SPEED-LIMITED PARTICLE-IN-CELL (SLPIC)
AND
GETTING TO THE ANSWER FASTER

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(U. COLORADO, TECH-X)

- PARTICLE-IN-CELL METHODS: POWERFUL FOR KINETICS, BUT LIMITING, ESP. ION-SCALE SIMULATIONS WITH KINETIC ELECTRONS
- SLPIC PROVIDES AN EXPLICIT METHOD TO ELIMINATE DISPARITY
- SLPIC ANSATZ CAPTURES THE REQUIRED PROCESSES WHILE IGNORING THE UNIMPORTANT
- SLPIC CAN BE SOLVED BY PARTICLE METHODS
- SLPIC SHOWN TO WORK ON SHEATH AND BREAKDOWN PROBLEMS

My long time connection with Livermore

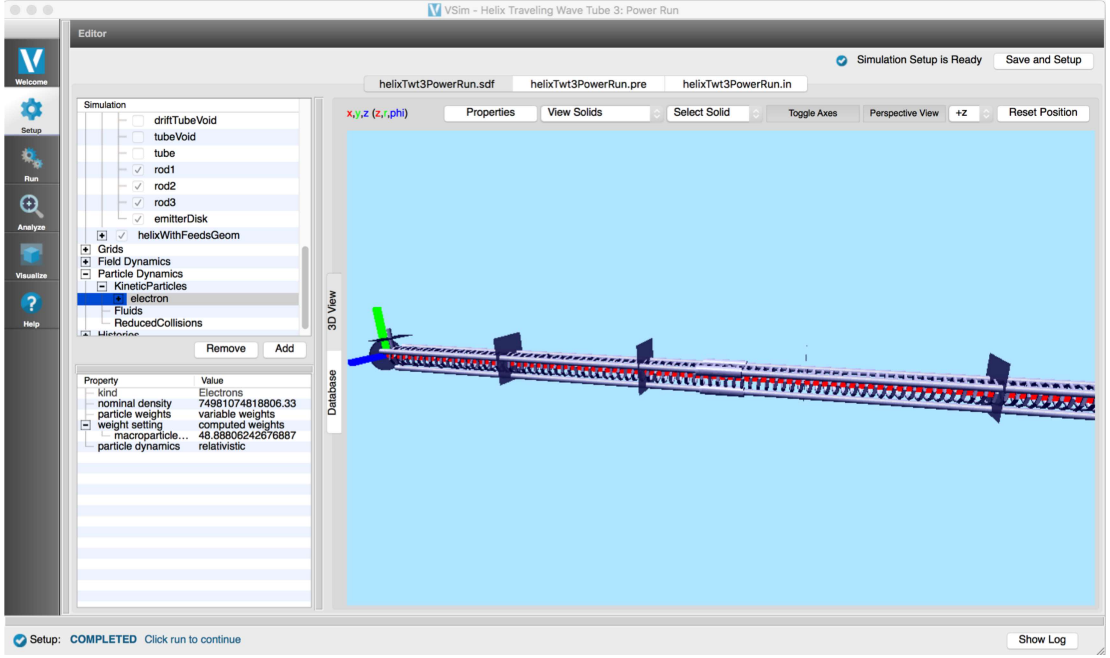
- Born March 15, 1953, 10:54 pm
  - St. Paul’s Hospital, 815 So. J St.
  - Delivered by Grace E. Devnich
  - Parents lived at 120 Vineyard Avenue
  - Dad (Mech Eng) worked at Cal. Res. and Dev.
- 70’s joint seminars with LBNL
- 2000’s: FACETS
- 2020: Visiting scientist?

Memorial today for Tri-Valley’s first woman doctor

https://www.eastbaytimes.com/2008/09/29/memorial-today-for-tri-valleys-first-woman-doctor/

Who am I, what is Tech-X?

- J Cary: Prof. Physics, U Colo; CEO, Tech-X
- Tech-X: Computational Physics company, Boulder, CO, ~40 emp. + cons.
  - ◆ VSim: structured mesh, cut-cell EM, particle in cell, DSMC, fluid. Emerging GPU, AVX.
  - ◆ USim: unstructured mesh, shock capturing, multiphysics fluid code: Hypersonics, HEDP.
  - ◆ RSim: emerging radiation modeling code front end
  - ◆ PSim: Self-consistent field, block co-polymers
  - ◆ Customers/Collaborators across education (e.g., WVa, UCD), government (e.g., CERN, prev LLNL), industry (e.g., Applied Materials)



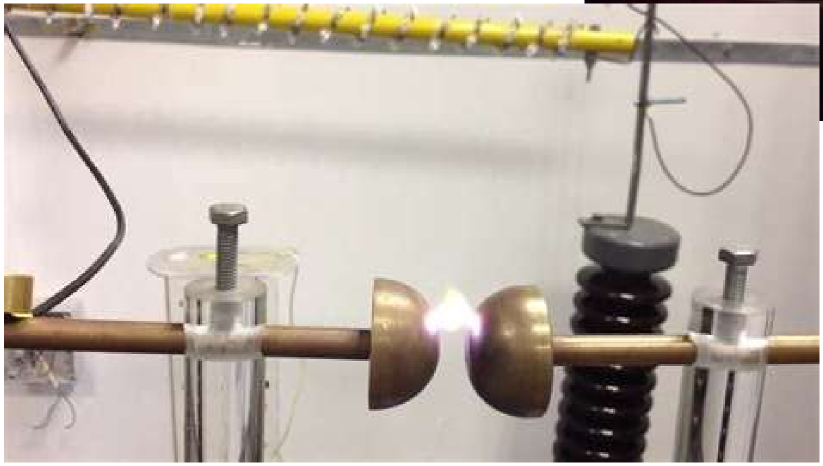
Simulation Setup is Ready

Property	Value
kind	Electrons
nominal density	74981074818806.33
particle weights	variable weights
weight setting	computed weights
macroparticle…	48.88806242676887
particle dynamics	relativistic

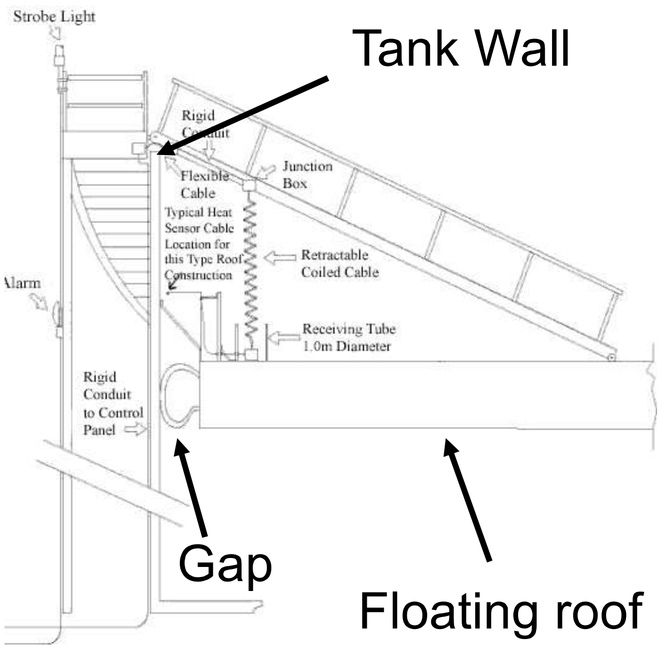
Setup: COMPLETED Click run to continue

Computing electrical breakdown (in complex shapes) has a wide array of applications

- To avoid:
  - Tank farm fires
  - Electrical power distribution
- To enable
  - Nanoparticle generation
  - Plasma medicine
- To learn:
  - Undergraduate physics labs



Oil tank: electric fields induced by lightning



- Lightning hits wall
- Induces electric field between wall and floating roof
- Floating roof sitting on a dielectric
- Put shorting straps between wall and roof
- Gap is 10’s of cm
- Shorting straps are a few cm in width
- Tank is 30m diameter
- How many are needed?
- Ultimately unsuccessful proposal

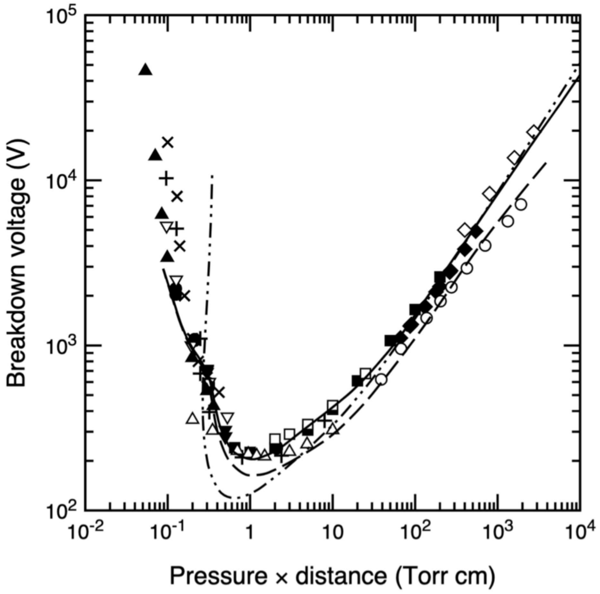
Phenomenon long known

- Paschen (1889) Breakdown voltage a function of pressure times gap separation
- Townsend (1896): “fundamental ionization mechanism”

- As pressure drops, not enough electron-ion pairs created by the transport (electrons zoom right through)
- As pressure rises too high, electrons lose energy to elastic scattering before attaining ionization energy

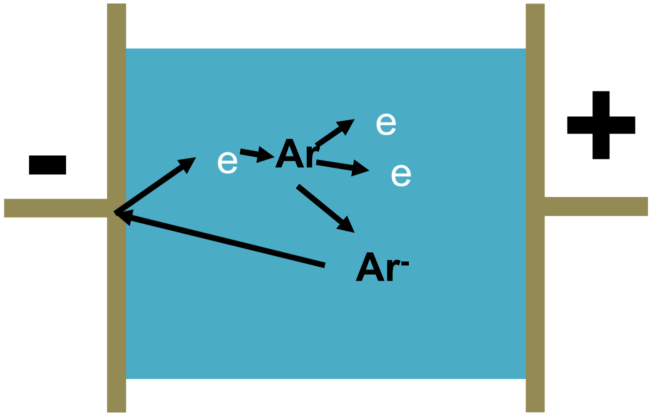
- Minimum voltage at some pressure-distance product.

Ar Paschen Curve
-Phelps 1999



Physics long known

- Electrons accelerated from cathode to anode, producing on average α ions.
- Ions accelerate traveling back towards cathode and cause secondary emission on average of γ electrons
- If $\alpha\gamma > 1$, the current grows exponentially
- Process time is some multiple of the time for an ion (slower species) to travel to the anode
- Well understood for plate geometry, but what about tank farms, high-voltage circuit breakers, electrostatic accelerators?
- Let's just code this up and get the answer!



Kinetic modeling is critical, but limited

- Electron distribution consists of multiple beamlets, with drops due to ionization, and long tails
- Need to model complex shapes with scale disparities
- One must model this for several ion transit times (physics recirculation time)
- And for explicit PIC, one has to have a time step smaller than the time for an electron to cross a cell

Particle-in-Cell methods are indispensable for plasma simulations

- PIC: Charged particles represented as macroparticles; interact with EM field. More later.
- PIC provides a representation of velocity space with minimal degrees of freedom
- Provides a way of giving velocity space representation that over multiple cells provides thousands of velocity space points
- Many advances to deal with noise (δf), numerical restrictions (implicit)

But at some point, maybe 100 ppc in 2d, 1000 in 3d, one can go to a continuum rep and eliminate noise.

Particle-in-Cell methods imply limits on time stepping, grid resolution

- $v_p \leq \Delta t$: Particles must not move over many grid cells in a time step to get an accurate force and to provide an accurate current
- $\omega_p \Delta t \leq 1$: otherwise get strong instability, i.e., plasma CFL,
- $\Delta x \leq \lambda_D$: Debye length resolution needed to prevent grid instability
- All very related
- For electromagnetics, also EM CFL, again related for relativistic particles

These numerical limits are not related to resolution requirements

- Cold plasma oscillations: wavelength determines the physics, not Debye length (yet have to resolve for stability)
- MHD: electrons mostly just cancel electric field
- Ion-acoustic modes (electrons basically Boltzmann response)
- Plasma sheaths (one-sided, chopped electron Maxwellians)
- Plasma discharges (resolve ion crossing time, mfp)

Current approach to avoiding limits is to apply implicit methods

- Mason RJ. Implicit moment particle simulation of plasmas. Journal of Computational Physics. 1981 Jun 1;41(2):233-44.
- Brackbill JU, Forslund DW. An implicit method for electromagnetic plasma simulation in two dimensions. Journal of Computational Physics. 1982 May 1;46(2):271-308.
- Friedman A, Langdon AB, Cohen BI. A direct method for implicit particle-in-cell simulation. Comments on plasma physics and controlled fusion. 1981;6(6):225-36.
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- Petrov GM, Davis J. A generalized implicit algorithm for multi-dimensional particle-in-cell simulations in Cartesian geometry. Physics of Plasmas. 2011 Jul;18(7):073102.
- S. Markidis, G. Lapenta, The energy conserving particle-in-cell method, J. Comput. Phys. 230 (1) (2011) 7037.
- Welch DR, Rose DV, Oliver BV, Clark RE. Simulation techniques for heavy ion fusion chamber transport. Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment. 2001 May 21;464(1-3):134-9.
- L. Chacon, G. Chen, D. Barnes, A charge-and energy-conserving implicit, electrostatic particle-in-cell algorithm on mapped computational meshes, J. Comput. Phys. 233 (2013) 1.
- Taitano WT, Knoll DA, Chacón L, Chen G. Development of a Consistent and Stable Fully Implicit Moment Method for Vlasov--Ampère Particle in Cell (PIC) System. SIAM Journal on Scientific Computing. 2013 Oct 28;35(5):S126-49.
- G.Chen, L.Chacon, “A multi-dimensional, energy-and charge-conserving, nonlinearly implicit, electromagnetic Vlasov–Darwin particle-in-cell algorithm”, Computer Physics Communications 197 (2015): 73-87.
- K. Noguchi, C. Tronci, G. Zuccaro, and G. Lapenta, “Formulation of the relativistic moment implicit particle-in-cell method,” Phys. Plasmas 14, 042308 (2007)
- And many more
- Two types: Direct, Moment
- Computationally intensive: matrix creation at each step (moment method)

Basic PIC methods – solve for distribution function by method of characteristics

- Conservation form

$$\partial_t f(\mathbf{x},\mathbf{v},t)+\nabla_x[\mathbf{v}f(\mathbf{x},\mathbf{v},t)]+\nabla_v[\mathbf{a}(\mathbf{x},\mathbf{v},t)f(\mathbf{x},\mathbf{v},t)]=0$$

- Advection form

$$\partial_t f(\mathbf{x},\mathbf{v},t)+\mathbf{v}\cdot\nabla_x[f(\mathbf{x},\mathbf{v},t)]+\mathbf{a}(\mathbf{x},\mathbf{v},t)\cdot\nabla_v[f(\mathbf{x},\mathbf{v},t)]=0$$

- Solution:

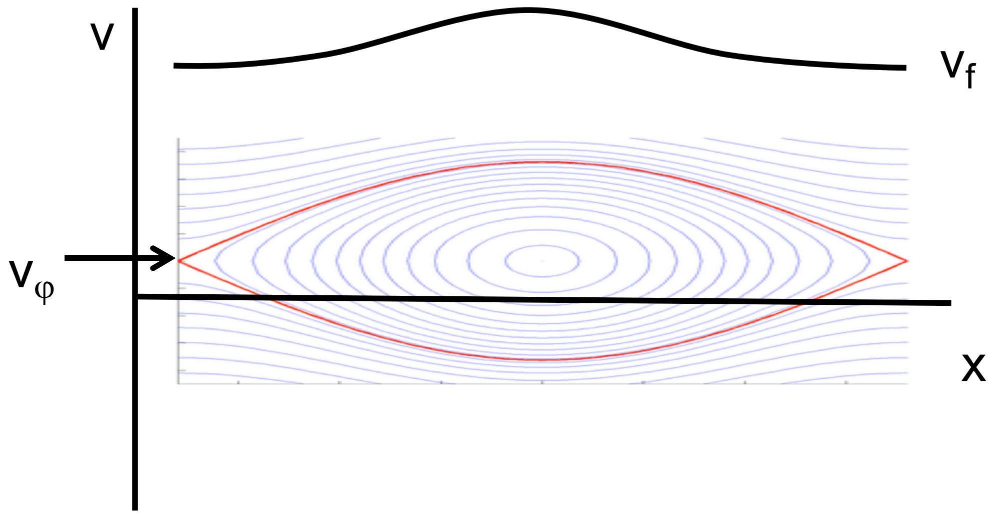
$$f(\mathbf{x},\mathbf{v},t)=\sum_p w_p\delta\left(\mathbf{x}-\mathbf{x}_p(t)\right)\delta\left(\mathbf{v}-\mathbf{v}_p(t)\right)$$

- w_p= particle weight
- x_p, v_p = particle trajectory, satisfying

$$\dot{\mathbf{x}}_p=\mathbf{v}_p \qquad \dot{\mathbf{v}}_p=\mathbf{a}(\mathbf{x}_p,\mathbf{v}_p,t)$$

- Discretize, put on grid, add fields…

Fast electrons are in equilibrium with slow (ion-scale) dynamics



- Resonance moving slowly with respect to particles at some velocity
- Particles at that velocity essentially in equilibrium with the perturbation
- Time derivative can be ignored

SLPIC is based on a simple ansatz

$$f(\mathbf{x},\mathbf{v},t) = \beta(\mathbf{x},\mathbf{v},t)g(\mathbf{x},\mathbf{v},t)$$

$$\partial_t\left[\beta g(\mathbf{x},\mathbf{v},t)\right] + \nabla_x[\beta \mathbf{v} g(\mathbf{x},\mathbf{v},t)] + \nabla_v[\beta \mathbf{a}(\mathbf{x},\mathbf{v},t)g(\mathbf{x},\mathbf{v},t)] = 0$$

$$\partial_t\left[g(\mathbf{x},\mathbf{v},t)\right] + \nabla_x[\beta \mathbf{v} g(\mathbf{x},\mathbf{v},t)] + \nabla_v[\beta \mathbf{a}(\mathbf{x},\mathbf{v},t)g(\mathbf{x},\mathbf{v},t)] = \partial_t\left[(1-\beta)g(\mathbf{x},\mathbf{v},t)\right]$$

- Choose β such that
  - For slow particles, β = 1, so RHS vanishes
  - For fast particles, β ➔0, but RHS unimportant compared with phase space derivatives
  - In both cases, RHS can be neglected

$$\partial_t\left[g(\mathbf{x},\mathbf{v},t)\right] + \nabla_x[\beta \mathbf{v} g(\mathbf{x},\mathbf{v},t)] + \nabla_v[\beta \mathbf{a}(\mathbf{x},\mathbf{v},t)g(\mathbf{x},\mathbf{v},t)] = 0$$

- Distribution evolves as if velocity *and* acceleration reduced for fast particles

Significant freedom in the prefactor

- Choose β such that
  - For slow particles, β = 1 (RHS vanishes)
  - For fast particles, β ➔0, RHS unimportant compared with phase space derivatives

$$\beta(\mathbf{x},\mathbf{v},t)=\frac{v_0}{\sqrt{v_0^2+v^2}} \qquad \beta\mathbf{v}=\frac{\mathbf{v}}{\sqrt{1+\left(v/v_0\right)^2}}$$

- Freedom to pick β to be a function of position
  - Variable grid: refine in plasma sheath, choose smaller β there
  - Increase β in time when faster phenomena appear

SLPIC equations can be solved in same way as original

$$g(\mathbf{x},\mathbf{v},t) = \sum_p w_p \delta\left(\mathbf{x} - \mathbf{x}_p(t)\right)\delta\left(\mathbf{v} - \mathbf{v}_p(t)\right)$$

$$\dot{\mathbf{x}}_p = \beta(\mathbf{x}_p,\mathbf{v}_p,t)\mathbf{v}_p \qquad \dot{\mathbf{v}}_p = \beta(\mathbf{x}_p,\mathbf{v}_p,t)a(\mathbf{x}_p,\mathbf{v}_p,t)$$

- Particle accelerate, move more slowly
- Follow same trajectories
- Transform back to get actual distribution function

$$f(\mathbf{x},\mathbf{v},t) = \beta(\mathbf{x},\mathbf{v},t)\sum_p w_p \delta\left(\mathbf{x} - \mathbf{x}_p(t)\right)\delta\left(\mathbf{v} - \mathbf{v}_p(t)\right)$$

- Slowing down the particles makes them more dense. The prefactor counteracts that.

But, solving with particles not a requirement. Could use continuum methods on the speed limited equation

SLPIC is NOT

- A coordinate transformation (would not change the way particles move through space)
- A delta-f approach (the weight does not vary in time; not separation into two distributions)
- Lowering the speed of light (particles still follow the same trajectories)
- Even necessarily a PIC approach. One could use continuum methods.

SLPIC is simply an ansatz that allows one to treat fast particles as if in equilibrium while treating slow particles exactly

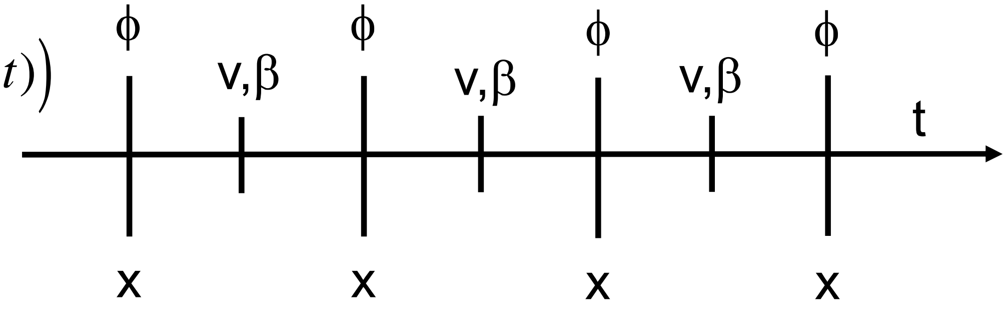
SLPIC fits into the DSMC-PIC cycle (almost – more later)

- Field solve (unchanged)
- Particles
  - Interpolate: same
  - Accelerate: modified acceleration, point-wise implicit algorithms solved by quartic for unmagnetized
  - Move: Just move less by β (could be implicit when β depends on x)
  - Deposit: change from standard pic is the variation of β from one end to other. More on this.
- Collisions are put in at end of particle push (makes this Direct Simulation Monte Carlo – Particle In Cell)

Complication: weight variation causes implicit dependence

$$f(\mathbf{x},\mathbf{v},t) = \beta(\mathbf{x},\mathbf{v},t)\sum_p w_p \delta\left(\mathbf{x}-\mathbf{x}_p(t)\right)\delta\left(\mathbf{v}-\mathbf{v}_p(t)\right)$$

$$W_{rho,p} = \beta_p w_p$$



- Charge weight: β(v), needed for weighting, not known at weighting time
- Not a problem for statics
- Need implicit particle solve for dynamics?
- But standard implicit PIC would require particles to move not much more than a cell, so would not apply without SLPIC

Complication: the “current weight” is constant

$$W_{j,p} = w_p$$

- Current weight is unchanged
- Still gives the rate at which particles cross the surface
- Collisions care about number out/number in (rational number)
- Collisions must take care to conserve the “current weight”
- Same issue with wall interactions, like secondary electron emission

$$\begin{aligned} w_{j,ce} &= \Delta V \frac{w_{j,pi}}{\Delta V} \frac{\beta_n(v_{ni}) w_{j,ni}}{\Delta V} \sigma(\mathbf{v}_{ni} - \mathbf{v}_{pi}) \|\mathbf{v}_{ni} - \mathbf{v}_{pi}\| \beta_e(v_{pe}) \Delta t \\ &= \Delta V \frac{w_{j,pi}}{\Delta V} \frac{w_{j,ni}}{\Delta V} \sigma(\mathbf{v}_{ni} - \mathbf{v}_{pi}) \|\mathbf{v}_{ni} - \mathbf{v}_{pi}\| \beta_n(v_{ni}) \beta_e(v_{pe}) \Delta t \quad (12) \end{aligned}$$

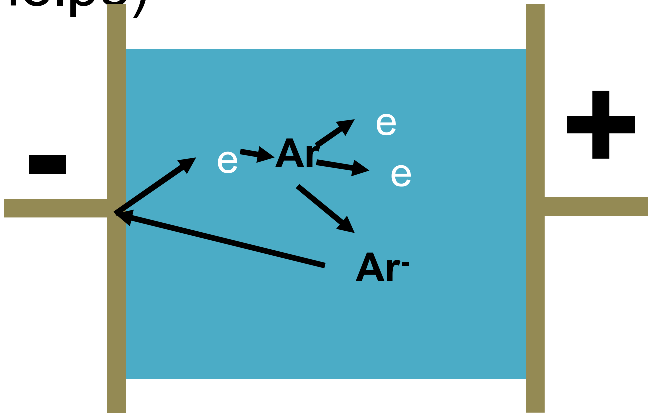
Verification: compare with PIC
Validation: compare with experiment

- Initiate with 0.625A/m^2
- Ionization
- Elastic collisions
- Excitation
- Secondary emission
- Energy gain = voltage
- SEY = 0.07 (Phelps)

$$v_{Ar} = \sqrt{2V/m_{Ar}}$$

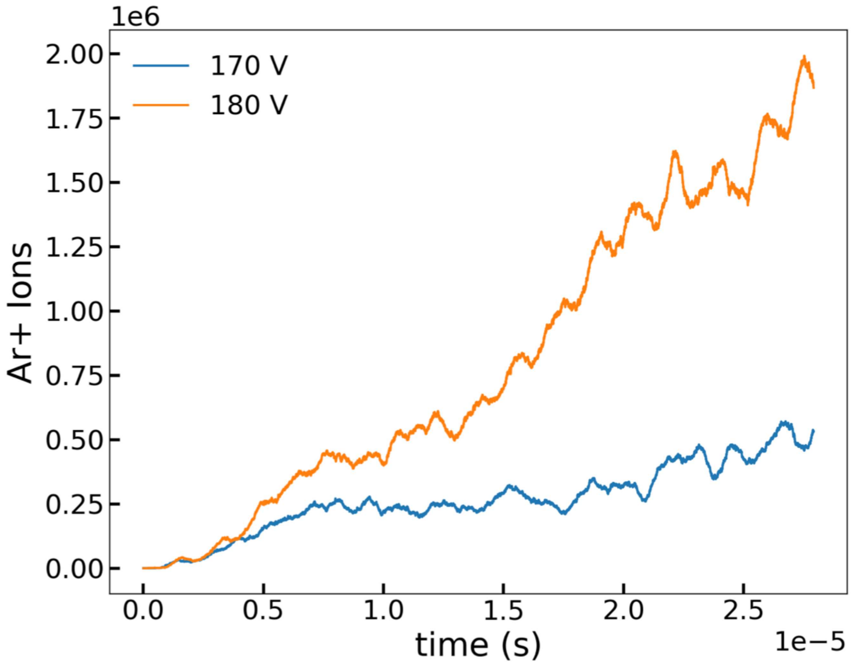
$$v_e = \sqrt{2V/m_e}$$

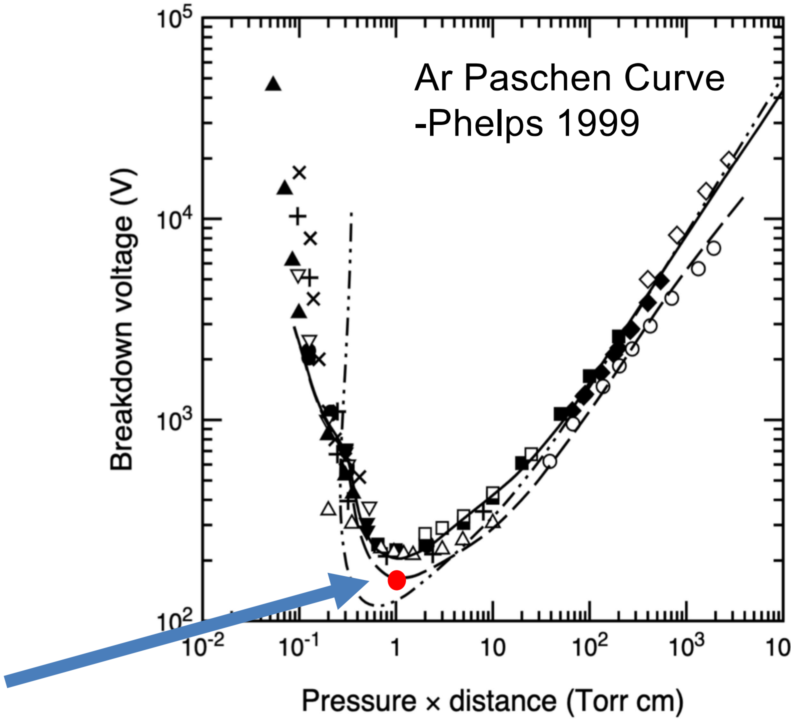
$$\sqrt{\frac{m_{Ar}}{m_e}} = 270$$



- Numerics - spatial
  - DSMC requires resolution of the mean free path
  - 1 Torr, 1 cm gap => 219 cells across gap
- Numerics – temporal
  - Simulate for 10 ion crossing times, look for exponential growth
  - Time step ~ cell size over max electron vel.
  - PIC: 4.7M time steps
  - SLPIC: *17.5k* time steps

Breakdown determined by presence/absence of exponential growth





Ar Paschen Curve
-Phelps 1999

- At 1 Torr breakdown occurs within 175 ± 5 V
- This agrees with experimental data

Computational savings > 100

- SLPIC simulation of (17.6k steps) took 64 cpu minutes
- PIC simulation (4.7M steps) took 8432 cpu minutes
- Speedup of 130x < 270x due to increased complexity of SLPIC
- Performance optimization underway

SLPIC should give big gains in computational speeds when

- $v_0 << v_e$
- Need not resolve electron plasma oscillations
- Especially good for
  - $T_e > T_i$
  - Large mass ions
- Examples
  - plasma sheath
  - free expansion
  - plasma thrusters

Multiple directions for SLPIC

- Applications
- Combine with implicit (energy conserving?)
- Use in continuum codes
- Inclusion of strong magnetic fields ($\omega_e \leq \Omega_e$)
- Collisions
- Spatial variation of β
- Combine with advanced computational devices (GPU, multi-/many core, AVX)

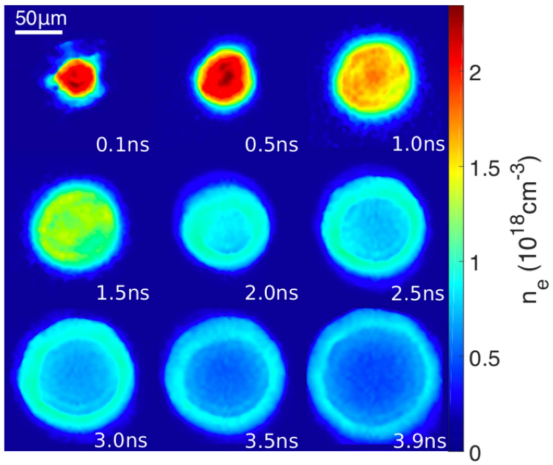
After V&V, time to do some new physics

- Just getting started

What else is going on in Colorado?

Group: long-time collaborator Greg Werner + 5 graduate students

New physics seen in low-density plasma formation (Wolfinger)



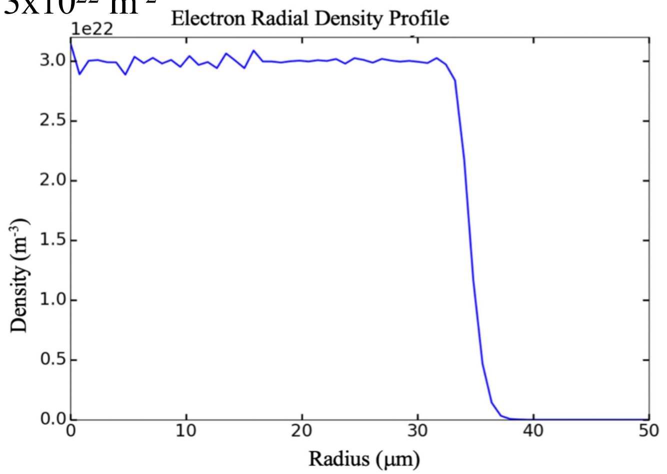
- Often formed by hydrodynamic expansion of plasma columns
- Low density plasmas require a different method

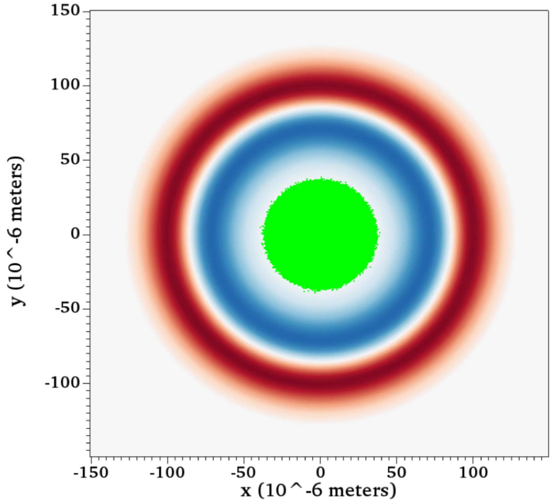
Figure: plasma column expansion and channel formation from Shalloo et al, 2019

Our work so far:

- 2D pic simulations with a single laser pulse
- optical field ionization of neutral gas
- collisions, self-consistent fields included

Figure: density profile created by a laser pulse of intensity 1.3x10^{20} W/m^2 in Hydrogen at 3x10^{22} m^{-2}



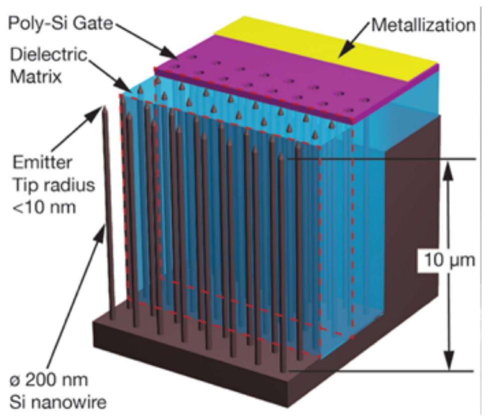


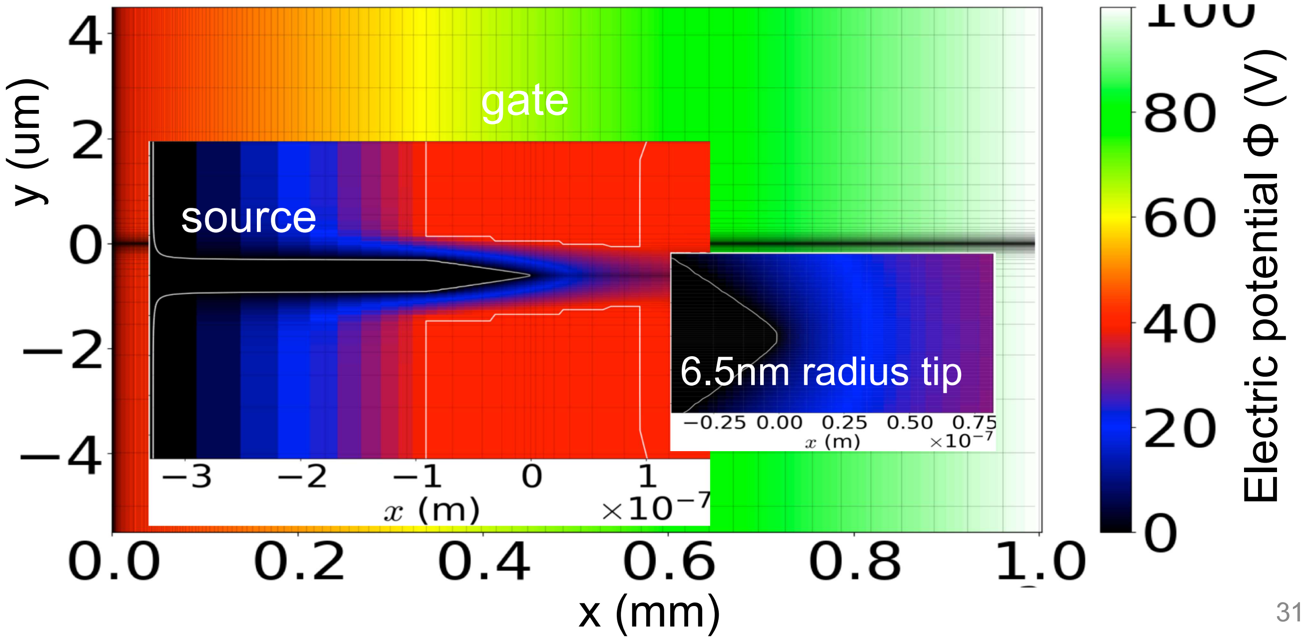
- We observe an EM pulse polarized in the direction of laser propagation
- Potential laser diagnostic
- Time-dependent ponderomotive force

Figure: EM pulse created by a laser of intensity 1.3x10^{20} W/m^2 in Hydrogen at 3x10^{22} m^{-2}. Electrons are in green, positive field in red, negative field in blue.

New modeling methods needed for proposed nanoscale vacuum channel transistors (NVCT) (Snelling)

- Vacuum devices + lithographic techniques
- Rad hard – can't hurt vacuum
- Use field emission (Fowler-Nordheim) from nm tips
- Scale disparity of <10 nm tip to (now) mm distance





The Real Summary

- Today just a taste of what is going on in my University research group
    - New algorithms: SLPIC
    - Predictions of target plasma formation, new physics discoveries
    - Nano-vacuum channel transistors
- And even more at Tech-X: Hypersonics, particle accelerators, plasma formation
- I hope this pandamnic ends at some point so that we can see each other in person