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1D Breakdown Simulations and Development of an Energy Conserving, Implicit PIC-DSMC Method

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Outline

- 1-D breakdown simulations
  - Electron source: Auger neutralization vs. Cold Field Emission
  - Differential Forward vs. Isotropic Scattering
- Energy-Conserving Vlasov-Poisson formulation
  - Momentum error control: Adaptive particle orbit substeps
  - Ion Acoustic Shock Wave test problem
  - Implementation of Realistic Boundary Conditions and Collisions
- Conclusions

1D Breakdown Simulations

1D Breakdown in Air

- 1D PIC-DSMC simulations
  - Fe cathode and Ag anode (for comparison to experiment)
  - Gap filled with air at STP
  - Simulate various gap sizes → Find breakdown voltage
  - Uniform grid, $\Delta x < \lambda_D$ at $n_e = 10^{21}\ m^{-3}$ (typical "breakdown"density)
  - Timestep = 5×10^{-15} s < CFL < mean collision time < $1/\omega_{pe}$
- Define "Breakdown": Exponential rise in current as voltage "collapses" and quasi-neutral plasma forms in gap
  - Simulations limited to 5 ns → Obtain upper limit $V_{breakdown}$
- "Trigger" breakdown with an initial, very low density uniform electron & ion plasma of $10^{17}\ m^{-3}$ ($\sim10^{-9} * n_{N2}$)

Gas Interactions Model

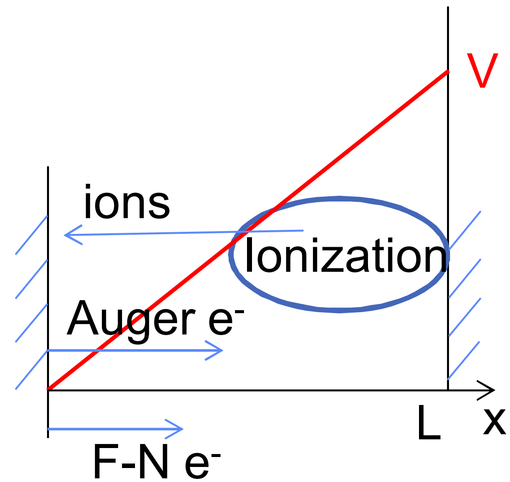
- Include e-N_2, e-O_2, e-N_2^+, and e-O_2^+ interactions
  - Elastic, Excitation
    - Alter electron energy distribution
    - Elastic collisions can be either isotropic or preferentially forward scattering
  - Ionization: $N_2 \rightarrow N_2^+$ and $O_2 \rightarrow O_2^+$
    - Source of ions & secondary electrons
    - Use *total* ionization cross section
    - Do not include double ionization ($N_2 \rightarrow N_2^{++}$ & $O_2 \rightarrow O_2^{++}$)
    - Do not include dissociative ionization ($N_2 \rightarrow N + N^+$ & $O_2 \rightarrow O + O^+$)
  - Recombination ($O_2 \rightarrow O + O^-$), Attachment ($N_2^+ \rightarrow 2N$ & $O_2^+ \rightarrow 2O$)
    - Sink for electrons, ions

Surface Model

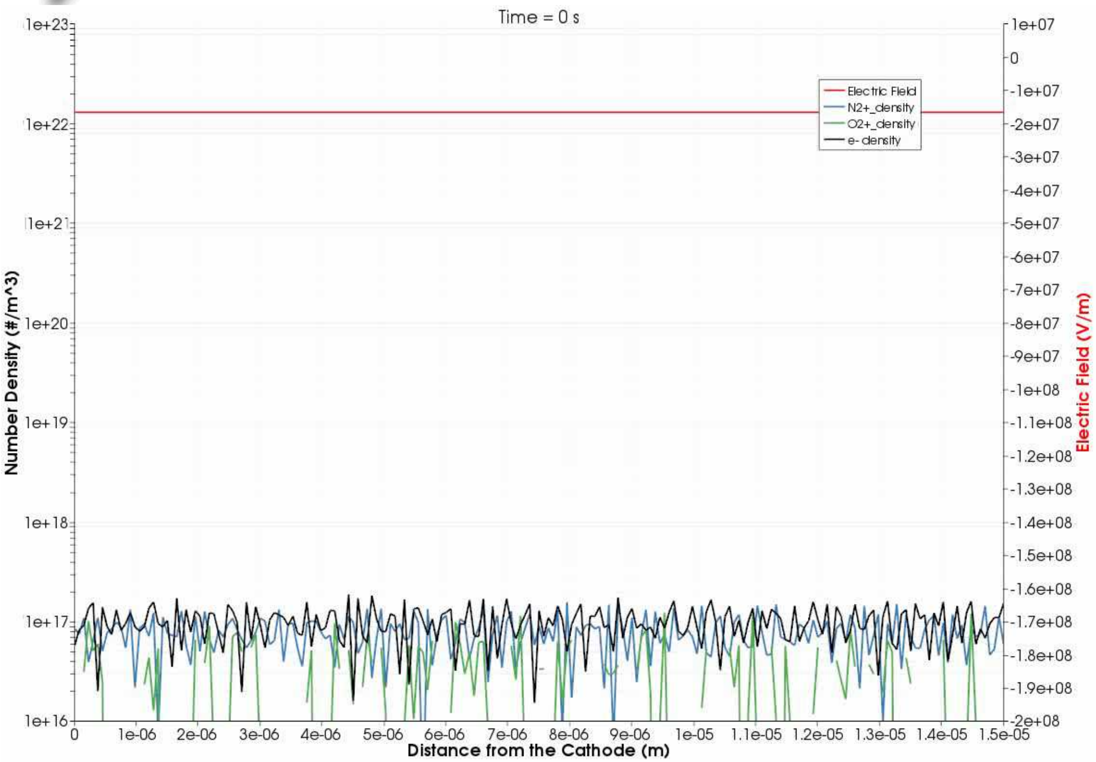
- Include Auger Neutralization
  - Upon approach to surface, Ion is neutralized and liberates secondary electron with probabilty γ_e
  - γ_{e,N_2^+}=0.026, γ_{e,O_2^+}=0.018 (Lieberman & Lichtenberg, 2005)
    - Function of the ion species' ionization potential & surface work function (use ϕ=4.5 for Fe)
    - Independent of kinetic energy below ~500 eV
    - Dependent on surface contamination
- Include Fowler-Nordheim field emission
  - Quantum tunneling through surface potential barrier accounting for local surface E-field, E_s

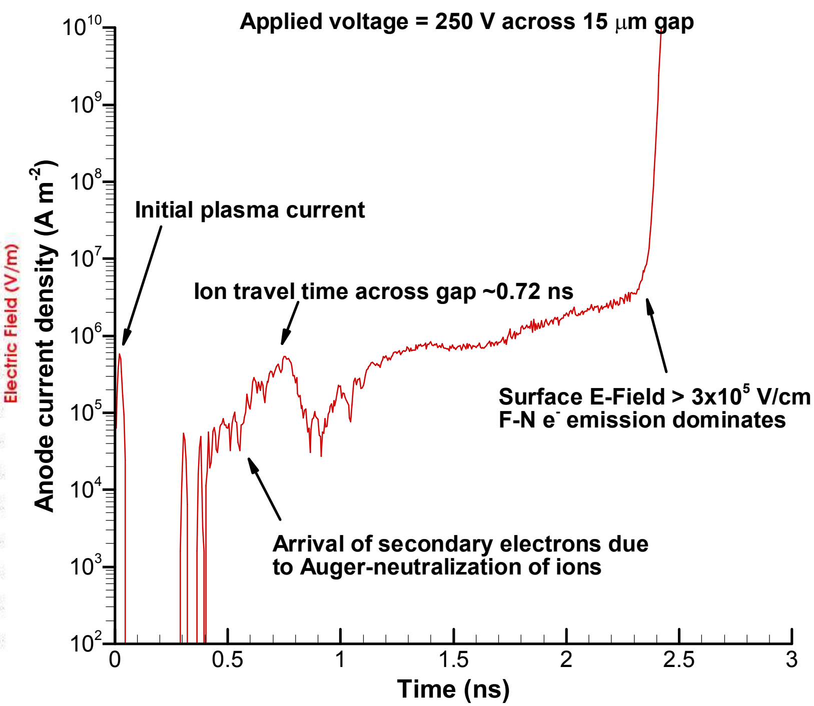
$$j = \frac{A[\beta E_s]^2}{\phi} exp\left(-\frac{B\phi^{1.5}v(y)}{[\beta E_s]}\right); \;\; v(y) \approx 0.95 - \left(\frac{C[\beta E_s]^{0.5}}{\phi}\right)^2$$

  - Assume β=50 (typical for polished metals)



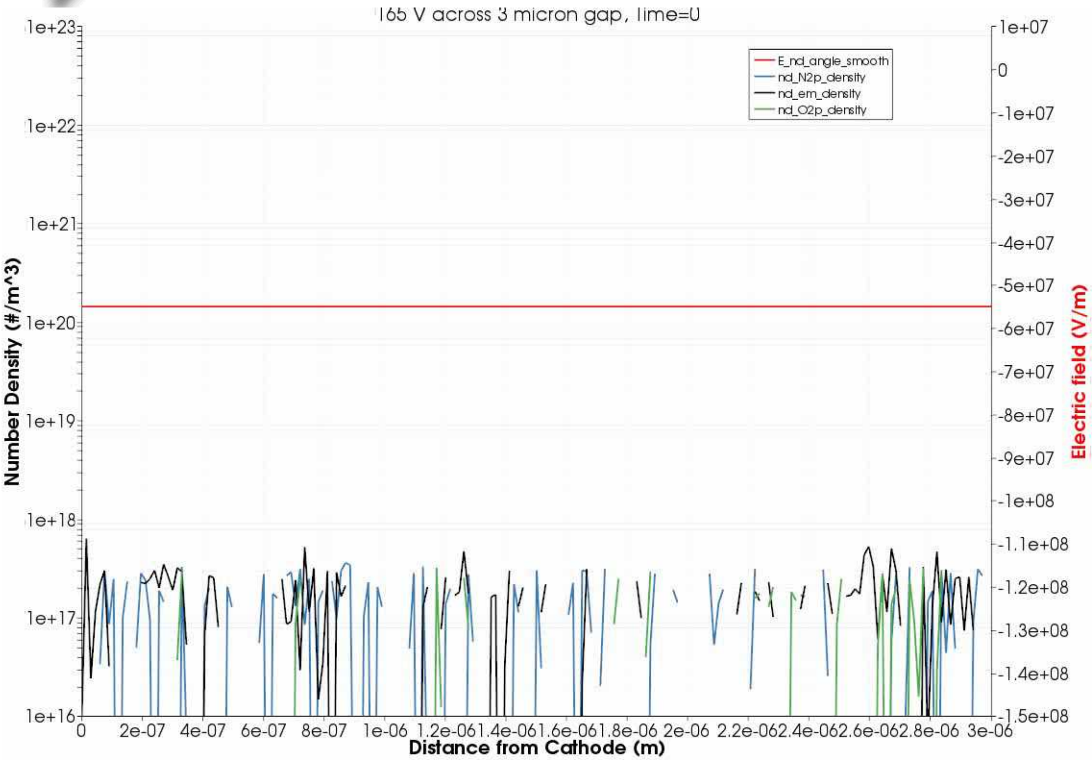
"Large" Gap Breakdown

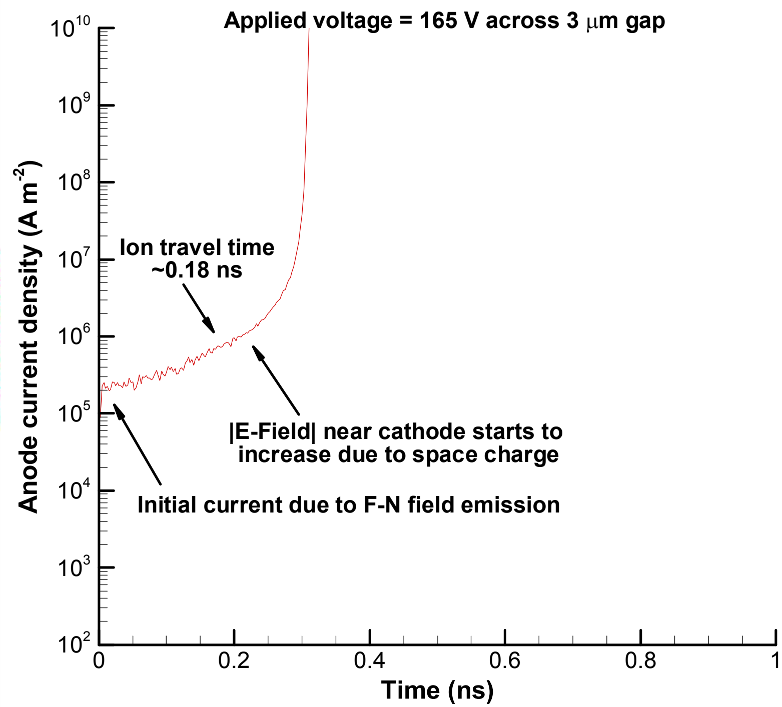




- Initial pulsing of current as ions transit gap and release electrons from cathode which then generate more ions
- Eventually quasi-neutral plasma established
  - Gap voltage drop only across sheath → Fowler-Nordheim emission accelerates breakdown

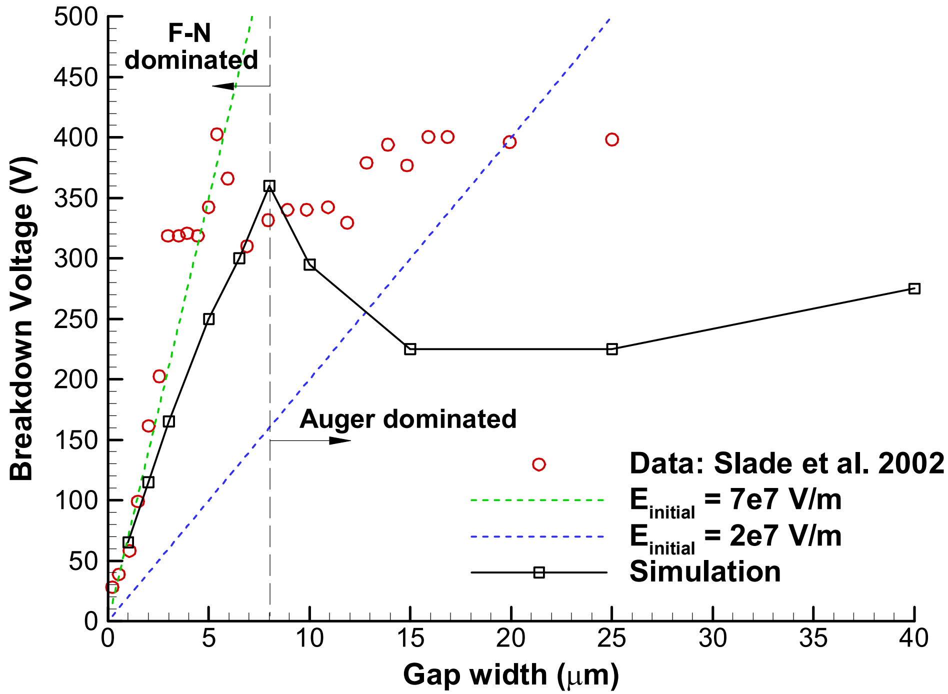
“Small” Gap Breakdown





- For small enough gaps, Fowler-Nordheim field emission dominate source of electrons
- Ionization of gap gas → Net charge buildup near cathode leads to increased field emission and breakdown

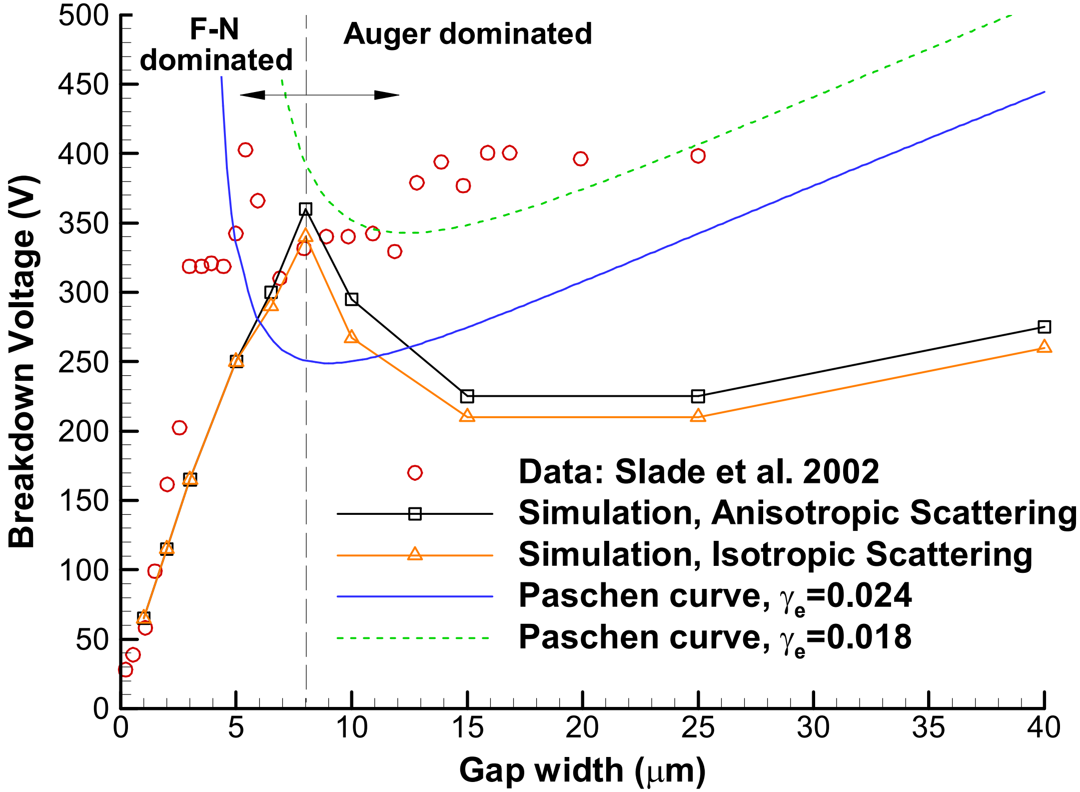
Breakdown vs. Gap size



- Small gaps: Fowler-Nordheim emission
  - Sensitive to Field Enhancement Factor due to microscopic roughness
  - Data requires initial field of 7×10^7 V/m; Simulation requires less initial field as gap size increases (but still Fowler-Nordheim dominated)
- Large Gaps: Auger neutralization electron flux
  - Sensitive to secondary emission coefficient and e^- - neutral interactions

Breakdown vs. Gap size

- Paschen curve coefficients fit to data & based on e⁻-gas interactions (net ionization rate)
- Discrepancy vs. theory (with γ_e=0.024) → Due to interaction physics model?
- Isotropic scattering model (vs. forward scattering) decreases simulated V_b by ~10%
  - Isotropic scattering results in longer e⁻ path length across gap due to backscatter events



Energy-Conserving Implicit PIC

Why Implicit PIC?

- Breakdown simulation timescale ~10×Ion transit time across gap
  - Computationally expensive
- Electric field changes over ~Ion timescales
  - But explicit schemes must still resolve electron motion timescales, e.g. ω_{pe}, for stability
- Implicit schemes will allow for much greater field solve timesteps and ion motion while still accurately capturing electron motion

Energy-Conserving Implicit PIC

- Based on work by Chen *et al.*†
  - Use Jacobian-Free Newton Krylov solver & particle enslavement to nonlinearly eliminate particle quantities
  - Vlasov-Poisson with Crank-Nicolson time discretization

$$\varepsilon_0\left(E_{i+1}^{n+1} - E_i^{n+1}\right) = \rho_{i+1/2}^{n+1}\Delta x$$

$$\frac{x_p^{n+1} - x_p^n}{\Delta t} = \frac{v_p^{n+1} + v_p^n}{2}$$

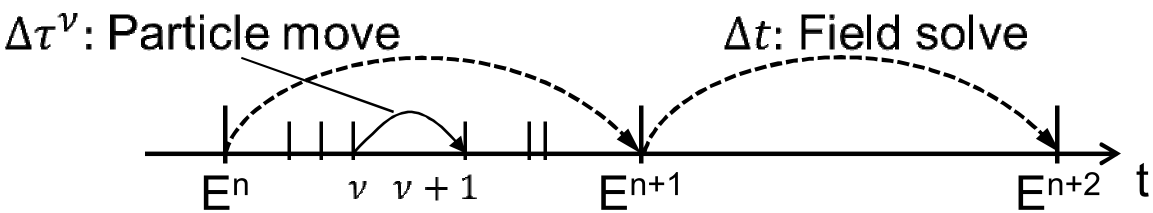
$$\frac{v_p^{n+1} - v_p^n}{\Delta t} = \frac{q_p}{m_p}\sum_i S\left(x_i - \frac{x_p^{n+1} + x_p^n}{2}\right)\frac{E_i^{n+1} + E_i^n}{2}$$

  - Energy conservation requires nonlinearly converged particles and fields
    1. Move particles using $E_i^{n+1,k} \rightarrow$ assemble $\rho_{i+1/2}^{n+1}$ and RHS
       a) Inner nonlinear iteration – use Picard iteration since it's not stiff
       b) Separate from field solve, can easily add adaptive substepping
    2. Solve for $E_i^{n+1,k+1}$
    3. Form residual

†Chen, G., Chacón, L., and Barnes, D.C., 2011. An energy- and charge-conserving, implicit, electrostatic particle-in-cell algorithm. JCP 230, 7018.

Adaptive Particle Orbit Substeps

- Algorithm doesn't enforce exact momentum conservation
- Control momentum errors by adapting timestep for integration of individual particle movement
  - Reduces particle tunneling

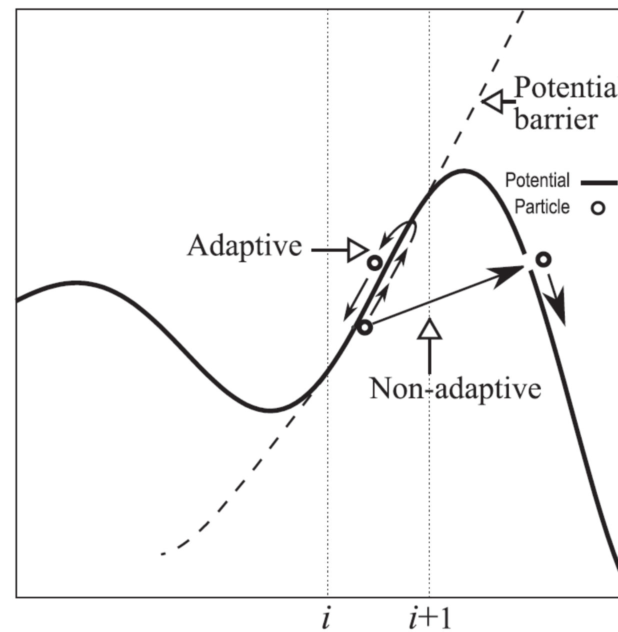


$$\frac{x_p^{\nu+1}-x_p^{\nu}}{\Delta\tau^\nu}=\frac{v_p^{\nu+1}+v_p^{\nu}}{2}$$

$$\frac{v_p^{\nu+1}-v_p^{\nu}}{\Delta\tau^\nu}=\frac{q_p}{m_p}\sum_i S\left(x_i-\frac{x_p^{\nu+1}+x_p^{\nu}}{2}\right)\frac{E_i^{n+1}+E_i^{n}}{2}$$

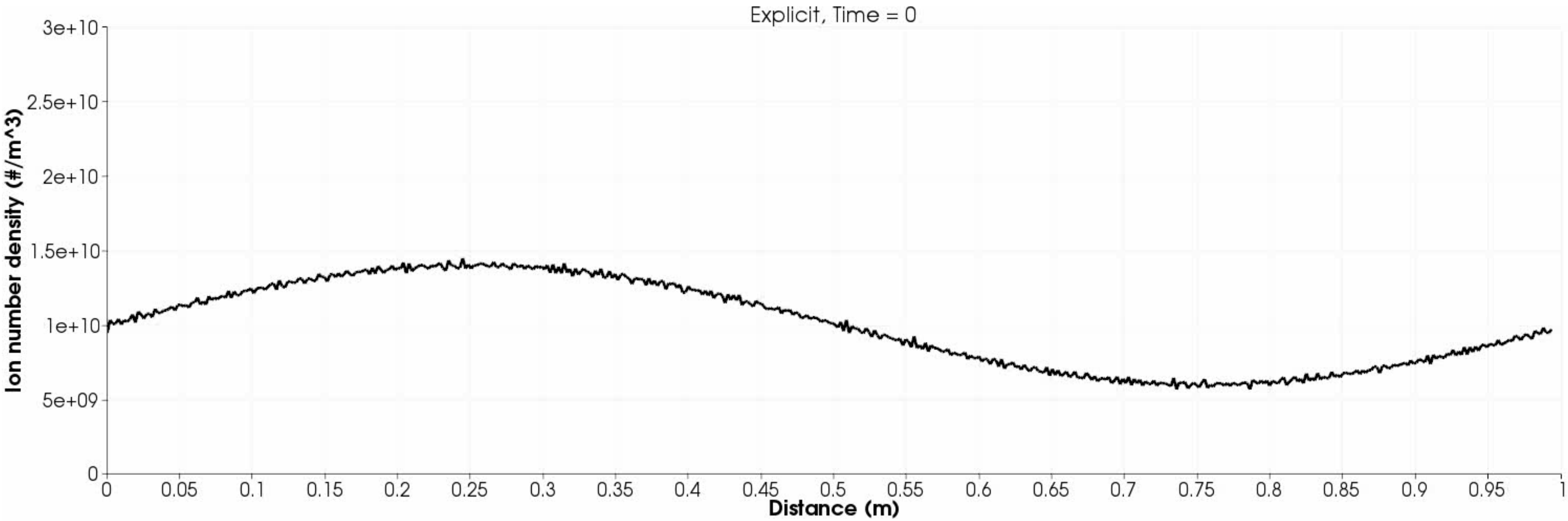
- Find $\Delta\tau^\nu$ to control local truncation

$$\|lte\|_2=\frac{q_p(\Delta\tau^\nu)^2}{2m_p}\left\|\begin{matrix}\frac{E_p^{n+1}+E_p^{n}}{2}\\ \frac{\partial E}{\partial x}v_p^\nu\end{matrix}\right\|_2\le\epsilon_0+\epsilon_r\Delta\tau^\nu\left\|\begin{matrix}v_p^n\\ \frac{q_pE_p^n}{m_p}\end{matrix}\right\|_2$$



Chen et al., 2011

Ion Acoustic Shock Wave Test



- Periodic boundaries, sinusoidal perturbation of initial density and velocity
- Ion acoustic shock dynamics develop over ion timescales
- Accurate explicit solution requires timestep resolution of plasma frequency even though fields vary “slowly” → Implicit could increase timestep by O(100)

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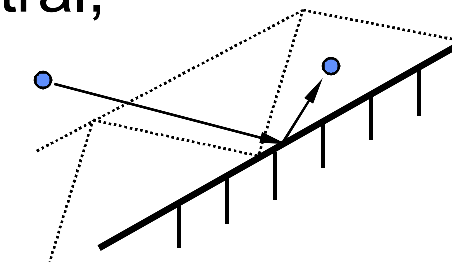
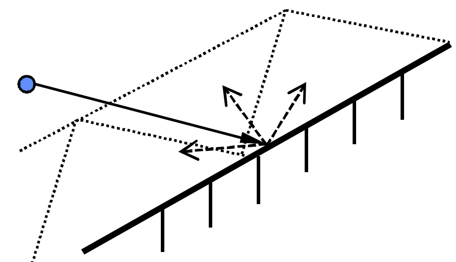
Stochastic/Charge Creation BC's

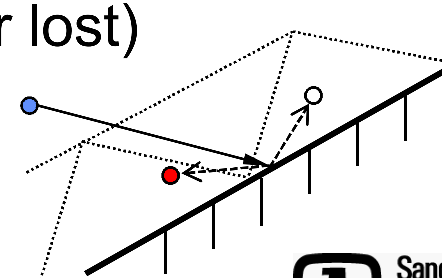
- Particle interaction while moving with neutral, deterministic boundaries not an issue:
  - Each iteration, if the particle hits the boundary it does the same thing. Eventually converges.



- Stochastic boundary (e.g. diffuse) for charged particles
  - Now each iteration the charge might end up in a different element. Convergence not assured.

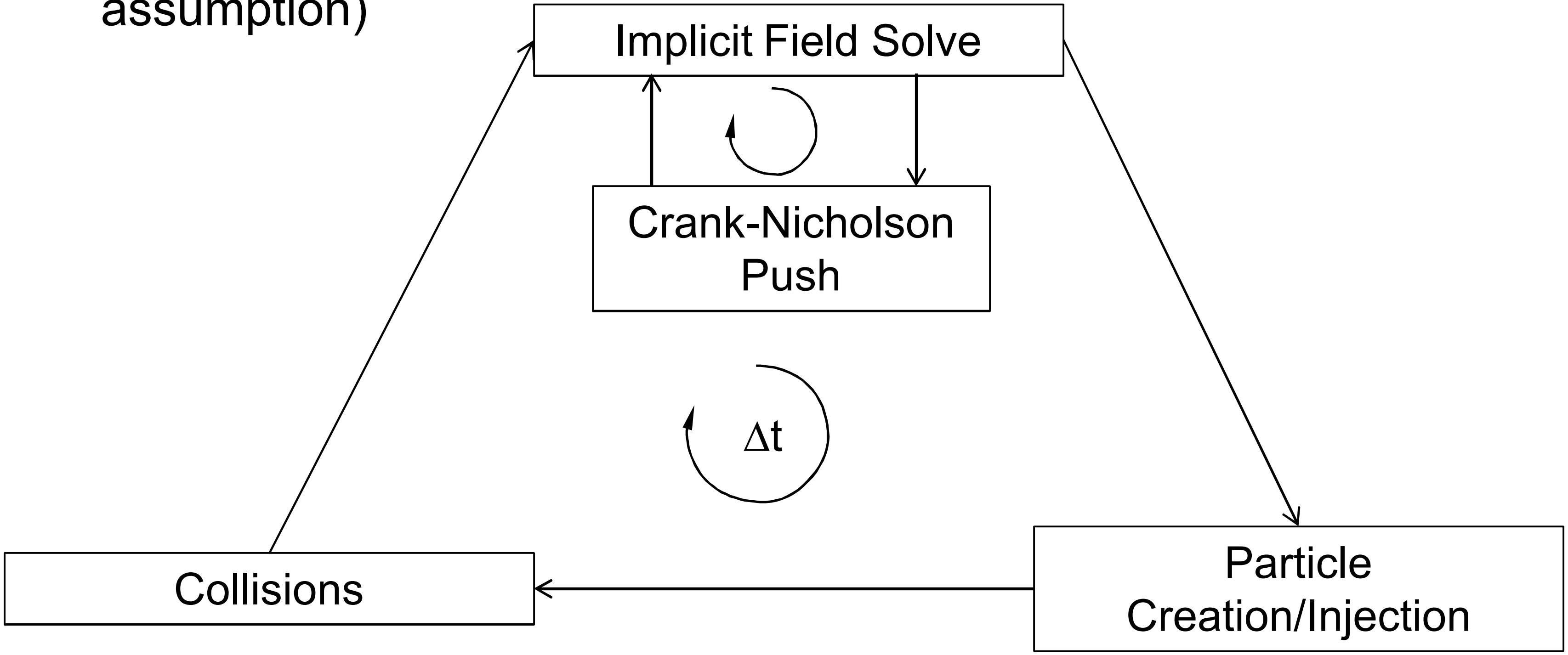


- Charge creation/destruction boundaries
  - Convergence problem if, on given iteration if the charge reaches the surface net charge created (or lost) which on the following field solve iteration prevents the original charge from reaching the surface



"Real" Simulations

- Lag charge creation/destruction → Create charge after field solve is converged & before interactions
- Lock in behavior of diffuse boundary for given particle (not implemented yet)
- Collisions decoupled from particle movement (typical collisional PIC assumption)



Conclusions

- Large Gaps:
  - Auger neutralization is primary source of initial e^-
  - Current "waves" as breakdown develops plasma in the gap
  - Preferential forward scattering *increases* V_b
  - Large discrepancy between simulation and experiment/theory indicates gas interaction model needs improvement
- Small Gaps:
  - Fowler-Nordheim field emission e^- flux source – no "trigger" plasma needed
  - Collisional processes with neutral gas not as important
- For all gap sizes, final breakdown occurs when quasi-neutral plasma forms a sheath and Fowler-Nordheim field emission results in huge currents

- Implicit, Energy Conserving PIC desirable for breakdown simulations b/c breakdown occurs over ion timescales
  - Must still resolve e^- timescales → Implicit allows much larger timesteps
  - Lag stochastic/charge-creation boundary conditions for "complicated" boundary conditions