

Motivation

In order to simulate transport phenomena in sputtering processes realistically, a spatial and temporal knowledge of the plasma density and electrostatic field configuration is needed. Due to relatively low plasma densities, continuum fluid equations are not applicable. We propose instead a particle-tracking method.

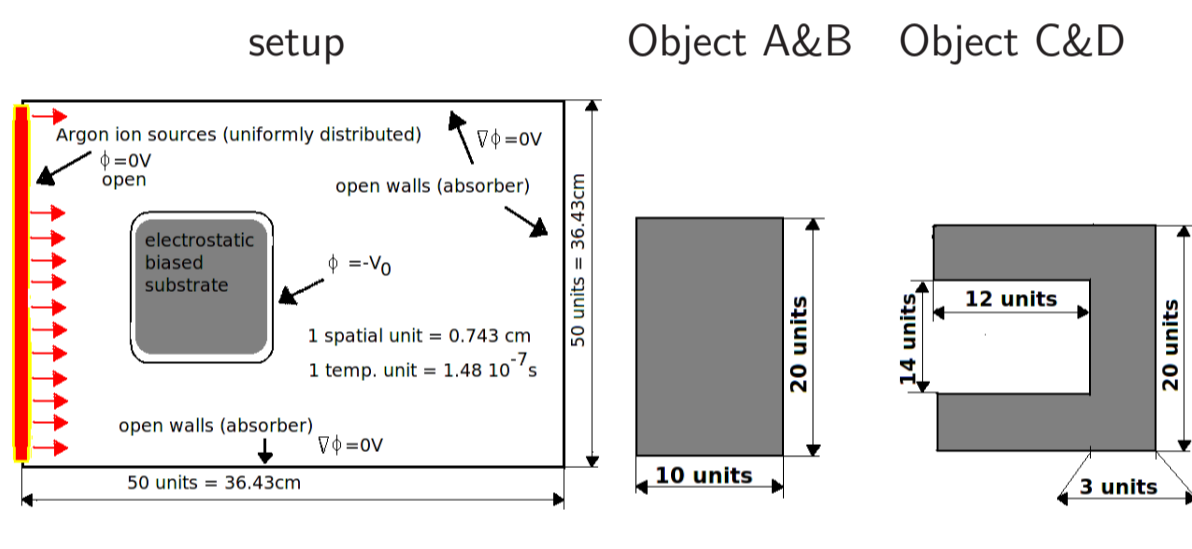
Problems

- ▶ Ion-electrostatic field feedback (selfregulating dynamic mechanism)
- ▶ Complex fields due to biased complex substrate geometries (electrostatic boundary conditions)

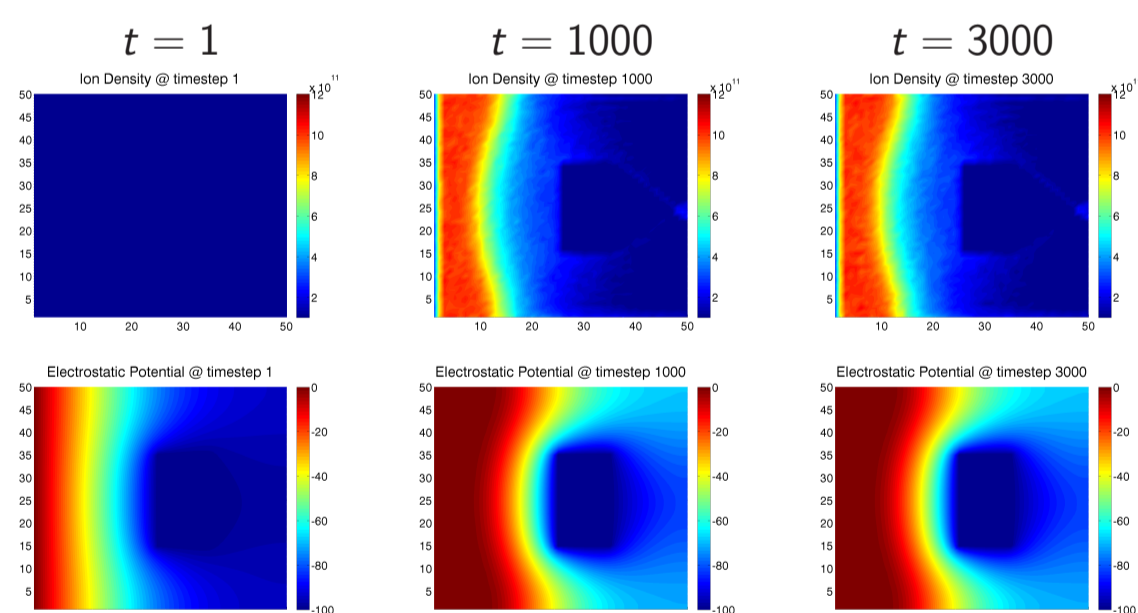
Solution Strategies

- ▶ Decoupling of ions and electrons (electrons behave like perfect fluid, due to low mass)
- ▶ Monte Carlo Particle-in-Cell simulations (of the order of 10 mio. particles)
- ▶ Optimized iterative potential solver

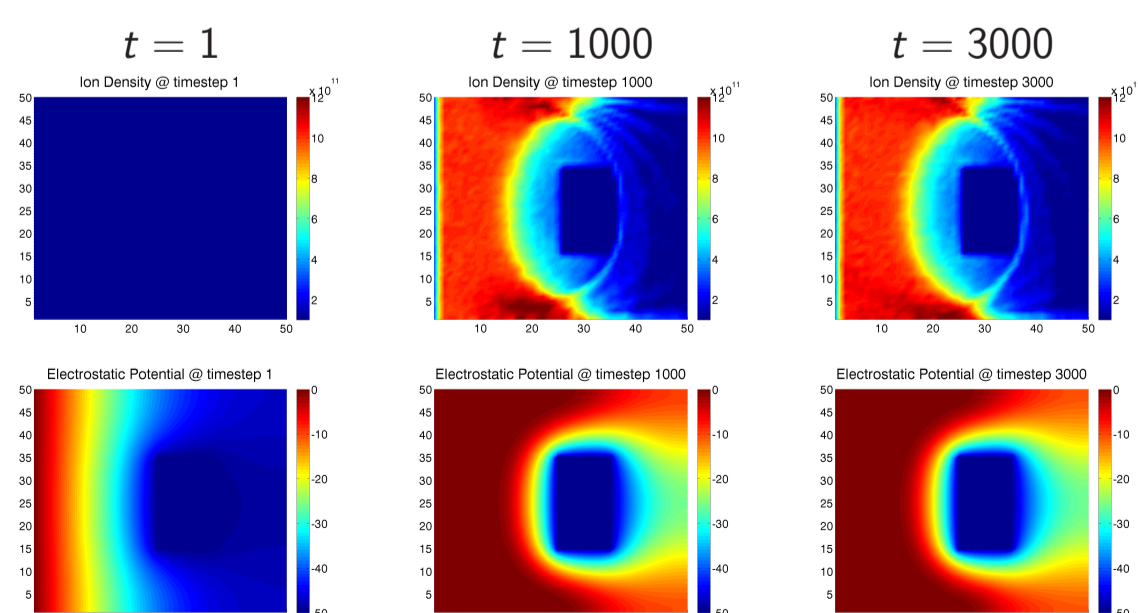
Experimental Setup



Results A: $U_{bias} = -100V, v_{drift} = 5000m/s$



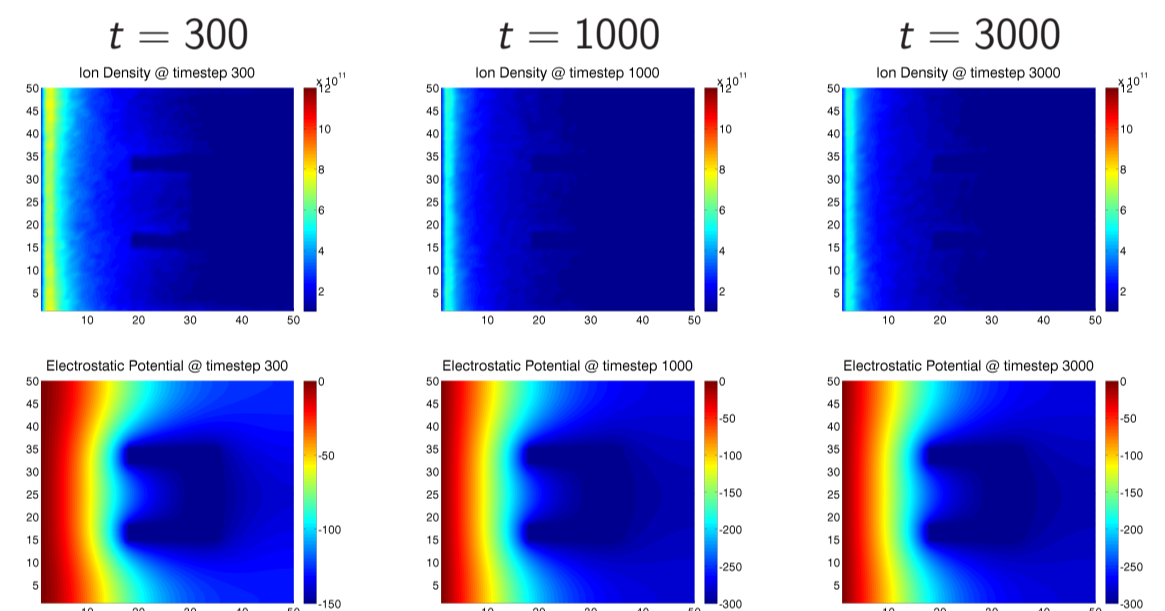
Results B: $U_{bias} = -50V, v_{drift} = 5000m/s$



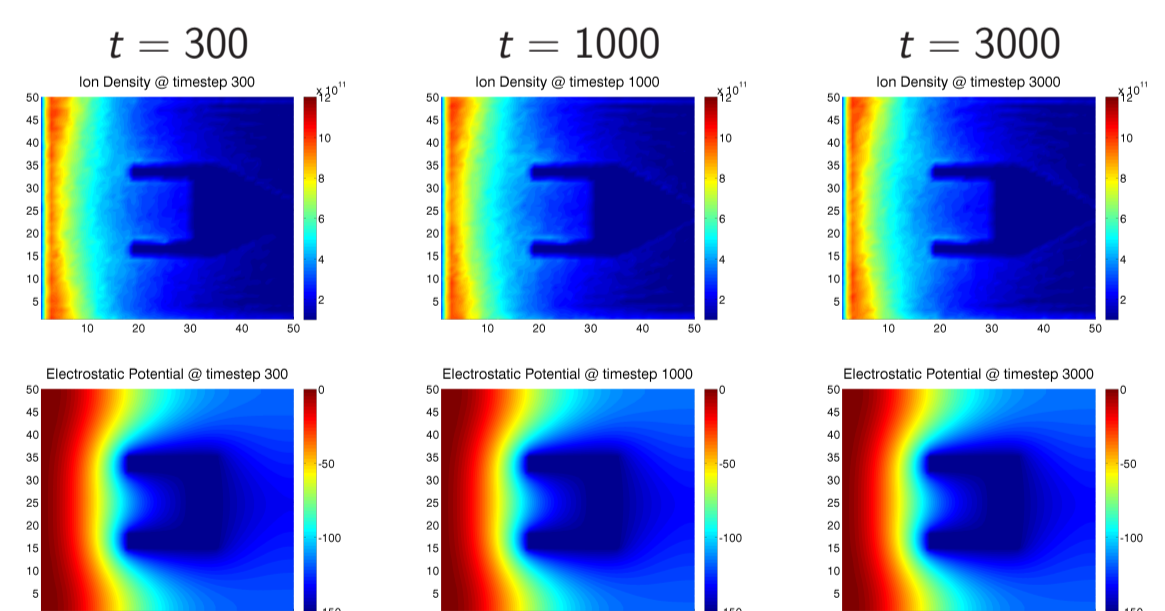
Fundamental Equations

- ▶ $\vec{F} = \underbrace{q \cdot \vec{E}}_{\text{our work}} + \underbrace{q \cdot \vec{v} \times \vec{B}}_{\text{neglected}}$ (Lorentz force on each particle)
- ▶ $\nabla \cdot \vec{B} = 0$ and $\vec{E} = -\nabla\Phi$ with $\nabla^2\Phi = -\rho/\epsilon_0$
- ▶ $\nabla \times \vec{B} = \mu_0\epsilon_0 \frac{\partial \vec{E}}{\partial t} + \mu_0 \vec{j}$ and $\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}$
- ▶ Ansatz: $\rho = e(Z_i n_i - n_e) = \rho(x, y, t)$ with Z_i : charge of ion i and density n
- ▶ Electrons as fluid: $n_e = n_0 \exp\left(\frac{\phi - \phi_0}{K_B T_e}\right)$
- ▶ Debye Length: $\lambda = \sqrt{\epsilon_0 T_e / n_0 e}$
- ▶ Thermal velocity of ions: $v_{th} = \sqrt{K_B T_e / M_{ion}}$
- ▶ Drift velocity of ions: v_{drift} : was varied between 5000 and 9000 m/s
- ▶ Operator discretization via finite difference scheme (spatial: in units of Debye Length, temporal: $0.1\lambda/v_{drift}$)
- ▶ Equation of Motion Solver: Leap Frog (symplectic integrator)

Results C: $U_{bias} = -150V, v_{drift} = 5000m/s$



Results D: $U_{bias} = -100V, v_{drift} = 9000m/s$



Conclusions (so far ...)

- ▶ We have developed an efficient Particle-in-Cell Monte Carlo Simulation of an argon plasma in C++.
- ▶ Simulations of arbitrary substrate geometries, ion sources and electrostatic boundary conditions are possible
- ▶ First hints of spatial ion distribution between target and substrate (electrostatic biased) as well as spatial selfconsistent electrostatic field configuration at equilibrium time (macroscopic time scales).
- ▶ Experimentally observed ion distribution has been qualitatively reproduced.