Error on field from PIC scheme and its effect on field emission

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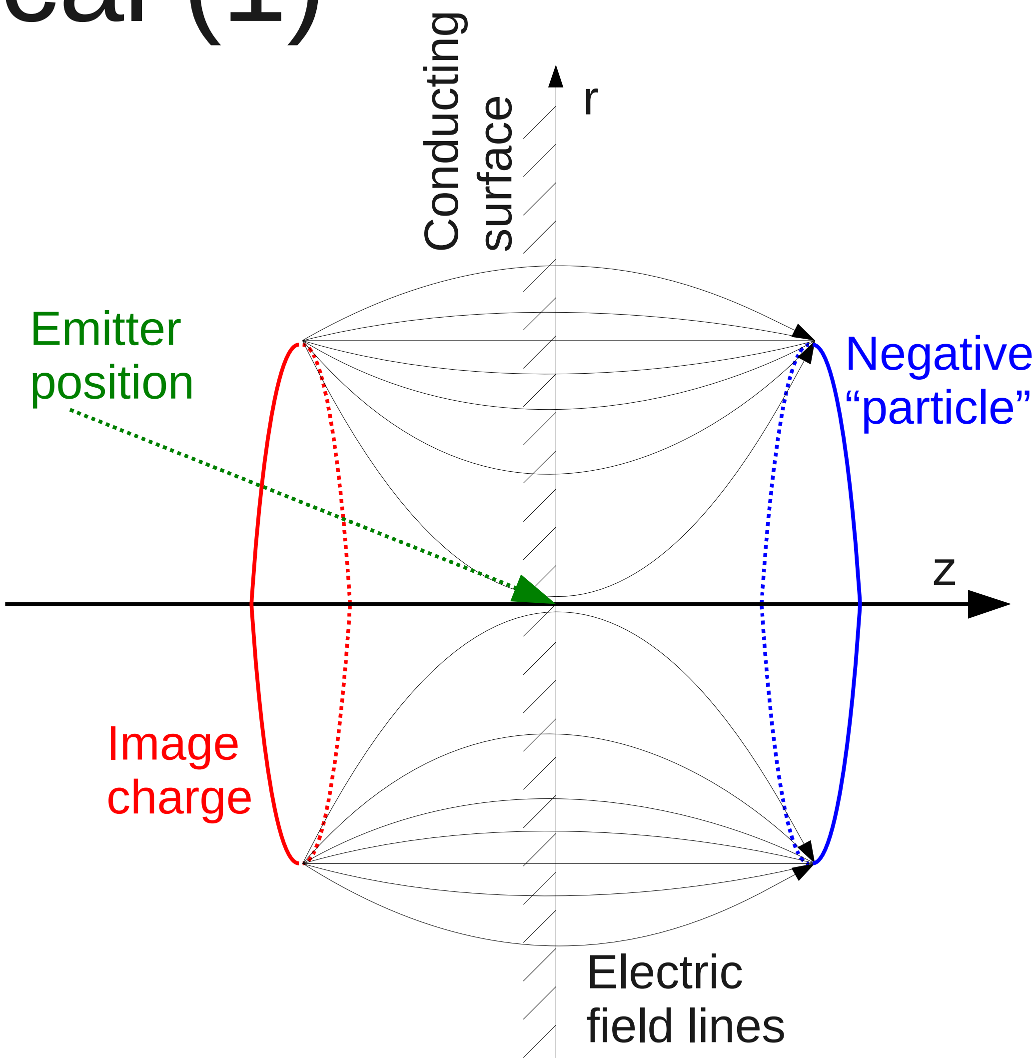
(+ update on time step 26/8)

Outline

- Field from a test particle at (z,r) observed at (0,0)
  - Analytical
  - PIC
- PIC field versus analytical field
- Effect on field emission in ArcPIC2D

Field from test particle on tip: analytical (1)

- Due to coordinate system, particles appears as infinitely thin circles with radius r at height z above surface
- Surface is perfectly conducting, so the boundary condition may be approximated by placing an identical but oppositely charged ring at -z
- We are interested in the field from a negative test particle located at (r,z) when observed at the emitter position (0,0)



Field from test particle on tip: analytical (2)

- This field may be calculated by summing up the field from infinitivly many charges dq distributed along the ring
- The single-particle field observed at position (x,y,z) from a particle located at (0,0,0) is given as:

$$\vec{E}=\frac{q}{k_e}\frac{\hat{R}}{R^2} \quad \text{where} \quad k_e=4\pi\epsilon_0$$

and the unit vector $\hat{R}=\frac{\vec{R}}{R}$ where

$$R=\sqrt{x^2+y^2+z^2}=\sqrt{r^2+z^2} \quad \text{and}$$

$$\vec{R}=r\,\hat{r}(\theta)+z\,\hat{z}=r(\cos(\theta)\,\hat{x}+\sin(\theta)\,\hat{y})+z\,\hat{z}$$
$$=x\,\hat{x}+y\,\hat{y}+z\,\hat{z}$$

- When swapping observation and test charge position, the sign of E is reversed
- The field from one particle on the emitter is then given as: $\vec{E}=\int\frac{dq}{k_e}\frac{-\hat{R}}{R^2}=$

$$\frac{\int_0^{2\pi}Q\,d\theta}{k_e 2\pi}\left(\frac{-z\,\hat{z}}{R^3}+\frac{\hat{x}\cos\theta+\hat{y}\sin\theta}{R^3}\right)=$$

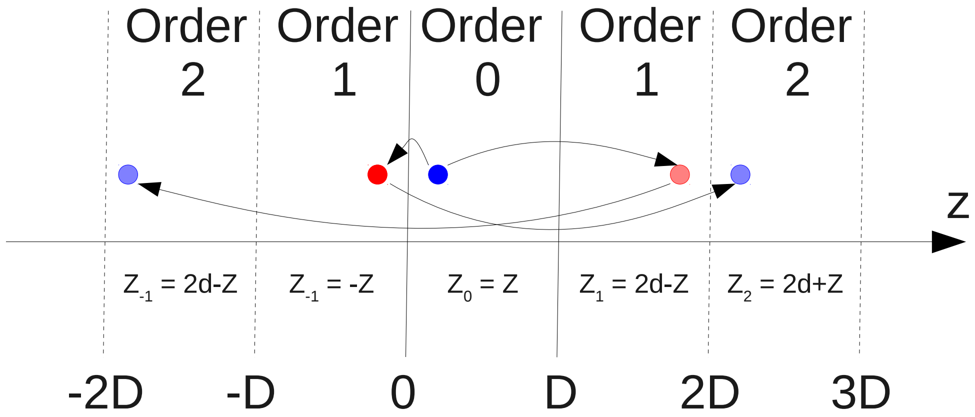
$$\frac{-Q\,z\,\hat{z}}{k_e R^3}=\frac{N_{sp}\,e\,z\,\hat{z}}{k_e R^3}$$

where $Q=\int dq=-N_{sp}e$ and

e is the electron charge,
N_{sp} the superparticle ratio

Field from test particle on tip: analytical (3)

- We have two perfectly conducting surfaces, so both requires an image charge
- The image charges are then mirrored on the other surface
- This leads to a series expansion of the field



$$Z_{-i} = -i * D + \left\{ \begin{matrix} D - z & i \quad odd \\ z & i \quad even \end{matrix} \right\}$$

$$Z_{+i} = i * D + \left\{ \begin{matrix} D - z & i \quad odd \\ z & i \quad even \end{matrix} \right\}$$

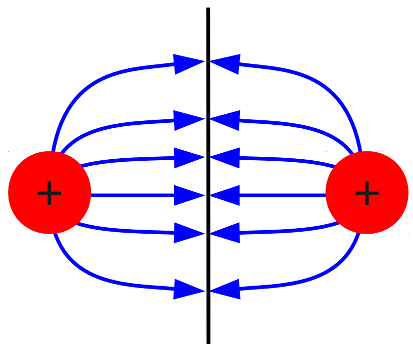
$$E_z = E_z(z_0) + \sum_{o=1}^{\infty} \left(E_z(z_{+i}) + E_z(z_{-i}) \right)$$

Field from test particle on tip: analytical (4)

- What is not taken into account in the analytical model is the r-boundary found in the simulation
- In the simulation, this is represented by a Neuman boundary condition at $r = R_{max} = nr$:

$$\frac{\partial \phi}{\partial r} = 0 \rightarrow E_r = 0$$

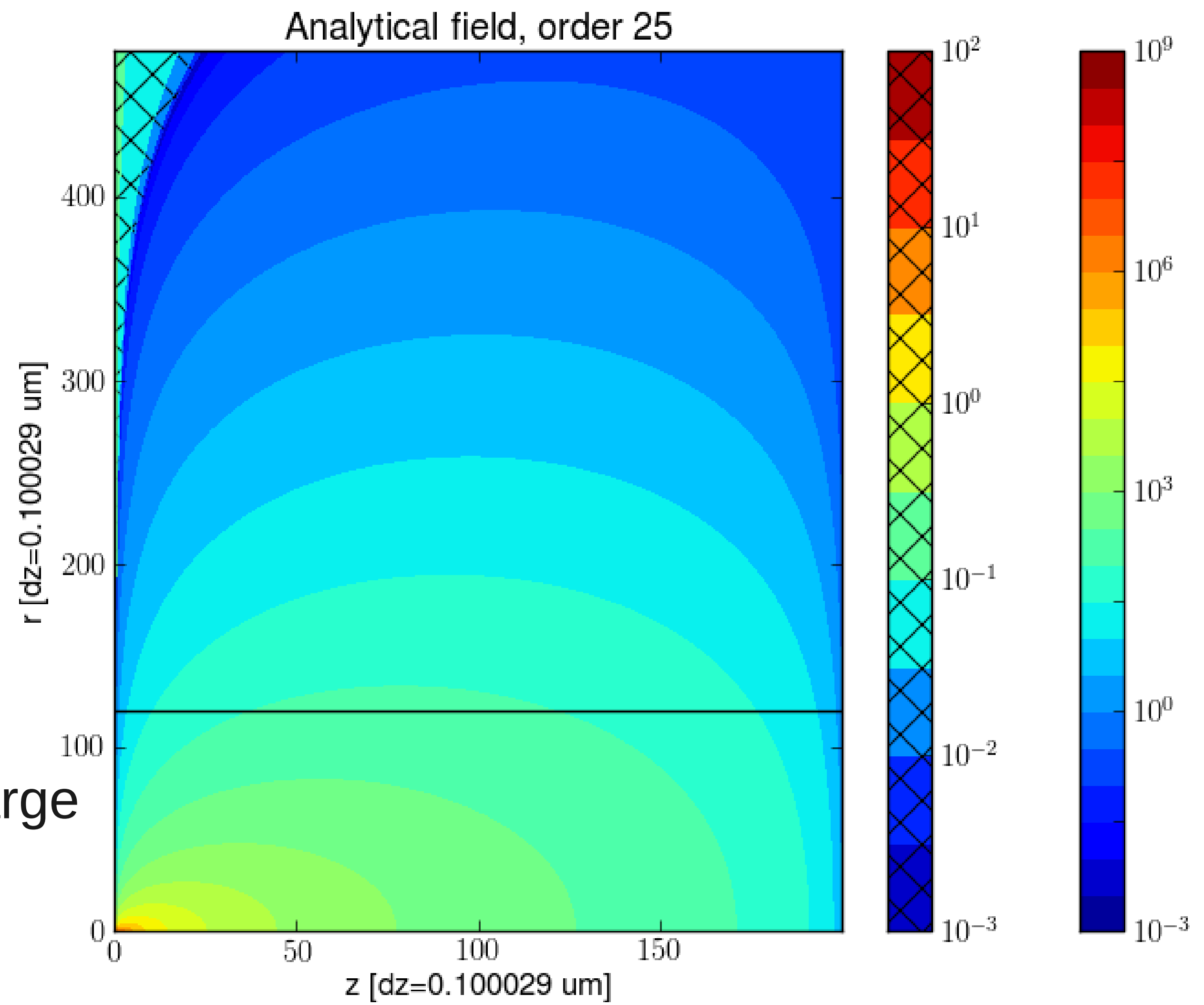
- In an analytical model, this can often be represented by a same-sign image charge



- I was not able to come up with a "mirror" charge distribution for this case
- Thus the analytic and numerical results differ at big r
- I am most interested in field at small r (big r fields anyway small)

Field from test particle on tip: analytical (5)

- The resulting field is shown on the right
  - Black line marks usual system size 12 µm
- Parameters:
  - N_{sp} = 21.35
  - Sum order = 25
  - D = 20 µm
- Note negative field at large radius
  - Happens due to image charge field – positive images with z>D, negative with z<0
  - Not important at small r

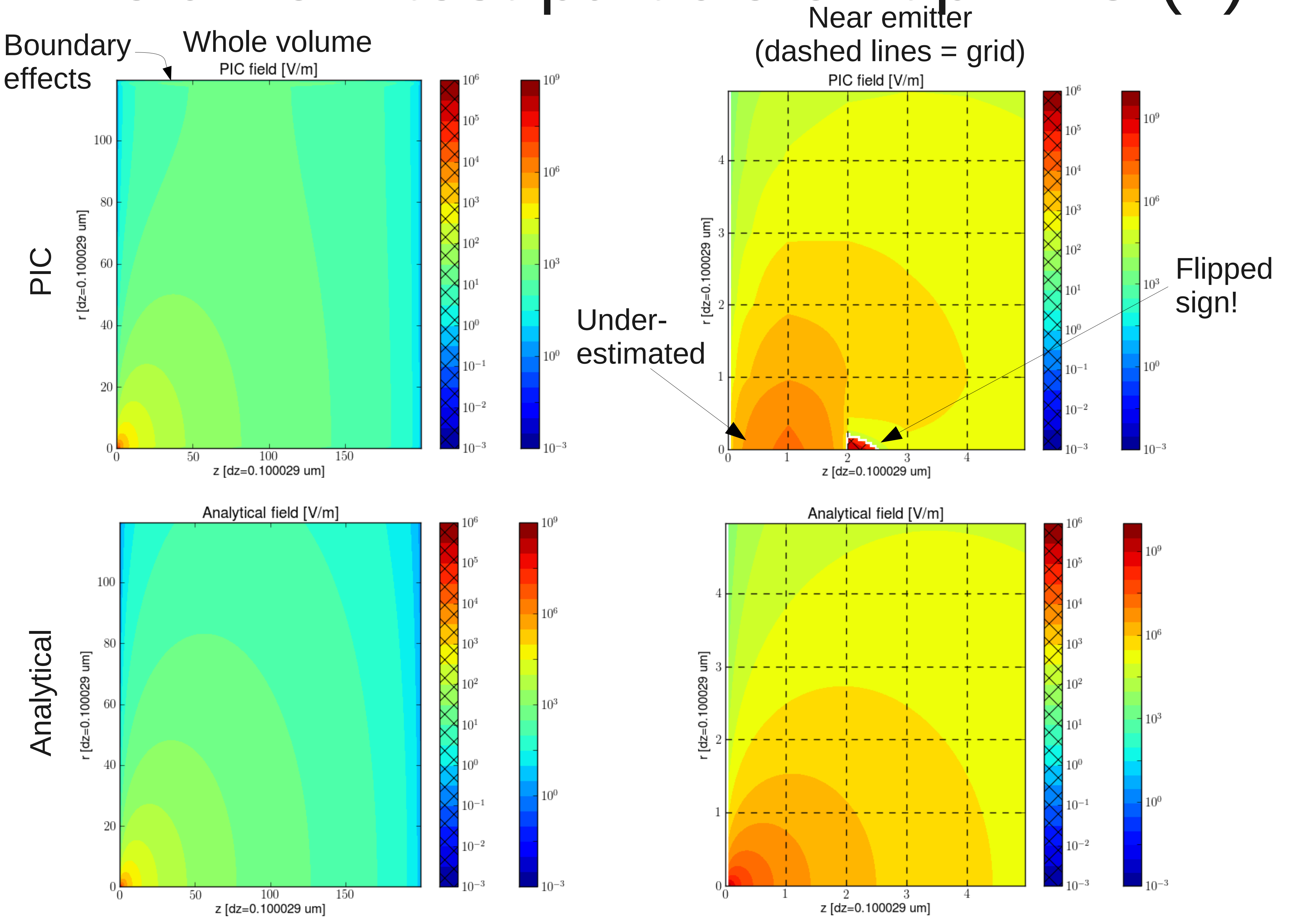


Field from test particle on tip: PIC (1)

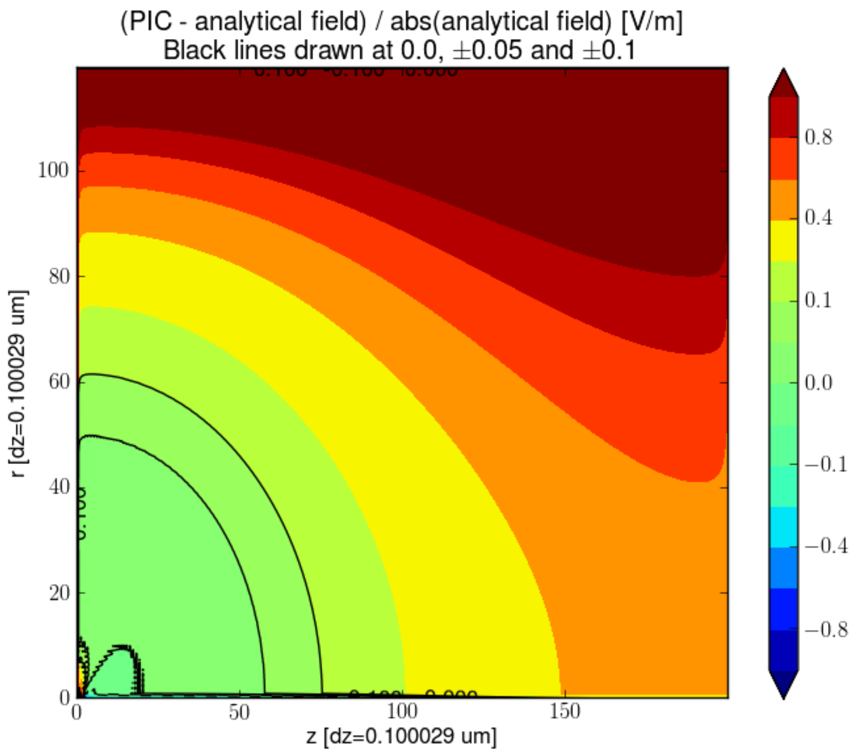
- In PIC:
  1. The charge is first interpolated onto the grid points
  2. Poissons equation solved on the grid points => potential
  3. Field calculated by derivative of potential on grid points
  4. Field interpolated to observer position

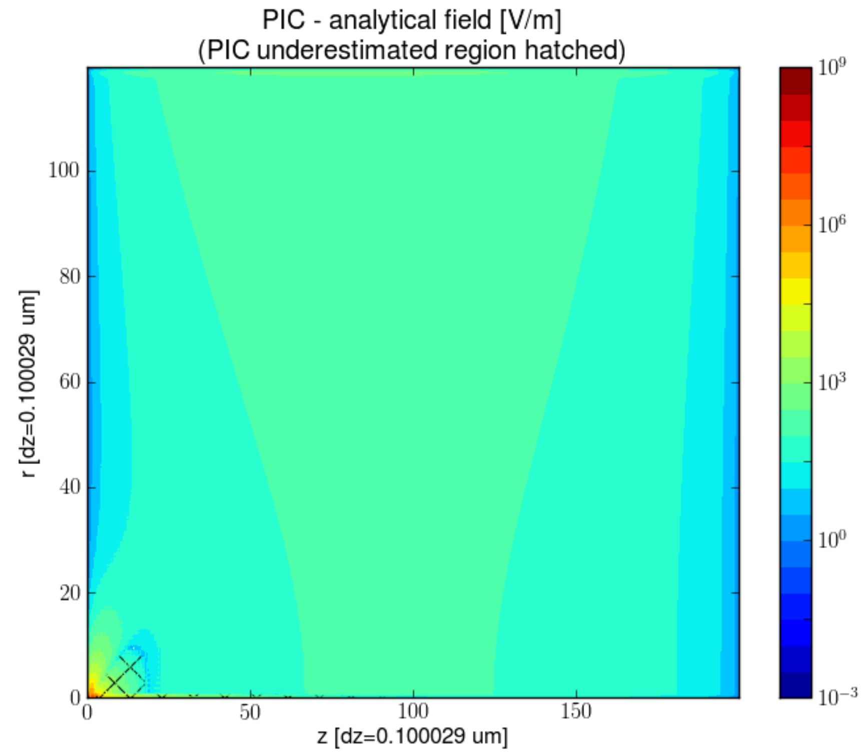
- This leads to underestimation of field and other inaccuracies at short range
- OK for plasma bulk
  (given that dz << typical length scale)
- Problematic at emitter
  - Relevant space-charge shielding charges very close
  - There may be effects of being at r=0 which is simultaneously a Neuman boundary and Dirichlet boundary
- Also, field close to r=dr is disturbed by Neuman boundary condition

Field from test particle on tip: PIC (2)



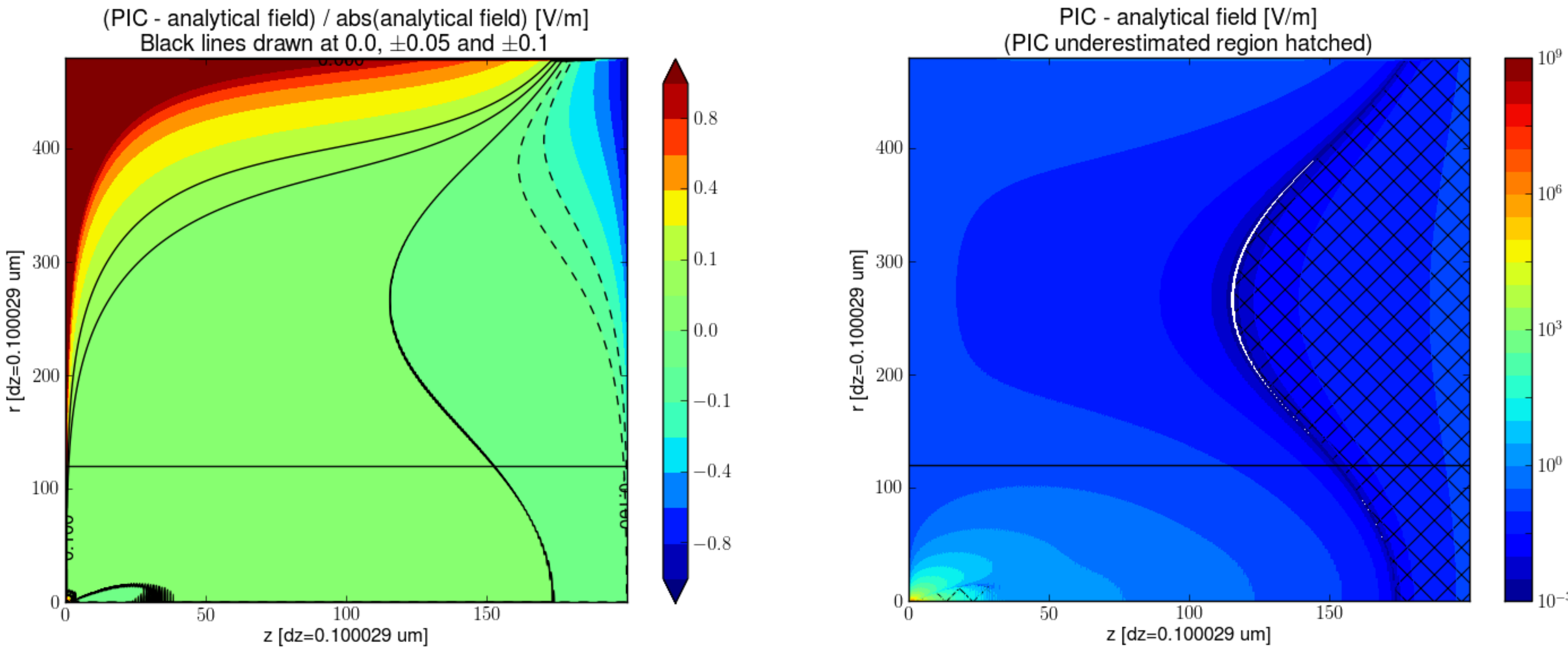
PIC field versus analytical field (1)





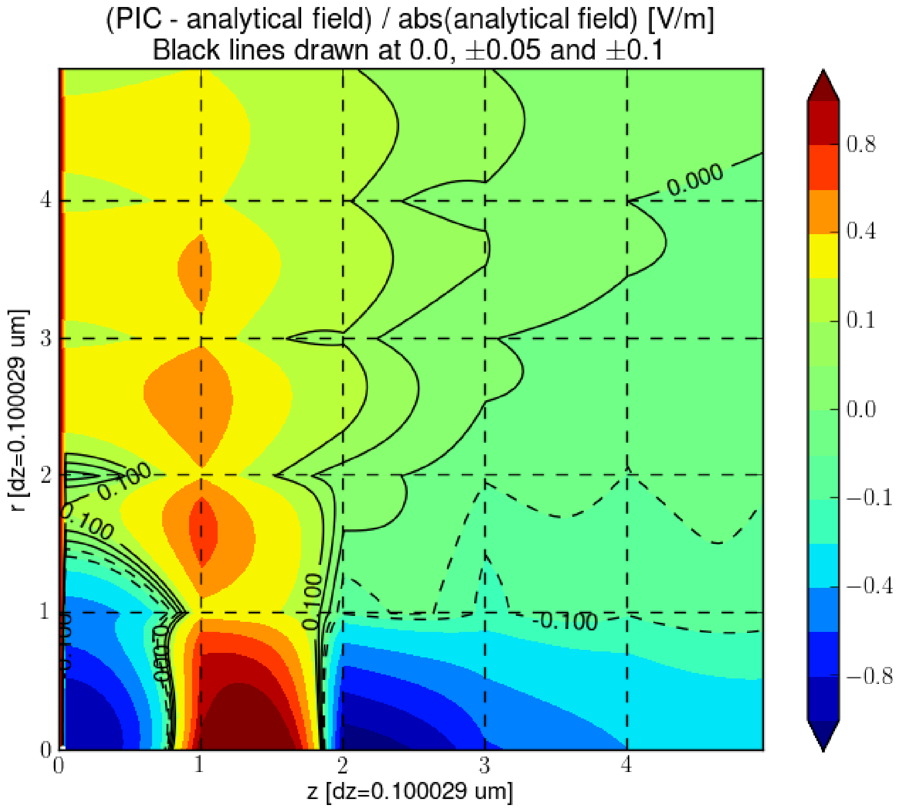
- See that it matches reasonably well far away
  - Boundary effects are visible, and large relative errors
  - These fields are however *absolutely* small (when observed from the emitter)

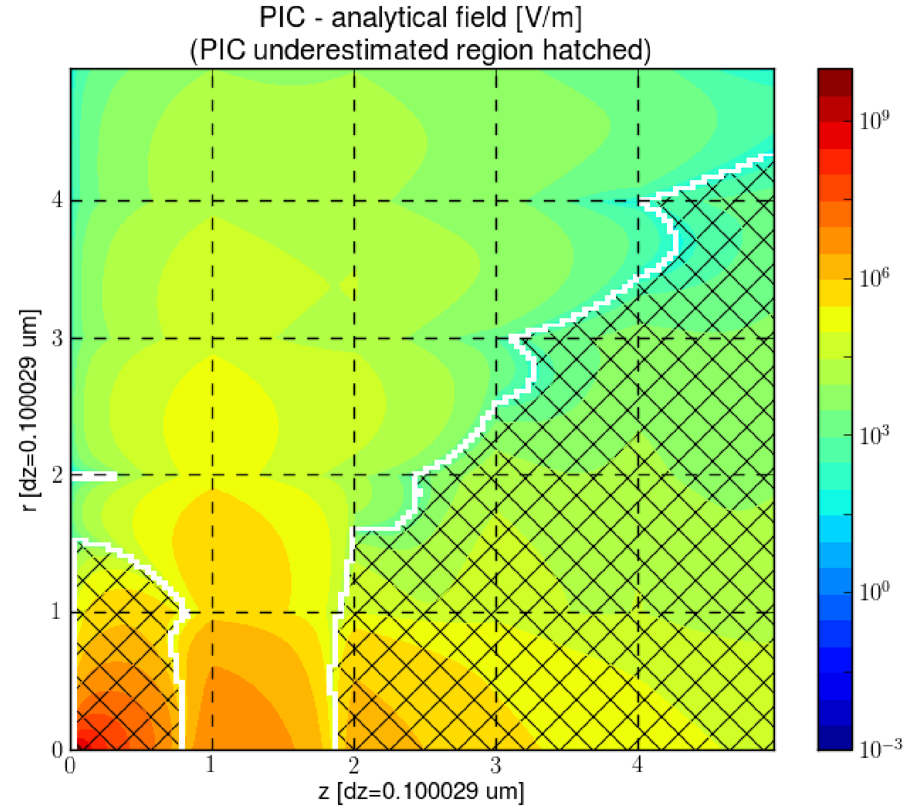
PIC field versus analytical field (2)



- Mitigation of boundary effect possible by extending the grid (assuming the arc has the same size)
- However this carries the penalty of slowing down the field solver (matrix size ~ (nr*nz)^2)

PIC field versus analytical field (3)

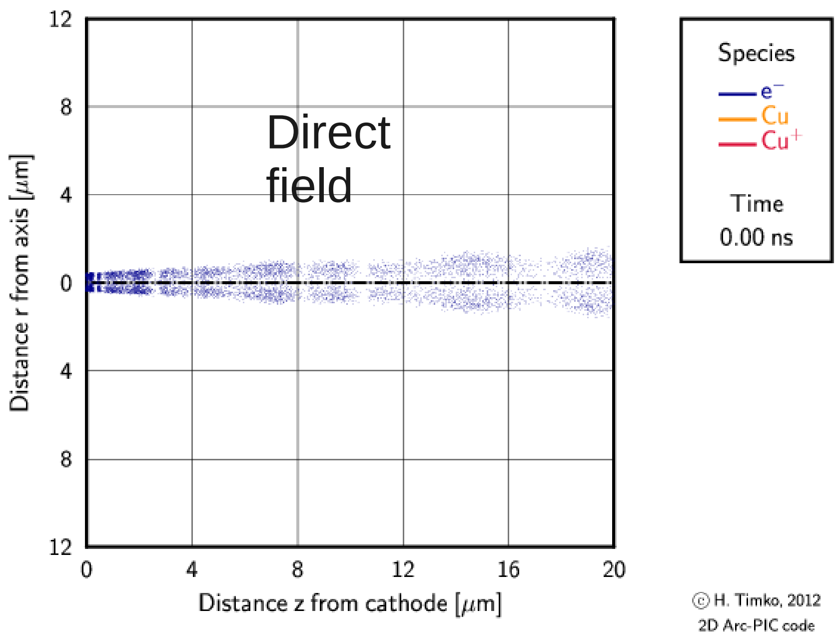


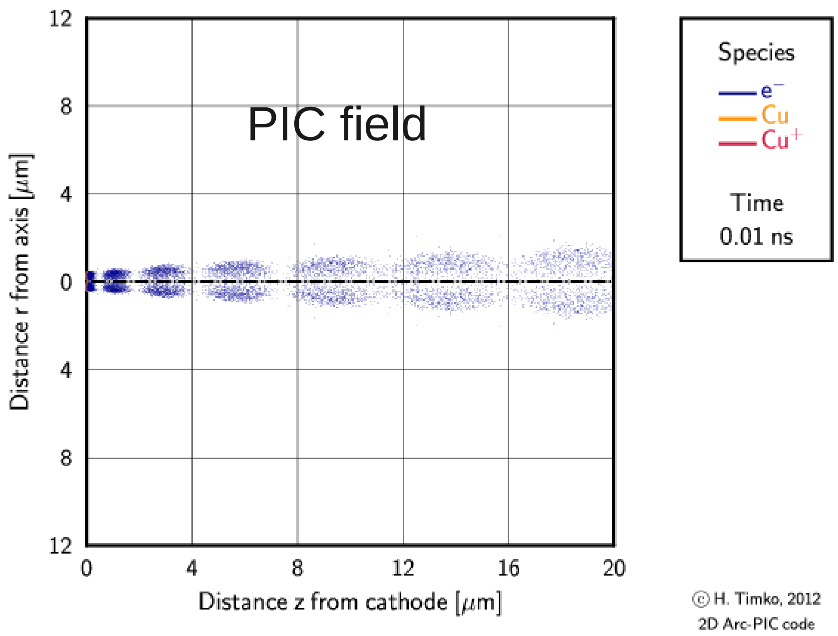


- Field very wrong close to emitter
  - This is where the recently emitted electrons are found...
  - Too-low field => overestimation of emission
    - These extra charges then leads to extra-much space charge -> emission quench
    - This again results in the observed pulsing during space-charge limited Fowler-Nordheim cold field emission

Effect on field emission in ArcPIC2D (1)

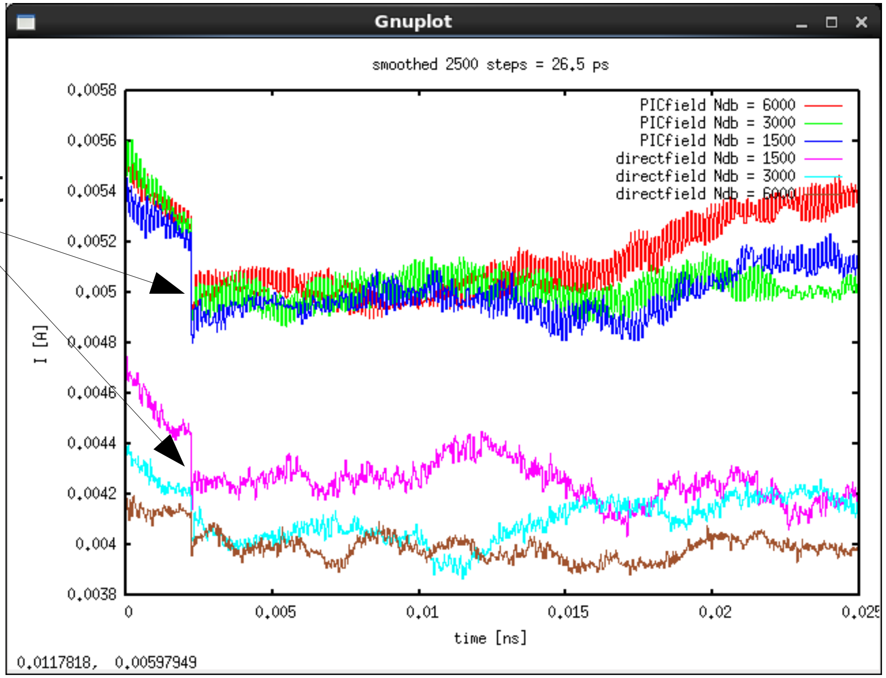
- I implemented a test emission model class in ArcPIC using the analytical expression to calculate the tip field
  - Only image charge at -z taken into account
  - No neutrals etc
  - Inter-electron and external field forces handled by PIC
- Still some instability due to field ~1/z^2
  - Sometimes evaluated with a “close” particle
  - Looks better
  - Less “structured” pulses



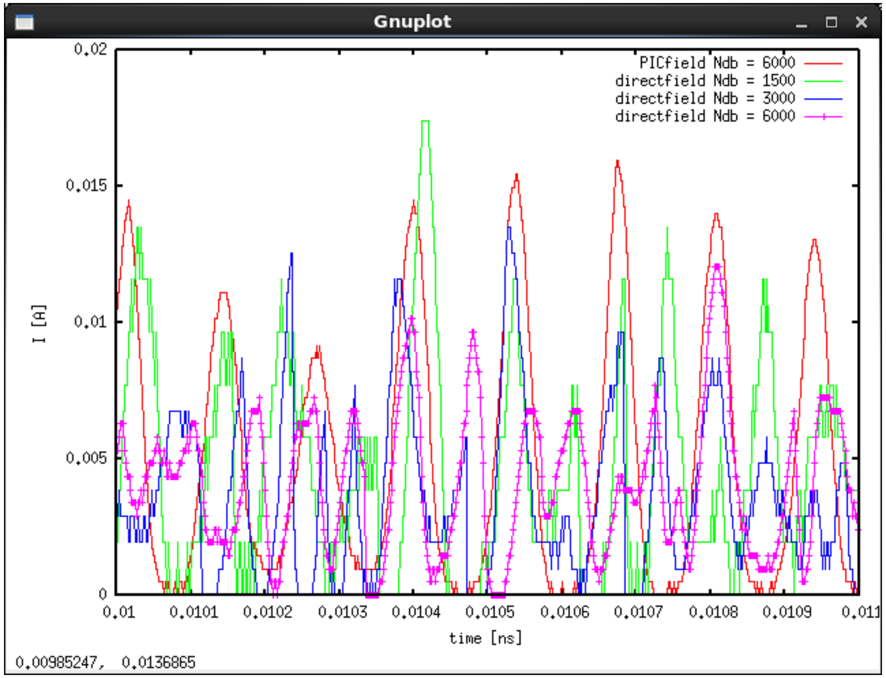


Effect on field emission in ArcPIC2D (2)

Due to first-step overshoot



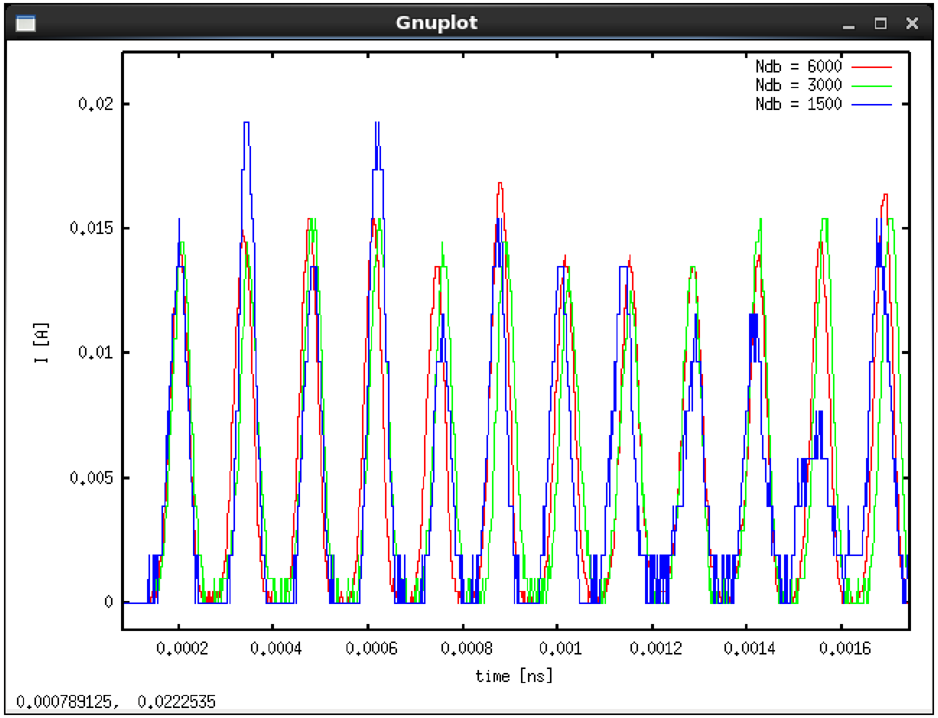
- Field emission current reduced significantly
- More random oscillations

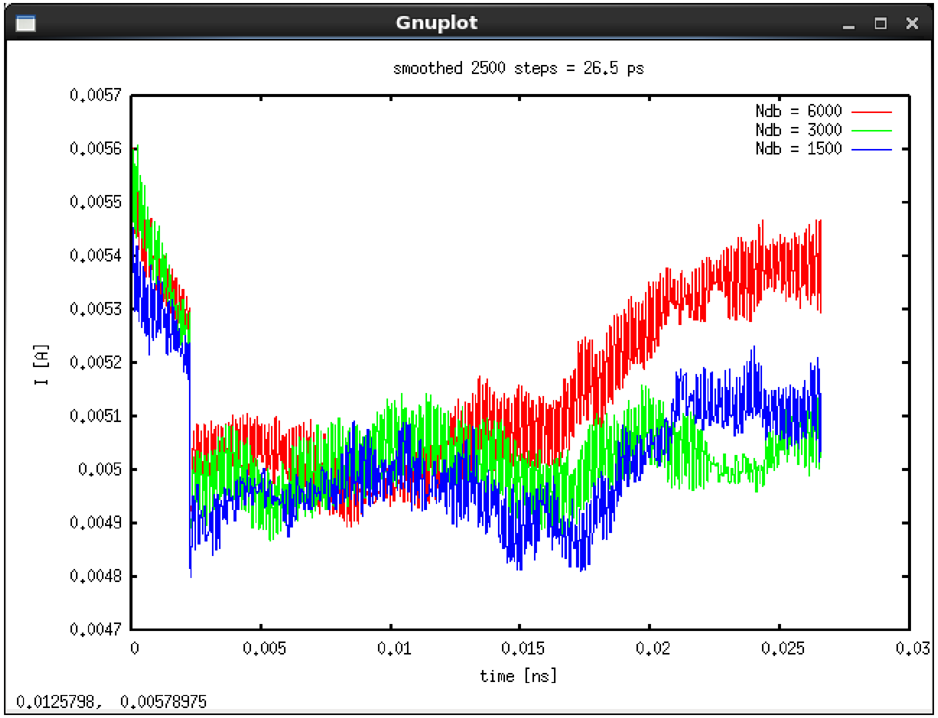


- TODO:
  - Expand test model to include neutrals & ions
  - Run breakdown simulation w/ this model

Appendix

Pulsing is NOT caused by statistics





... but as expected, the higher-Ndb runs are less noisy

Pulsing NOT caused by time step

- See that current well converged in dt
- Increasing dt leads to cycle “emission -> acceleration -> emission”, increasing the average current
- Small dt leads to only 0-1 electrons emitted per time step
- Grid convergence may be more interesting
  - Analytic result is basically an infinite grid, but still noisy (not single frequency tough)