PIC-MCC Gun Code Simulations of a Surface Conversion H^- Source

Edwin Chacon-Golcher[1]

Kevin J. Bowers[2]

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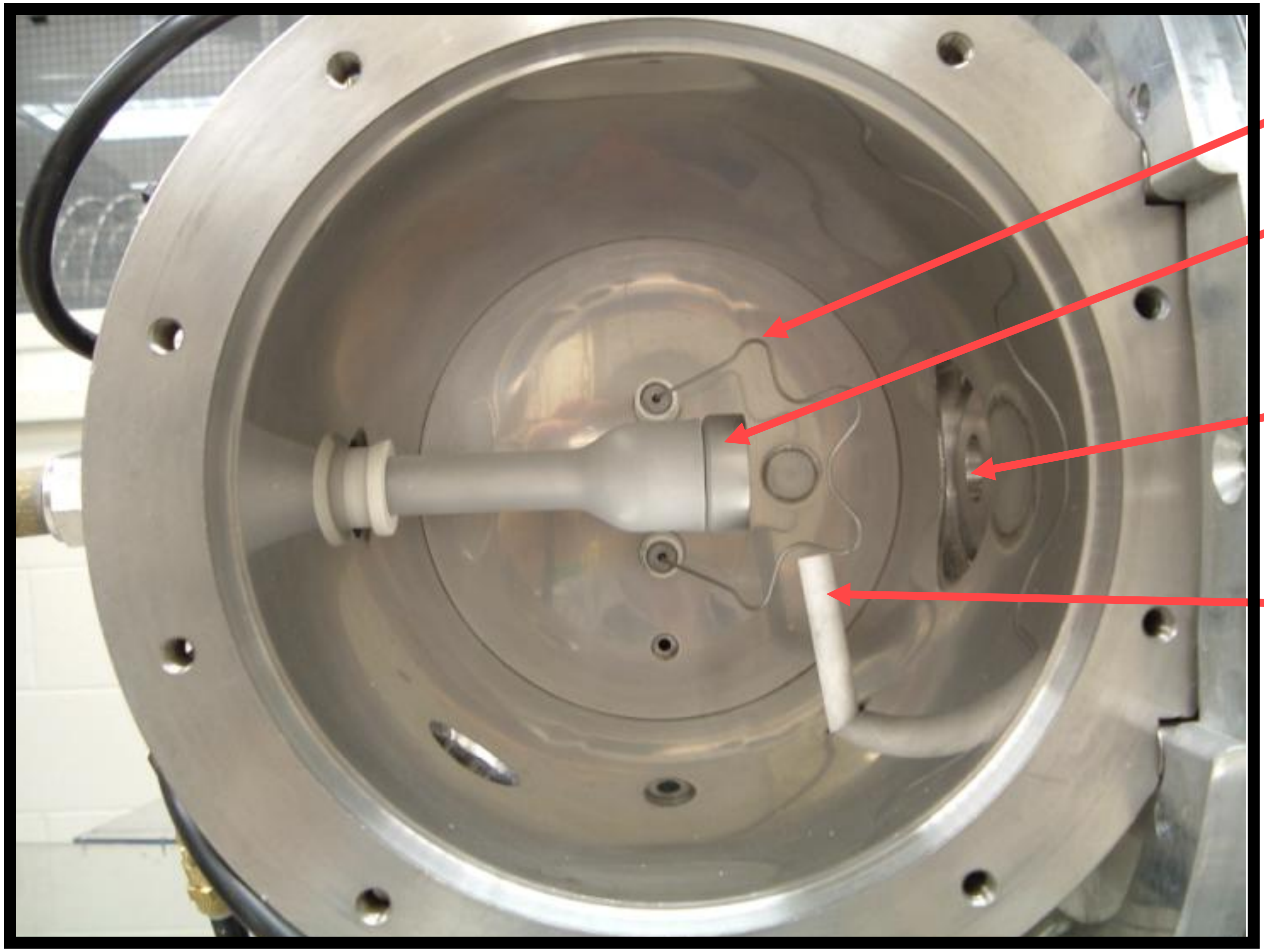
1: LANL, 2: Guest Scientist, currently at D.E. Shaw, NY

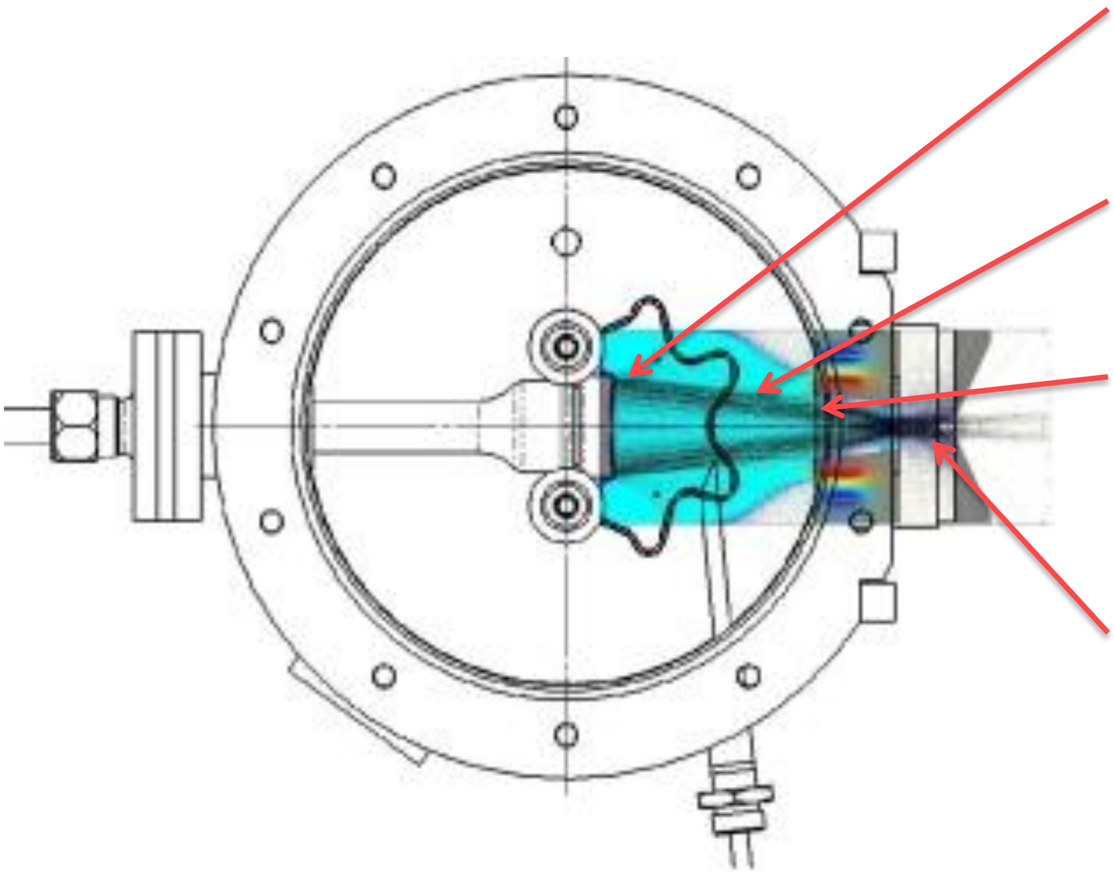
Some Context:
Aerial View of LANSCE

More Context:
The Ion Source



- Filament.
- Converter electrode.
- Repeller electrode.
- Cesium dispenser.

Problems of interest



- Converter surface-plasma interaction
- Beam-plasma interaction
- Formation of diffusive sheaths and effects on the beam
- Identifying zones of insufficient neutralization that may cause beam loss

Simulation Strategy:
Particle-in-Cell with Monte Carlo Collisions

Injection of seed electrons at filament surface

Allocation of charge to grid nodes through a bilinear charge assignment scheme with subsequent calculation of the charge density per node.

Computation of the potential field with a split Fourier-tridiagonal method and subsequent computation of the electric field by central differencing

Particle advance of position and velocity with the leap frog method using bilinearly interpolated scalar and vector potentials

Application of boundary conditions: absorption, reflection or generation of new particles.

Application of Monte Carlo collisions for ionization, scattering, neutralization, etc.

Generation of diagnostic files.

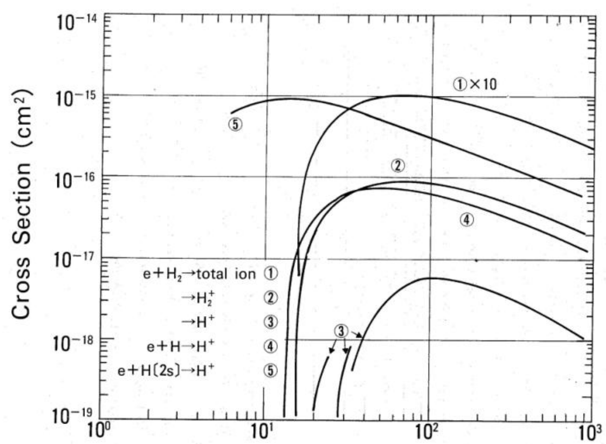
Adjustable physical parameters:

- Discharge current (up until virtual cathode formation)
- Cross-section scaling (up to experimental uncertainty)
- Neutral gas pressure (up until uncertainty)
- Secondary emission coefficients
- Velocity spreads of surface-generated particles (determined by surface and ambient temperature

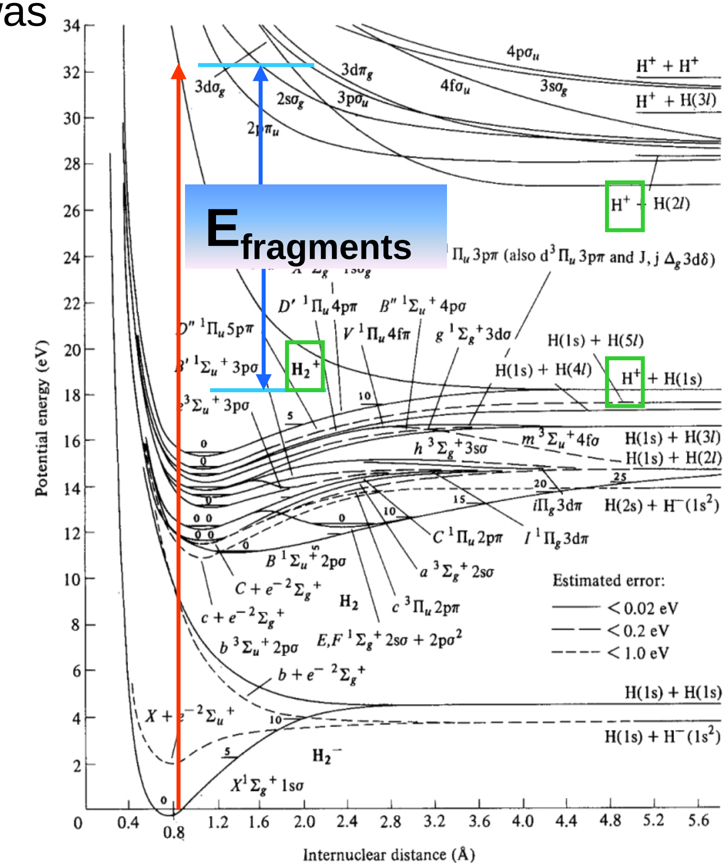
Plasma Chemistry Modeling

- A molecular hydrogen Monte Carlo package was developed to model discharge processes, including detailed kinetics and kinematics.

- The package is based on the "null collision" approach.(ref. Vahedi & Surendra. *Computer Physics Communications* 87. 1995)



Ref. Tawara et al. Institute of Plasma Physics. Nagoya Univ. Report IPPJ-AM-46



Ref. Lieberman & Lichtenberg. *Principles of Plasma Discharges and Materials Processing*. John Wiley & Sons. 1994. p. 222

Specific Reactions Included

Ionization reactions:

$$e^- + H_2 \rightarrow H_2^+ + 2e^-$$
$$e^- + H_2 \rightarrow H^+ + H + 2e^-$$
$$e^- + H \rightarrow H^+ + 2e^-$$

Charge exchange reactions:

$$H^+_{2\,fast} + H^0_{2slow} \rightarrow H^+_{2slow} + H^0_{2\,fast}$$
$$H^+_{fast} + H^0_{slow} \rightarrow H^+_{slow} + H^0_{fast}$$
$$H_2^+ + H^0_{2slow} \rightarrow H_3^+ + H^0$$

Rotational and vibrational molecular excitation reactions:

$$e^- + H_2 \rightarrow H_2(J = 0 \rightarrow 2) + e^-$$
$$e^- + H_2(\nu = 0) \rightarrow H_2(\nu = 1,2,3) + e^-$$
$$H^+ + H_2(\nu = 0) \rightarrow H^+ + H_2(\nu = 1,2,3)$$
$$e^- + H_2 \rightarrow H_2(B^1\Sigma_u^+) + e^-$$
$$e^- + H_2 \rightarrow H_2(C^3\pi_u) + e^-$$
$$e^- + H_2 \rightarrow H_2(B''^1\Sigma_u^+) + e^-$$
$$e^- + H_2 \rightarrow H_2(c^3\pi_u) + e^-$$
$$e^- + H_2 \rightarrow H_2(b^3\Sigma_u^+) + e^-$$
$$e^- + H_2 \rightarrow H_2(a^3\Sigma_g^+) + e^-$$
$$e^- + H_2 \rightarrow H_2(D^1\pi_u) + e^-$$
$$e^- + H_2 \rightarrow H_2(D'^1\pi_u) + e^-$$

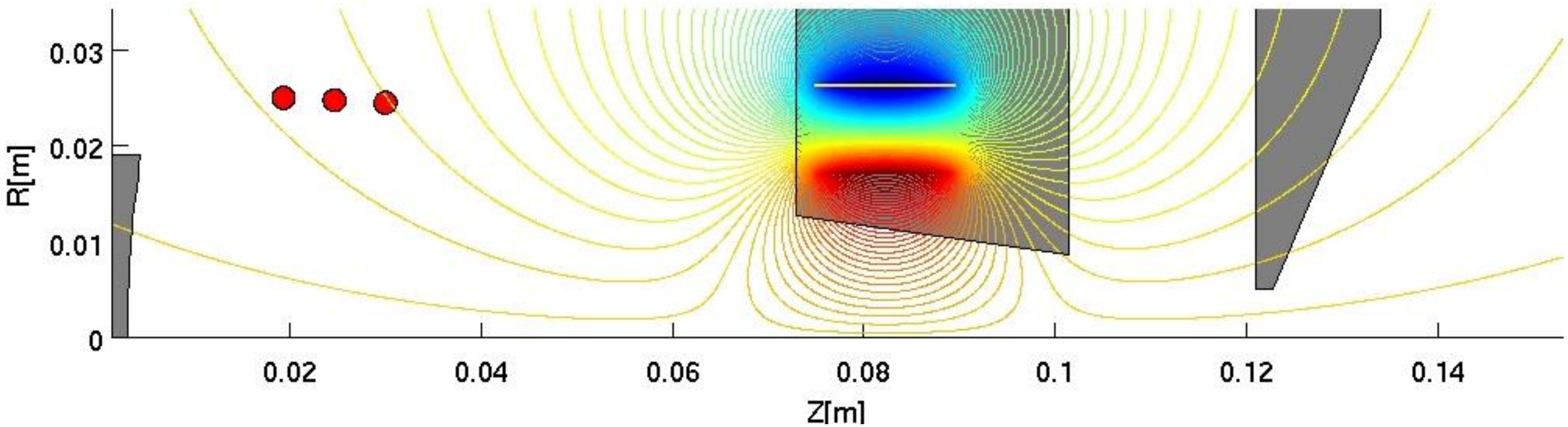
H- destruction reaction:

$$H^- + H_2 \rightarrow H^0 + H_2 + e^-$$

All these reactions can initiate and/or sustain a plasma discharge, extract some energy the plasma and account for important destruction mechanisms.

The model includes static magnetic fields produced by a ring magnet

Magnetic field line plot:



The vector potential is computed by direct summation of the contributions of a set of current-carrying rings on the surface of the magnet.

$$\vec{A}(\vec{x}) = \frac{\mu_0}{4\pi} \iiint \frac{\vec{J}(\vec{x}')}{|\vec{x} - \vec{x}'|} d^3\vec{x}'$$

Particle Advance

The equations of motion were derived from a Lagrangian formulation for a charged particle in an EM field:

$$L(r,z,\dot{r},\dot{z},\dot{\phi}) = \frac{1}{2}m(\dot{r}^2 + \dot{z}^2 + r^2\dot{\phi}^2) - q\Phi(r,z) + qr\dot{\phi}A_\phi(r,z)$$

Using the canonical momentum p_ϕ,

$$p_\phi = mr^2\dot{\phi} + qrA_\phi(\vec{x})$$

the equations of motion become:

$$\frac{d}{dt}v_z = -\frac{\partial}{\partial z}\left[-\frac{qp_\phi}{m^2}\left[\frac{A_\phi(r,z)}{r}\right] + \frac{q}{m}\Phi(r,z) + \frac{1}{2}\left(\frac{q}{m}\right)^2 A_\phi^2(r,z)\right]$$

$$\frac{d}{dt}v_r = \frac{p_\phi^2}{m^2}\left(\frac{1}{r^3}\right) - \frac{\partial}{\partial r}\left[-\frac{qp_\phi}{m^2}\frac{\partial}{\partial r}\left[\frac{A_\phi(r,z)}{r}\right] + \frac{q}{m}\Phi(r,z) + \frac{1}{2}\left(\frac{q}{m}\right)^2 A_\phi^2(r,z)\right]$$

which are integrated with leapfrog. This method exactly conserves the canonical angular momentum.

Homogeneous Poisson Solver

A split FFT/tridiagonal approach is used to solve for the electrostatic potential produced by a collection of charge. This yields a "homogeneous" solver in the sense of forcing potential values of zero at the edges of the solution region.

Upon substituting the discrete inverse *sine* transform formula for ϕ and ρ into the discretized Poisson's equation, the following tridiagonal system of equation results:

$$\left(\frac{1}{(\Delta r)^2}+\frac{1}{2r\Delta r}\right)\tilde{\phi}_{r+1,k}-\left(\frac{2}{(\Delta r)^2}+\frac{4}{(\Delta z)^2}\sin^2\left(\frac{\pi k}{2N_z}\right)\right)\tilde{\phi}_{r,k}+\left(\frac{1}{(\Delta r)^2}-\frac{1}{2r\Delta r}\right)\tilde{\phi}_{r-1,k}=-\frac{\tilde{\rho}_{r,k}}{\varepsilon_0}$$

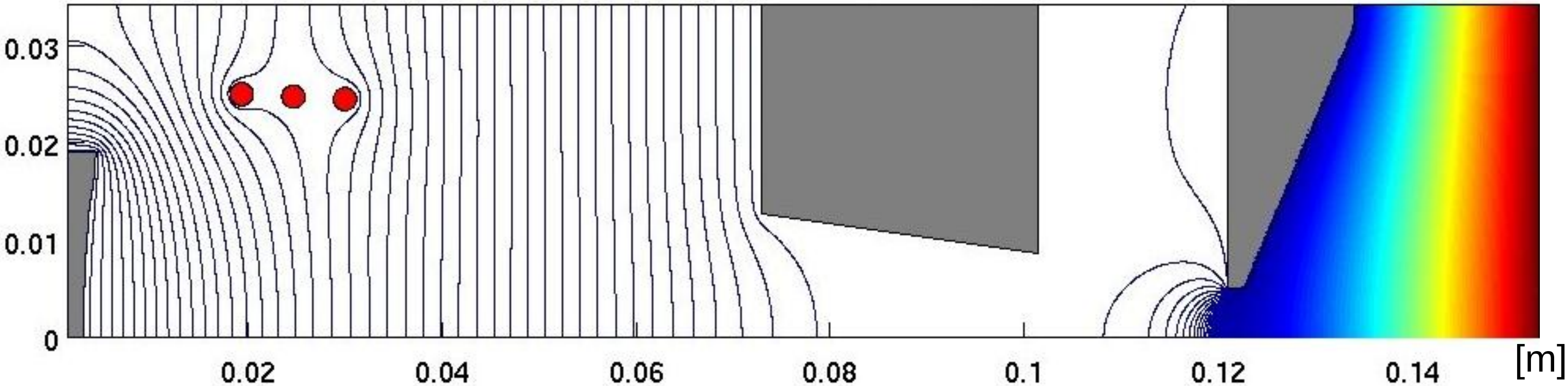
The axis of symmetry is treated through Gauss's Law.

$$\frac{4}{(\Delta r)^2}\tilde{\phi}_{1,k}-\left(\frac{4}{(\Delta r)^2}+\frac{4}{(\Delta z)^2}\sin^2\left(\frac{\pi k}{2N_z}\right)\right)\tilde{\phi}_{0,k}=-\frac{\tilde{\rho}_{0,k}}{\varepsilon_0}$$

Thus, the homogeneous Poisson equation is solved by sine transforming rho, solving the tridiagonal linear system above and finally inverse transforming the result.

Arbitrary Inhomogeneous Boundary Conditions

Plot of equipotentials when no particles are present:



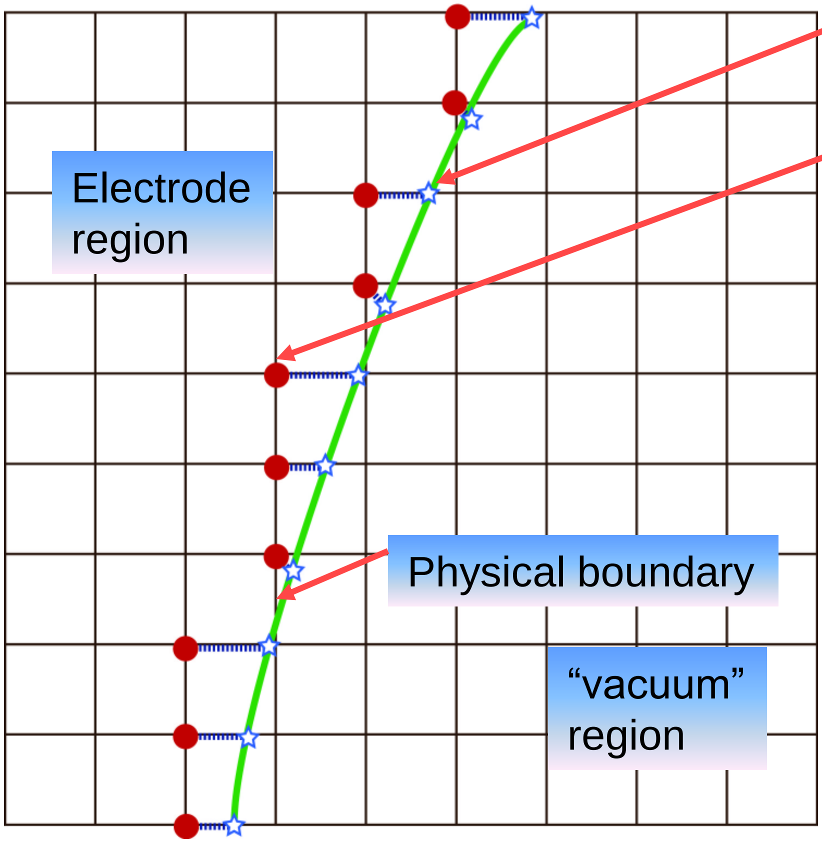
Arbitrary, mixed boundary conditions (Dirichlet and Neumann) can be set anywhere on the solution region, including the true positions of physical boundaries.

After the homogeneous solution of Poisson's equation is found, charge is allocated at specific nodes to enforce general conditions of type

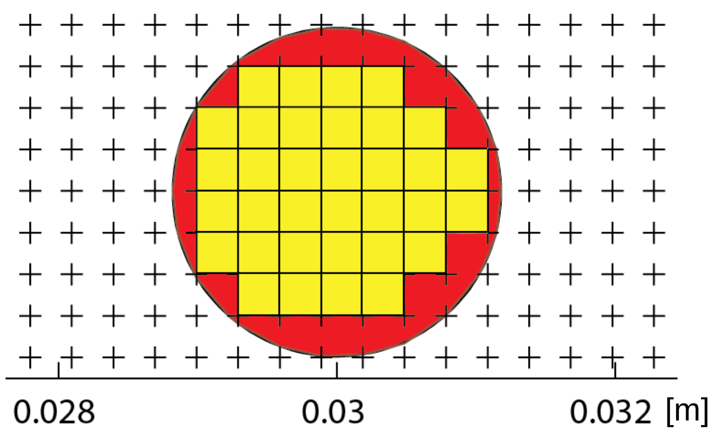
$$\boxed{\gamma = \alpha\phi + \beta\hat{n}\cdot\nabla\phi}$$

Then the homogeneous solver is applied again with the modified charge configuration. This yields the end solution.

Physical Boundaries are Represented Smoothly (without stair-stepping)



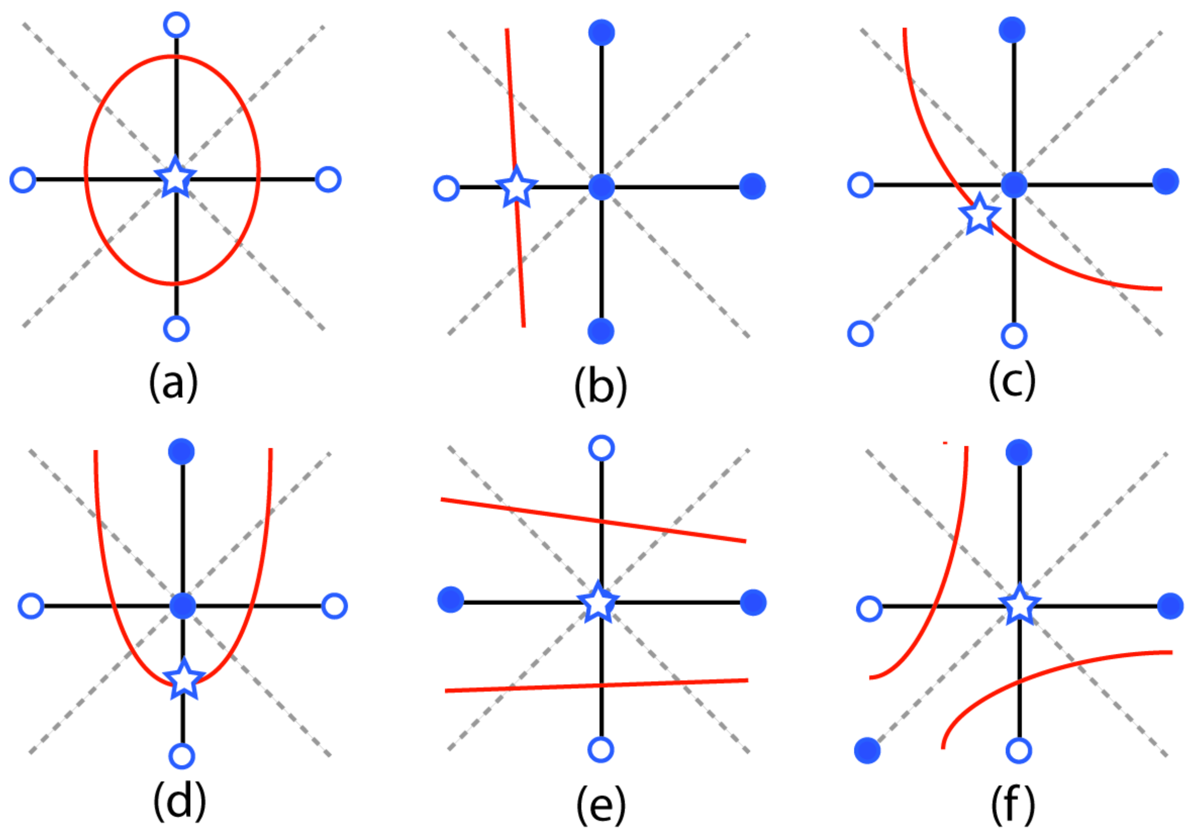
- Points on the physical boundary where boundary conditions are enforced.
- Points on logical boundary (strictly exterior) where charge is allocated to enforce boundary conditions
- Below: comparison between a stair-stepped representation of a filament held at a constant potential and the smooth representation. Surface equipotential is shown and tightly conforms to the boundary.



Selection of points on the physical boundary

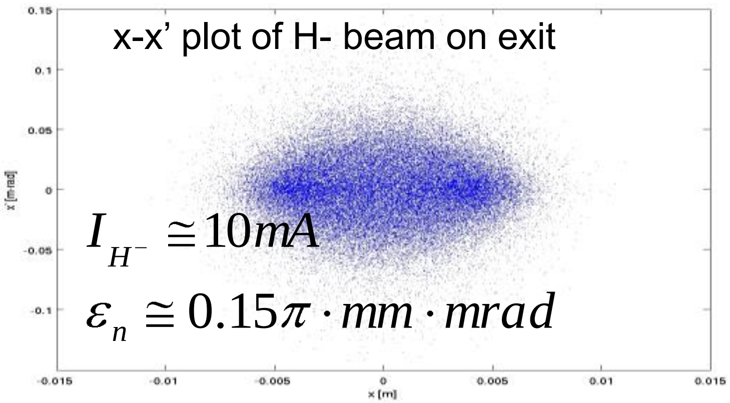
- Algorithm searches for the "edge nodes" on the electrodes and selects a corresponding point on the physical boundary where the boundary condition will be enforced.

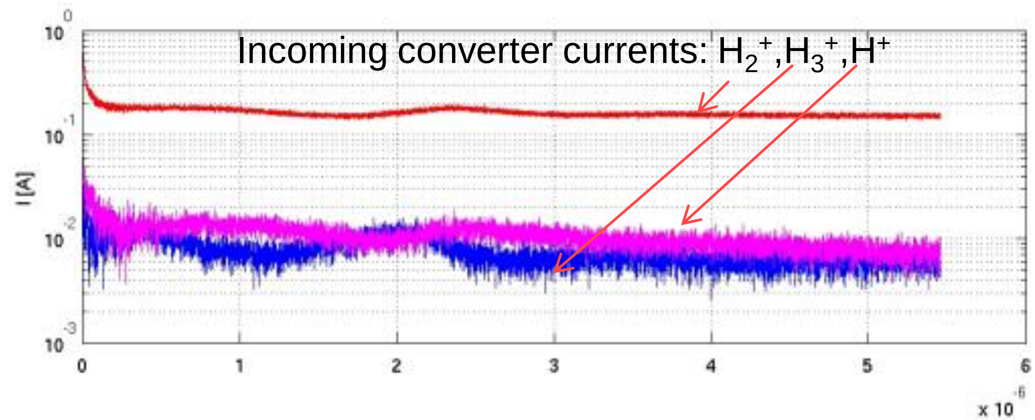
- All 16 possible cases fall into a few categories shown on the right.
  - Full dots: inside the electrode.
  - Blank dots: outside.
  - Stars: where the potential is enforced.

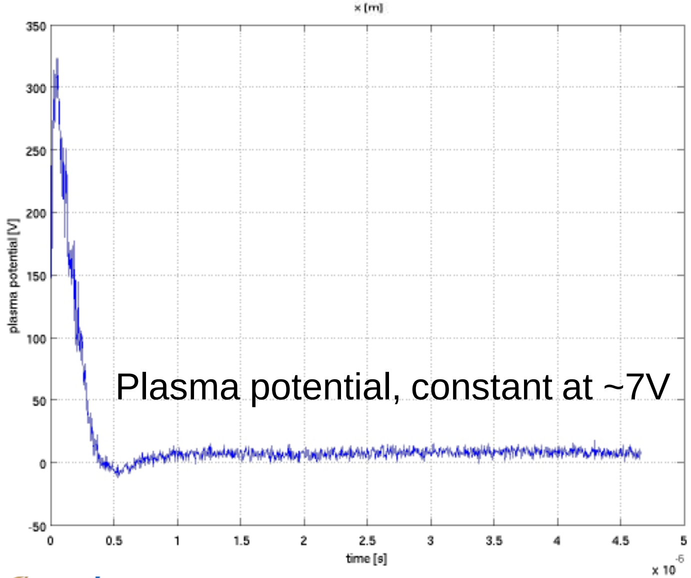


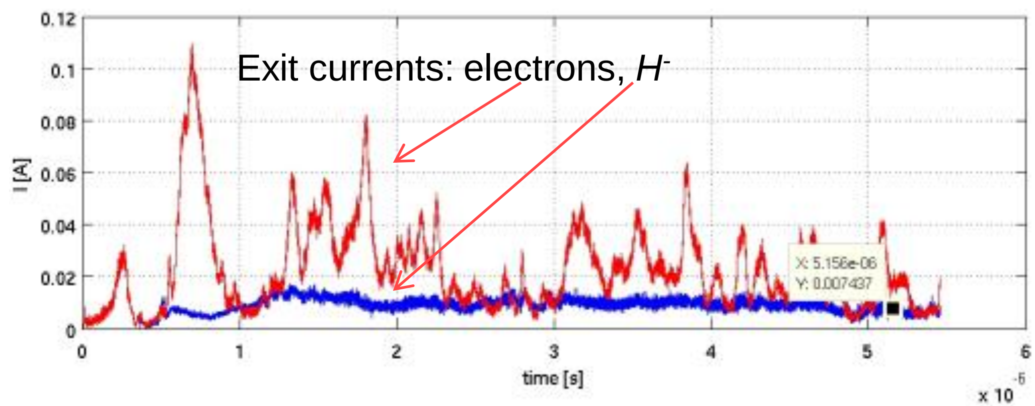
Experimental Comparisons

Simulation with ~40 million particles, over 800,000 time steps, 8-processor run.









Some animations: Configuration space and longitudinal phase space of the *H*⁻ beam