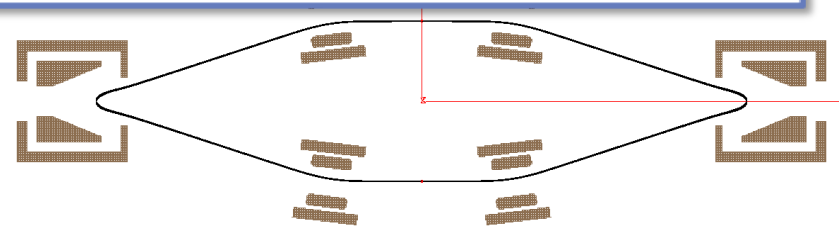
PAs Require 1428.455 MB RAM

Computation quality TQual

TQual = 3

TQual = 103

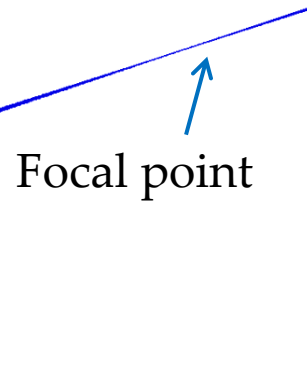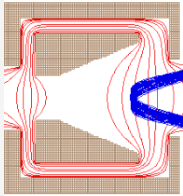- TQual ≥ 103 mandatory to account correctly for velocity reversals
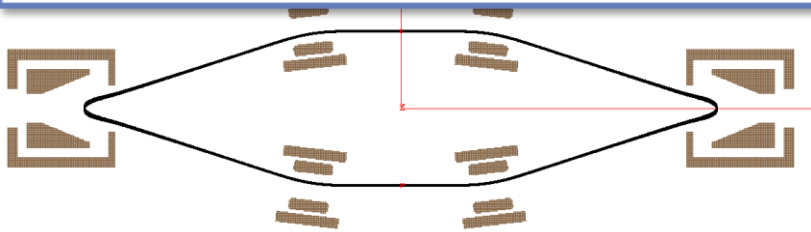
Focusing properties of the cones and deflectors

Cone

Focal point

o Similar to an optical spherical mirror

o Focus in two directions (y and z)

Deflector

Horizontal plane

Vertical plane

Focal points
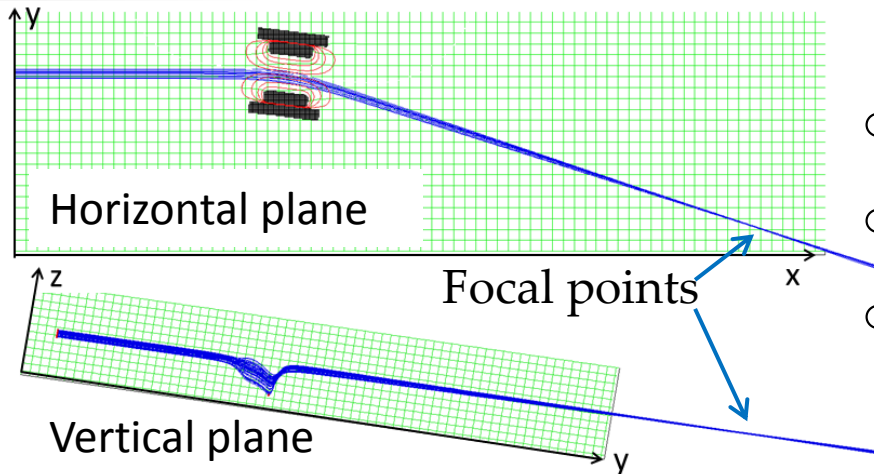
o Deflection and focus in horizontal plane

o Higher deflection angle, shorter focus

o Weak focus effect in vertical

Expected stable trajectories

Reduced quantities

$$\xi_m = \frac{qV_m}{E_k} \qquad \xi_D = \frac{qV_D}{E_k}$$

$+V_D$

$-V_D$

V_m
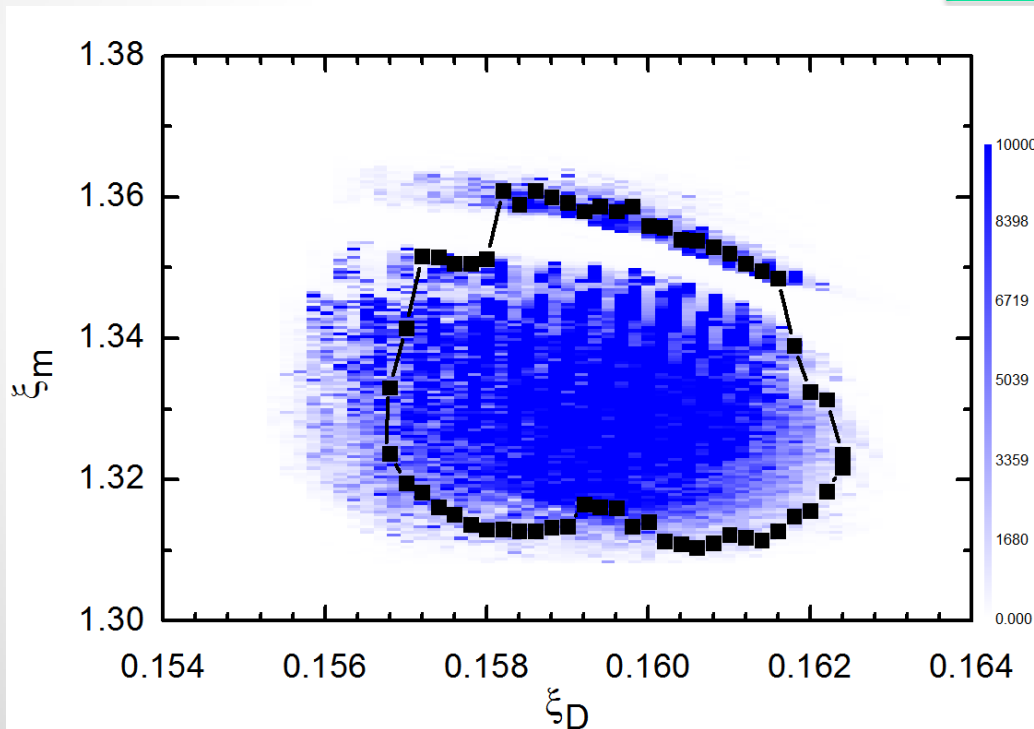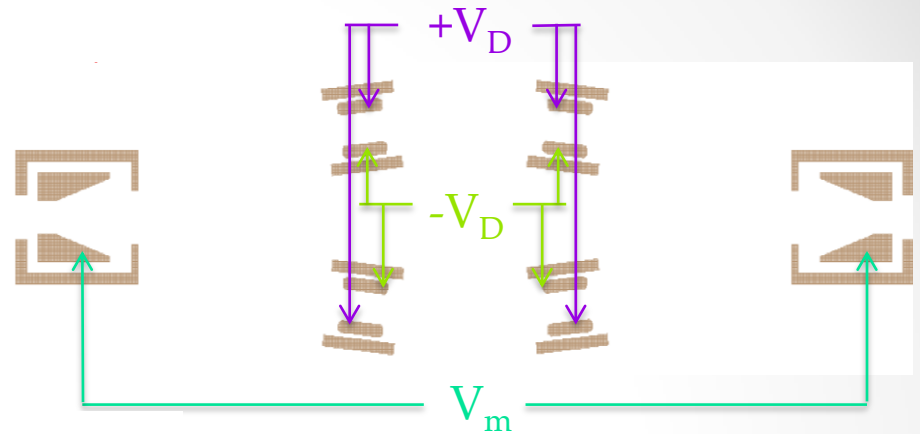
Lua code : *My work (2006)*

- Change VD by fixed steps
- Dichotomy algorithm for Vm :
  - search for storage/No storage border

- Change VD and Vm by fixed steps
- Calculate all trajectories
- More than 48h computation time

M. Ji's work

Acceptance of the Mini-Ring
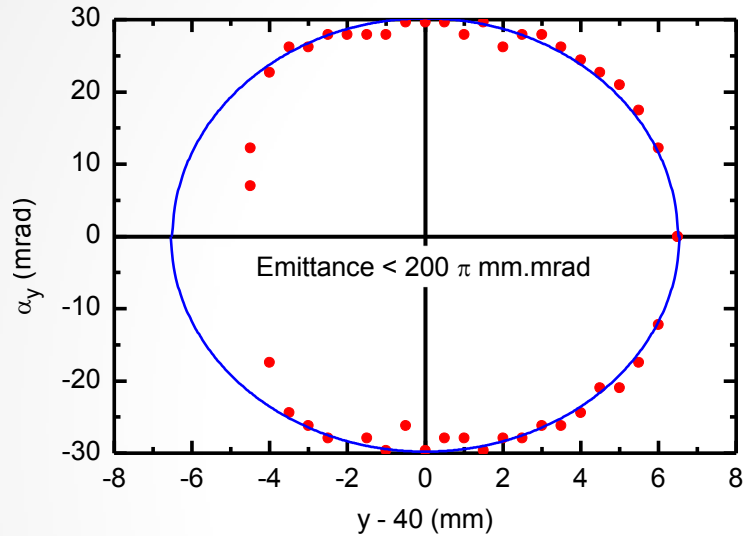
Lua code :

- Change y or z by fixed steps

- Dichotomy algorithm for α_y and α_z :
  - search for storage/No storage border

« advanced » strategies for geometry optimization

- ## Geometry files
  - o Change the Cone shape
  - o Change the deflector positions
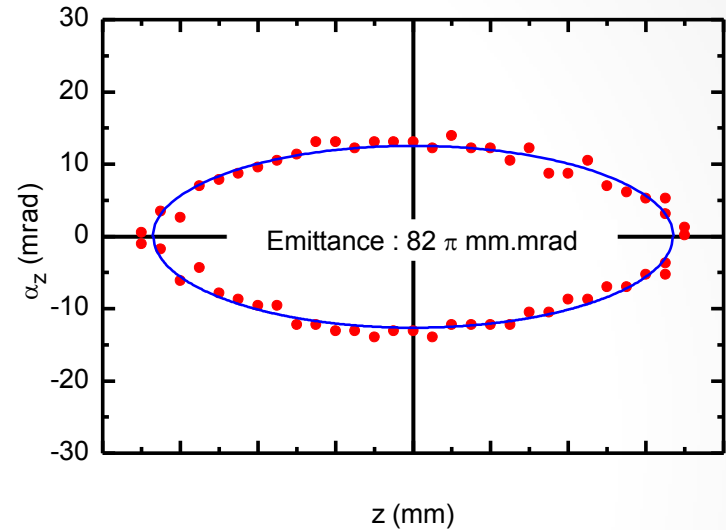 - o Change the Cone positions

- ## Lua code to control ion trajectory parameters and electrode voltages
  - o Ion Stability diagrams
  - o Acceptance of the Mini-Ring

- ## Lua code to change geometry files and run ions
  - o Time computing savings in batch mode?

« advanced » strategies for geometry tests

- Algorithm

```
                    ┌─────────────────────────────────┐
      ┌────────────►│      Create geometry file       │
      │             └─────────────────────────────────┘
      │                            │
      │                            ▼
      │             ┌─────────────────────────────────┐
      │             │            Create PA#            │
      │             │            →gem2pa              │
      │             └─────────────────────────────────┘
      │                            │
      │                            ▼
 ┌──────────┐       ┌─────────────────────────────────┐
 │  Change  │       │             Refine              │
 │ geometry │       └─────────────────────────────────┘
 └──────────┘                     │
      ▲                            ▼
      │             ┌─────────────────────────────────┐
      │             │           Create Fly2           │
      │             └─────────────────────────────────┘
      │                            │
      │                            ▼
      │        ┌──────────────────────────────────────────┐
      └────────│  Fly ions to Calculate stability diagram,│
               │      Using the dichotmy algorithm        │
               └──────────────────────────────────────────┘
```
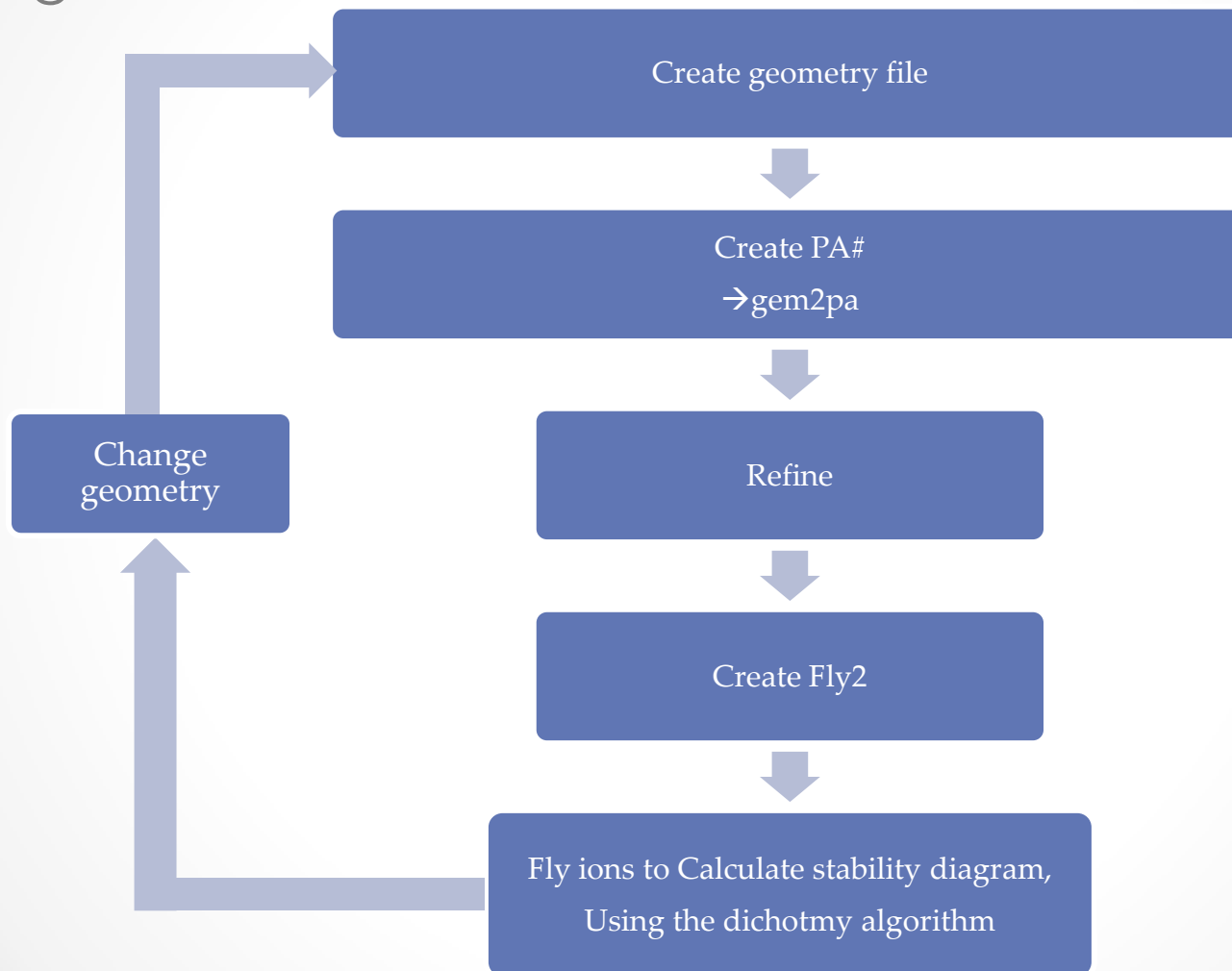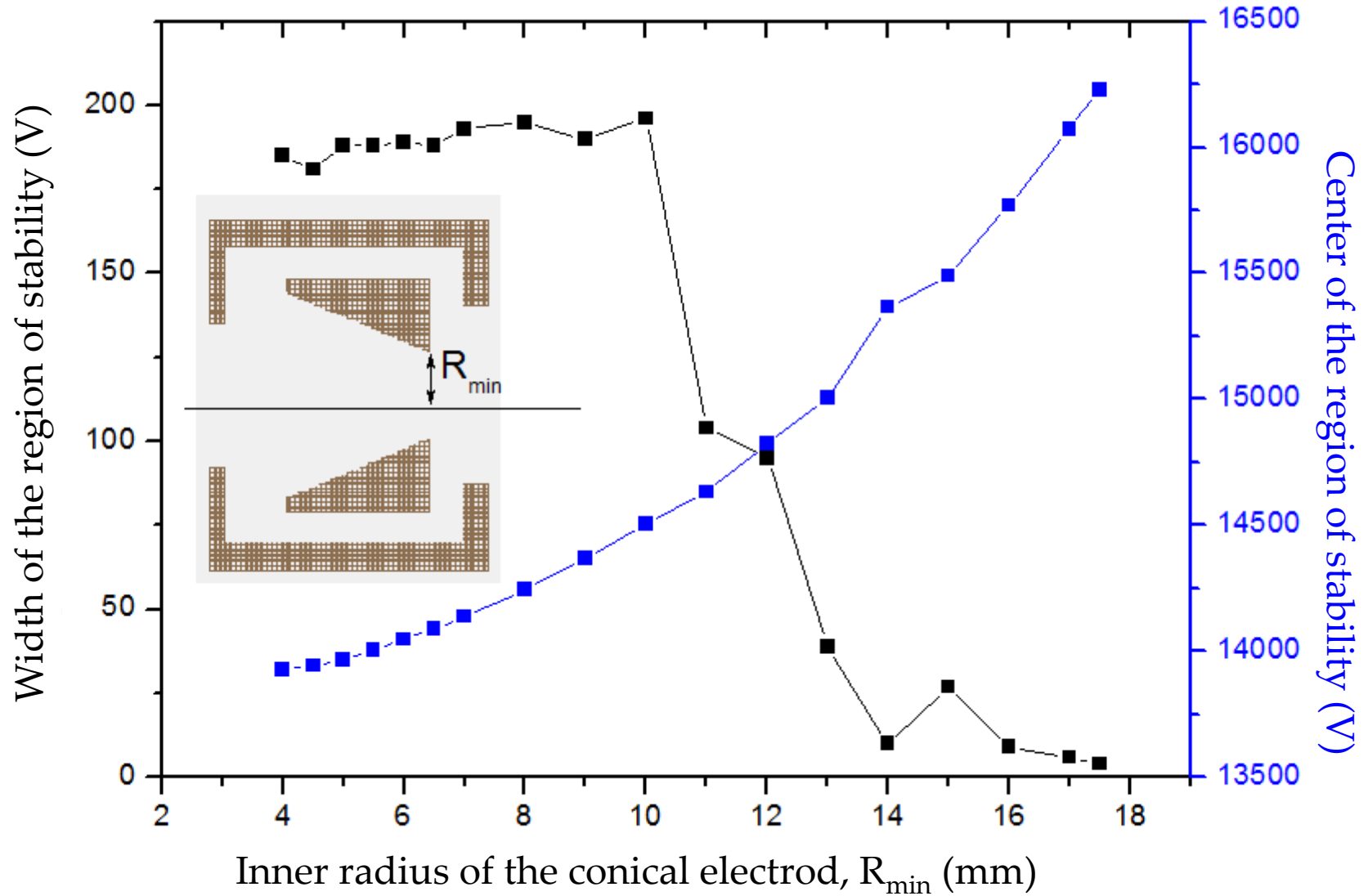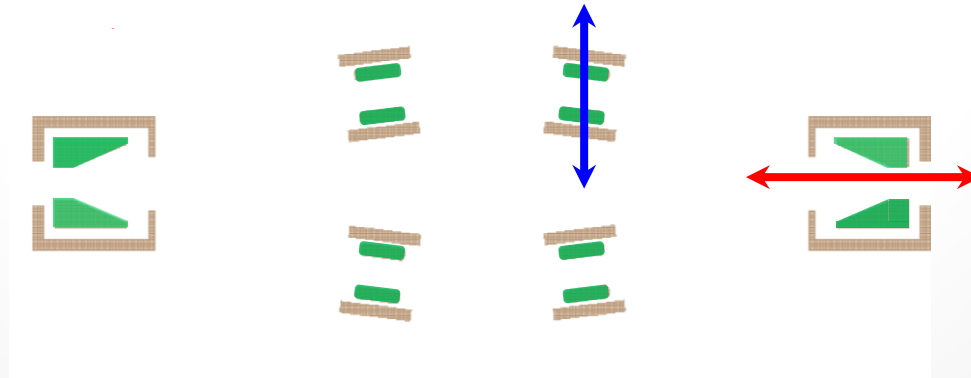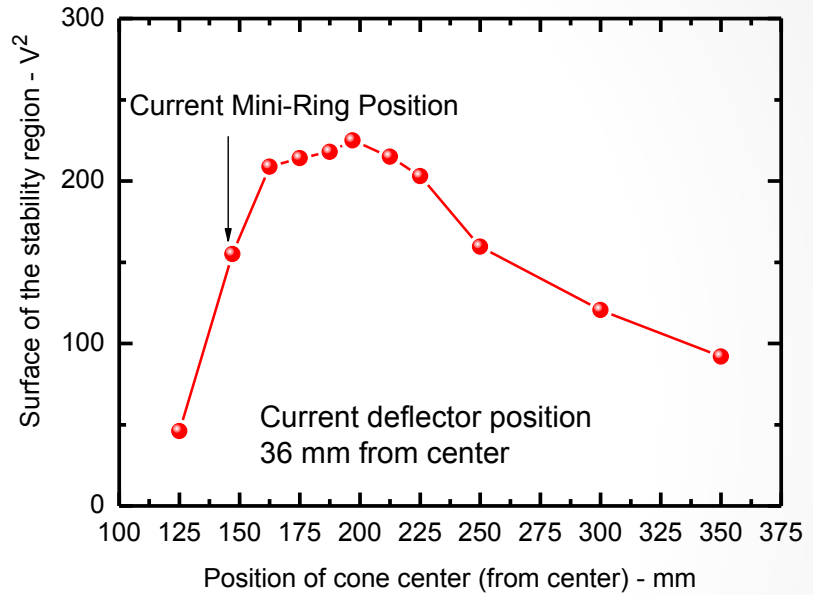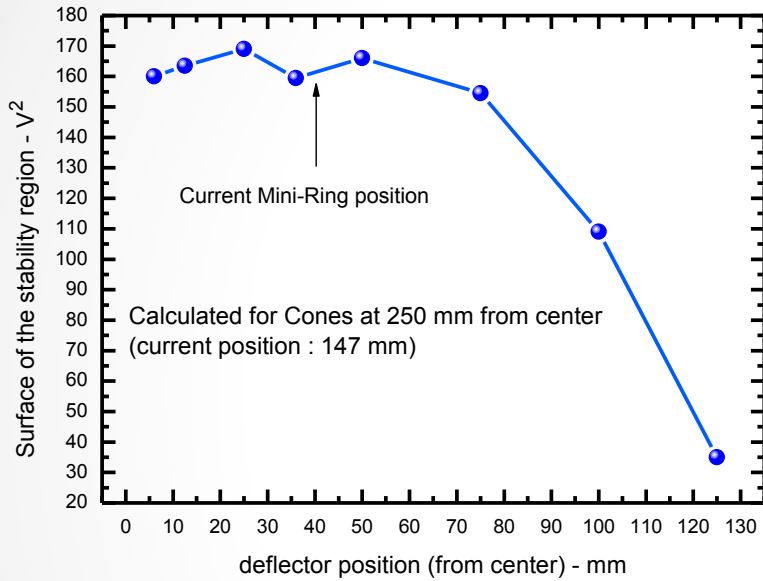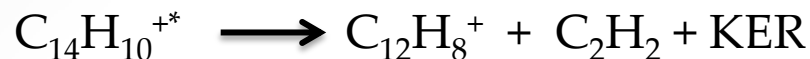
Design of the cones

Simulation of the stability regions in the conetrap mode for 10 keV beam

Positioning of the Deflectors and the Cones

Simulation of unimolecular dissociation

$$C_{14}H_{10}^{+*} \longrightarrow C_{12}H_8^+ + C_2H_2 + KER$$

Fixed excitation energy $\Longrightarrow$ Exponential decay law $N(t) = N_0 \exp(-t/\tau)$

Random fragmentation time with exponential distribution

```
Frag_Time = Frag_LifeTime*ln(1/simion.rand())
```
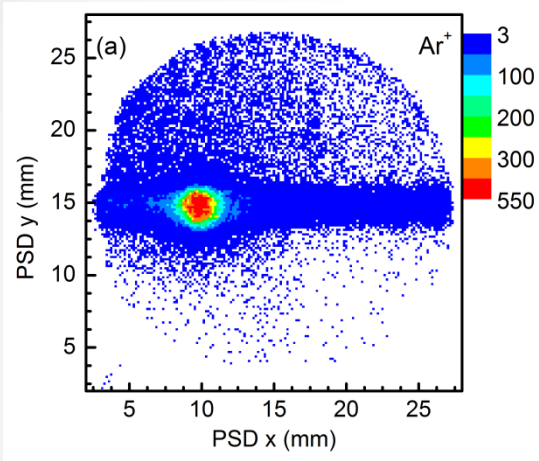
Random direction of the velocity

```
local speed = ke_to_speed(Frag_ke,ion_mass)
local phi = 2* math.pi*simion.rand()
local theta = math.pi*simion.rand()
ion_vz_mm = ion_vz_mm + speed * cos(theta)
ion_vx_mm = ion_vx_mm + speed * sin(theta)* cos(phi)
ion_vy_mm = ion_vy_mm + speed * sin(theta)* sin(phi)
```
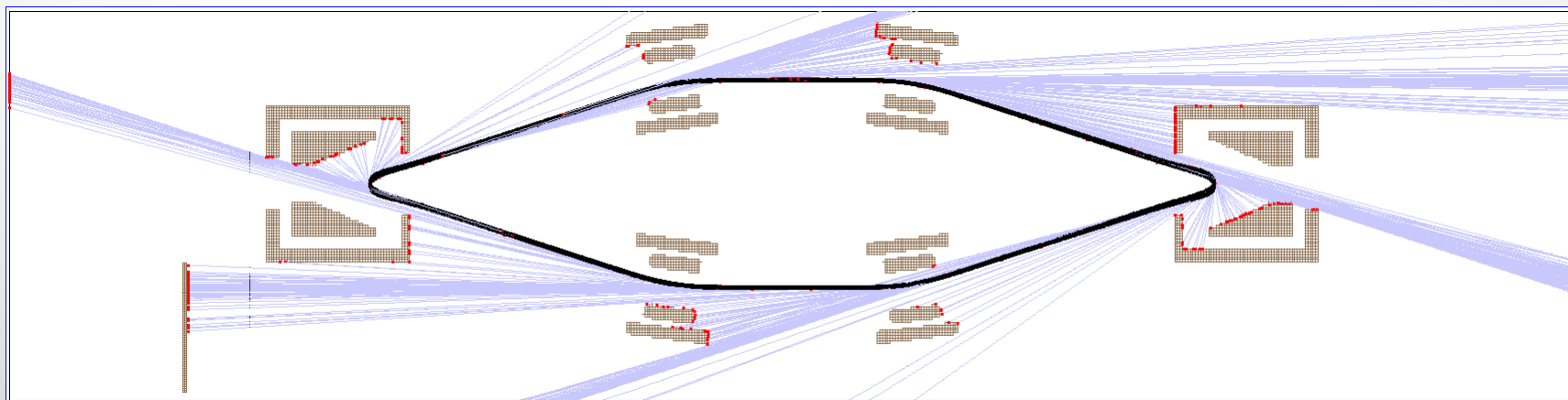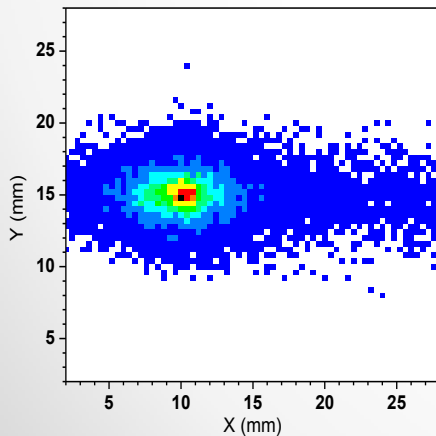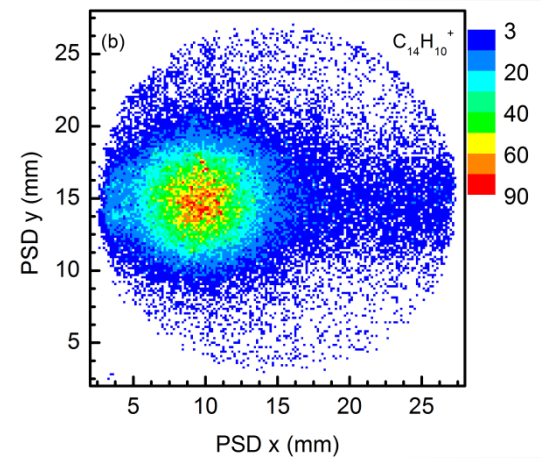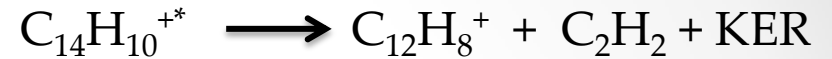
Kinetic Energy Release (KER)

Ar$^+$ beam

$$C_{14}H_{10}^{+*} \longrightarrow C_{12}H_8^+ + C_2H_2 + KER$$
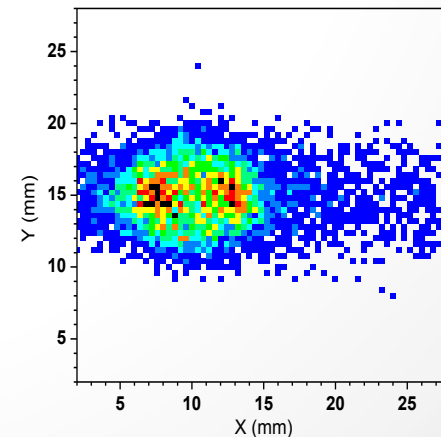
Experiment

Simion simulations
(MingChao Ji)

100 000 ions
56h comp. Time

Conclusion