SAND2015-3016C

AN OVERVIEW OF THE MCSWARM MONTE-CARLO AIR CHEMISTRY CODE*

Steve Swanekamp, Steve Richardson,
Justin Angus, and David Mosher[a)]

Plasma Physics Division
Naval Research Laboratory
Washington, DC 20375

K.L. Cartwright, T.D. Pointon, and B.V. Oliver

Sandia National Laboratories
Albuquerque, NM 87123

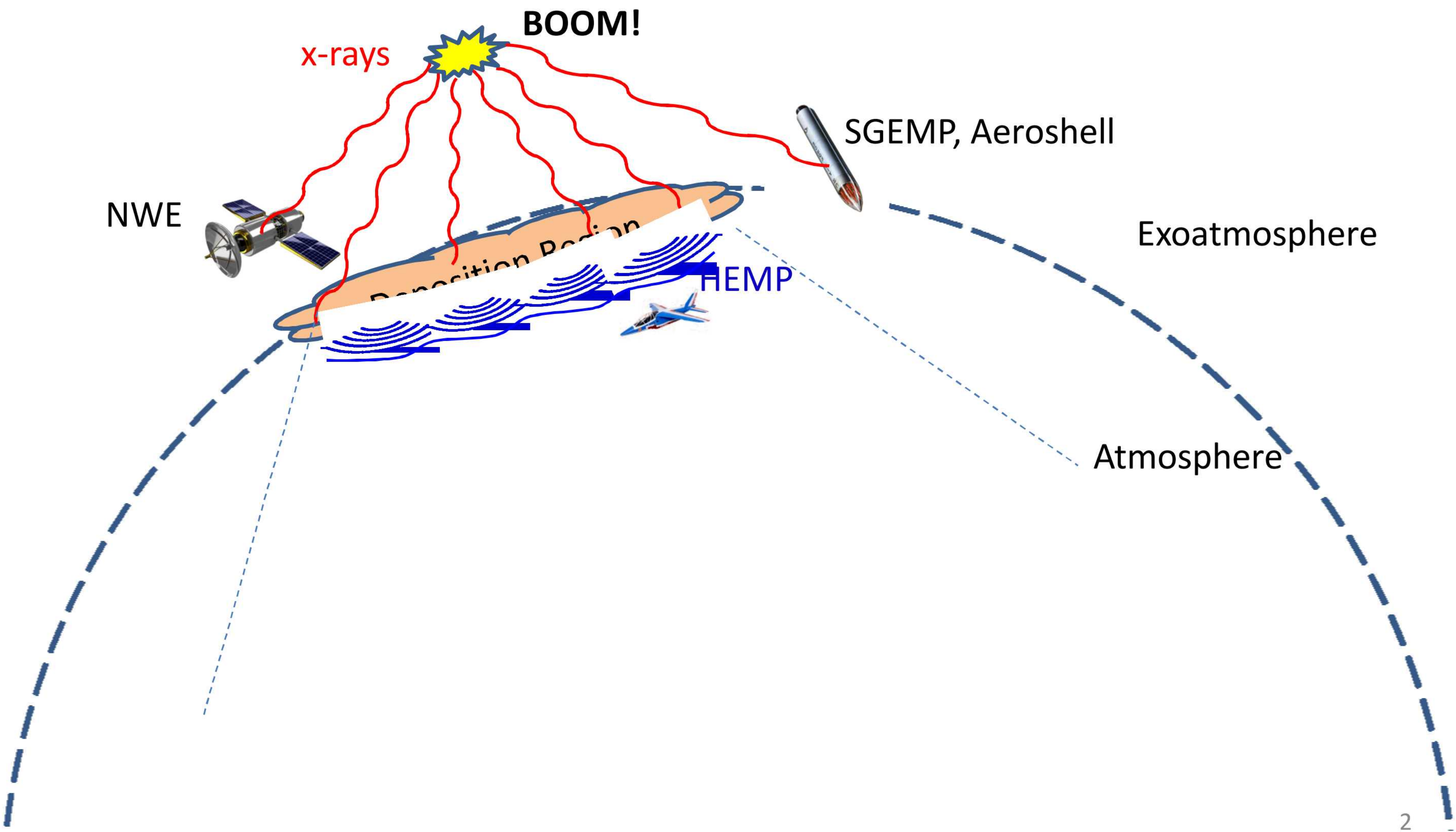
prepared for HEART 2015 Chantilly, VA April 21-24, 2015

*Work supported by Sandia National Laboratories, a multiprogram laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC

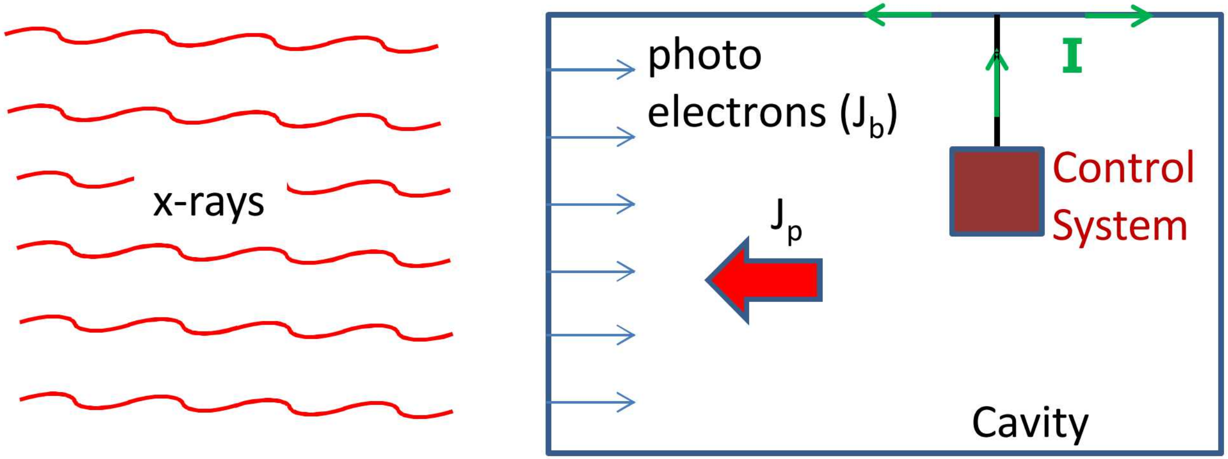
Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

a) An independent consultant through Engility Corp., Chantilly, VA.

X-rays generated from a nuclear detonation drive a number of important effects

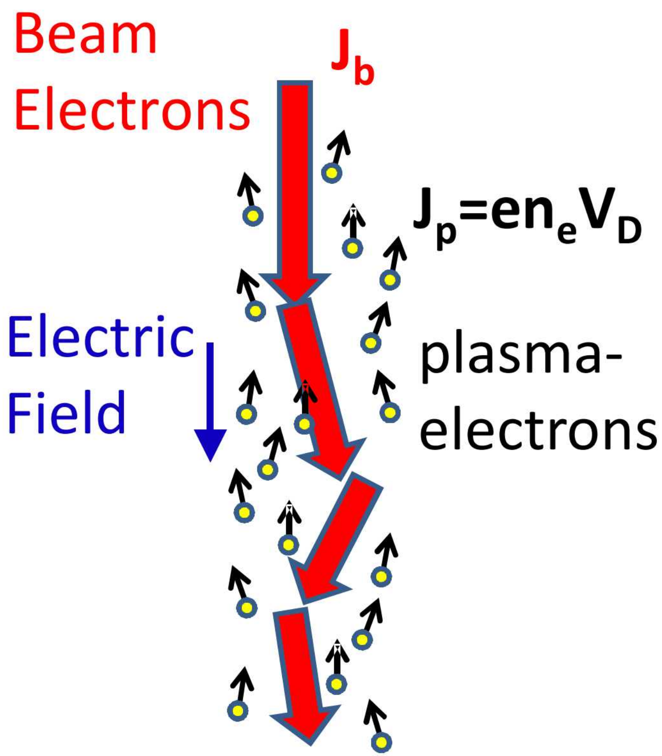


Air chemistry is one of the main focuses for System-Generated EMP



- Gas pressures from p=0 to 1 atm inside the cavity
- Warm x-rays drive off photoelectrons which drive transient currents inside a cavity
- Interaction of a high-energy electron beam with air is key piece of the puzzle
- Photoemission process is also crucial.

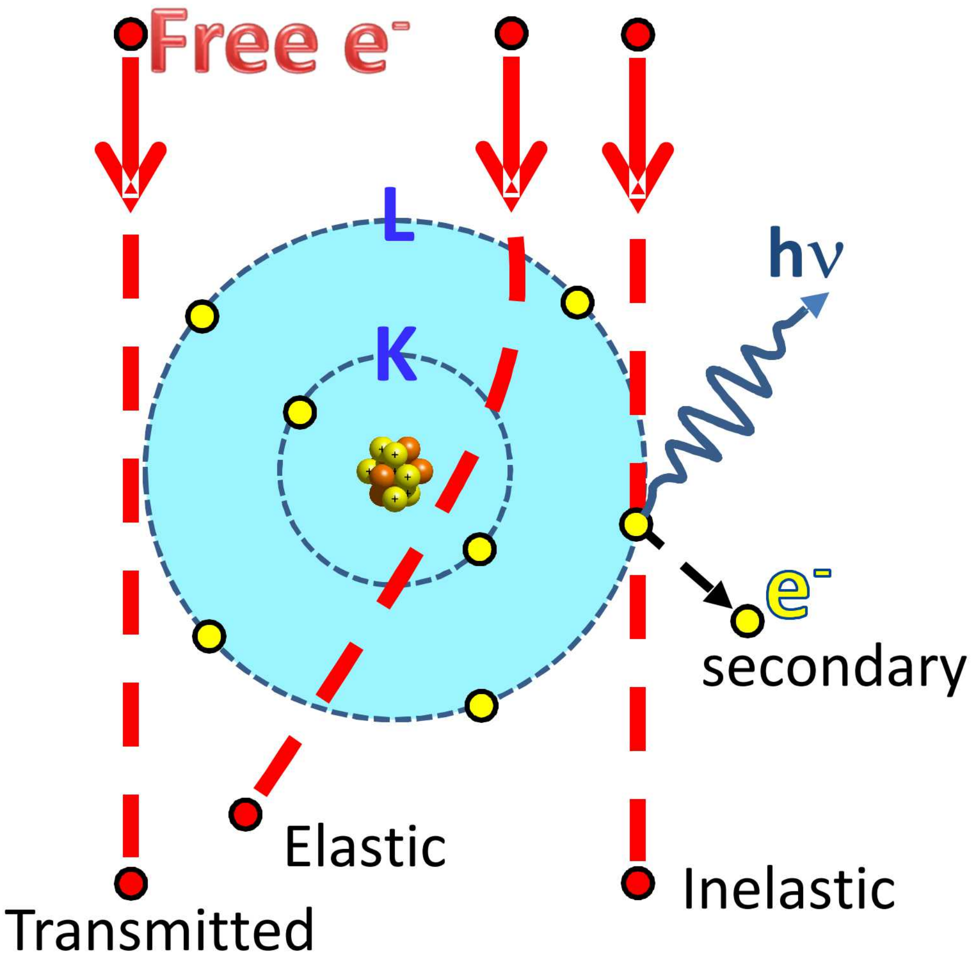
The NRL MCSwarm Monte-Carlo code is developed to self-consistently model air-chemistry and return current



$$J_{net} = J_b - J_p$$

- The size of J_p depends on the how quickly plasma electrons can respond to the rapidly rising electric field
- SGEMP magnitude depends on J_{net}
- Coupling a gas-chemistry model to electromagnetic PIC is a way to model SGEMP
- MCSwarm is being rewritten in a modular class-based style to make it easier to couple with other codes (PIC)
  - Sandia PIC codes EMPHASIS and Quicksilver is first test case

MCSwarm follows electrons in gas on a collision by collision basis



- Collisions are kinetic and nonlocal – important at low pressure
  - all collisions are with unexcited neutral gas
- Elastic collisions
- Inelastic collisions
  - N_2 and O_2 have many rotational and vibrational modes
  - electronic excitations and ionization
  - dissociation

Sandia has funded the development of MCSwarm

- Rewrite MCSwarm in a modular class-based style to make it easier to couple with other codes (PIC)
- Work with SNL and NRL to make MCSwarm open source and available to the weapons effects community
- Use MCSwarm coupled with EMPHASIS to continue model validation with direct e-beam experiments
- Think about how to use direct electron beam injection to complement integrated experiments

Future improvements

- Couple MCSwarm with other PIC codes (ICEPIC, LSP, etc)
- Continue validation effort with ongoing NRL experiments
- Improve MCSwarm algorithm to treat exponential electron density growth without exponential growth in particle number
- Use variance reduction techniques to increase computational efficiency
- Add reverse reactions, superelastic collisions, other processes and electron-electron collisions
- Continue with code validation

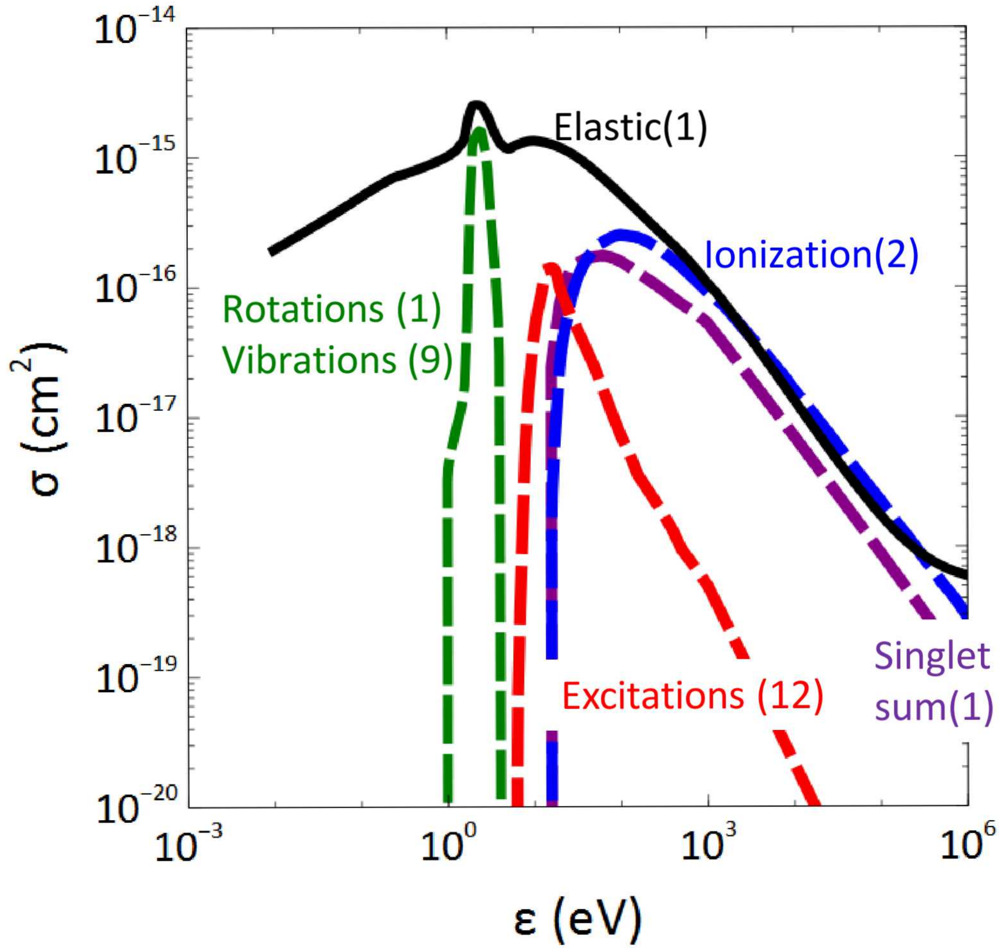
This work builds on a history of beam-gas-interaction studies at NRL

- Ion-focused electron beam transport in atmosphere for SDI in the 1980's
- SNL-supported measurements of ionization by ion beams in 1990's
- DTRA-supported measurements of ionization by electron beams in early 2000's
- AWE-supported studies for paraxial diode development (2004)
- Direct electron-beam injection into gas for gas-chemistry validation (2006-2008)
  - very attractive from cost considerations
  - useful as a test bed for diagnostic development for integrated shots
  - useful surrogate for integrated tests?
- Current AWE-funded program for large-area 1 MeV, 1 kA/cm^2 electron beam to test aeroshells

Cross sections

Neutral N_2 cross sections used in MCSwarm

All these reactions are important for accurate electron-energy distribution function f(ε) (eedf)



Scattering angle is chosen by sampling an approximate form for the differential cross section

- Cross section form is consistent 1-Born approximation with a screened potential

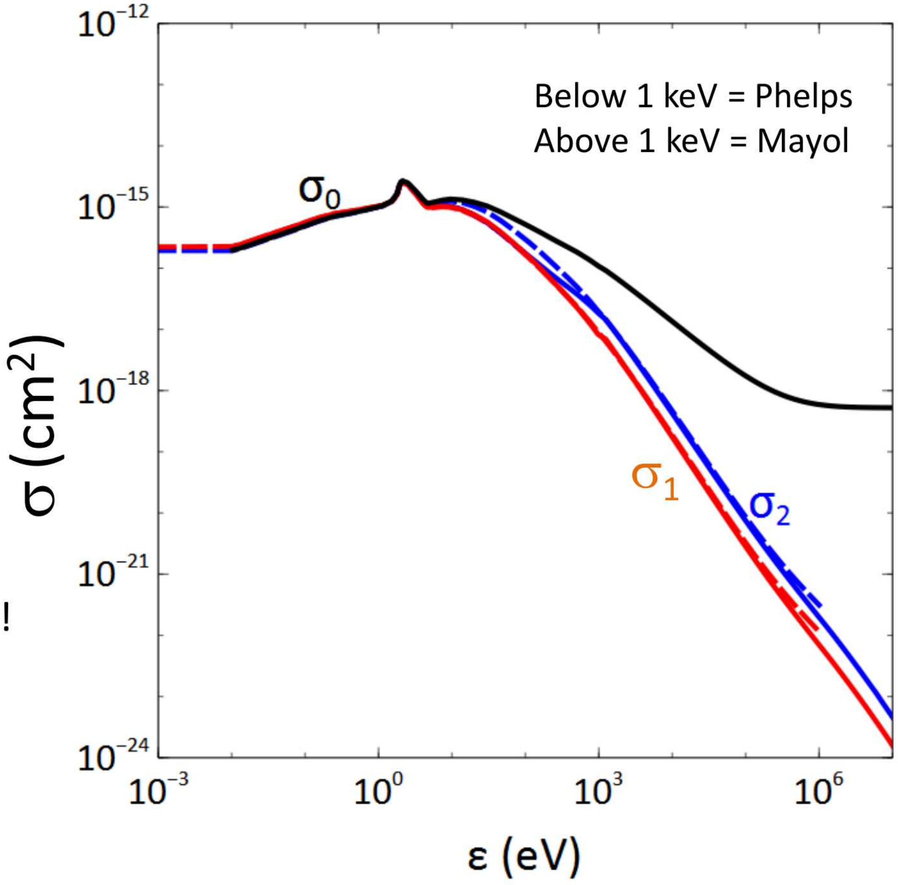
$$\frac{d\sigma}{d\Omega} = \frac{\sigma_0(\varepsilon)}{4\pi} \frac{\left(1-\xi^2\right)}{\left(1-\xi\cos\theta\right)^2}$$

- The screening parameter, ξ, is chosen to match measured momentum transfer cross section

$$\frac{\sigma_1}{\sigma_0} = \int_{-\pi}^{\pi} (1-\cos(\theta)) \left(\frac{1}{\sigma_0} \frac{d\sigma}{d\Omega} \right) 2\pi \sin(\theta) d\theta$$
$$= \frac{(1-\xi)}{2\xi^2} \left[(1+\xi) \ln \frac{1+\xi}{1+\xi} - 2\xi \right]$$

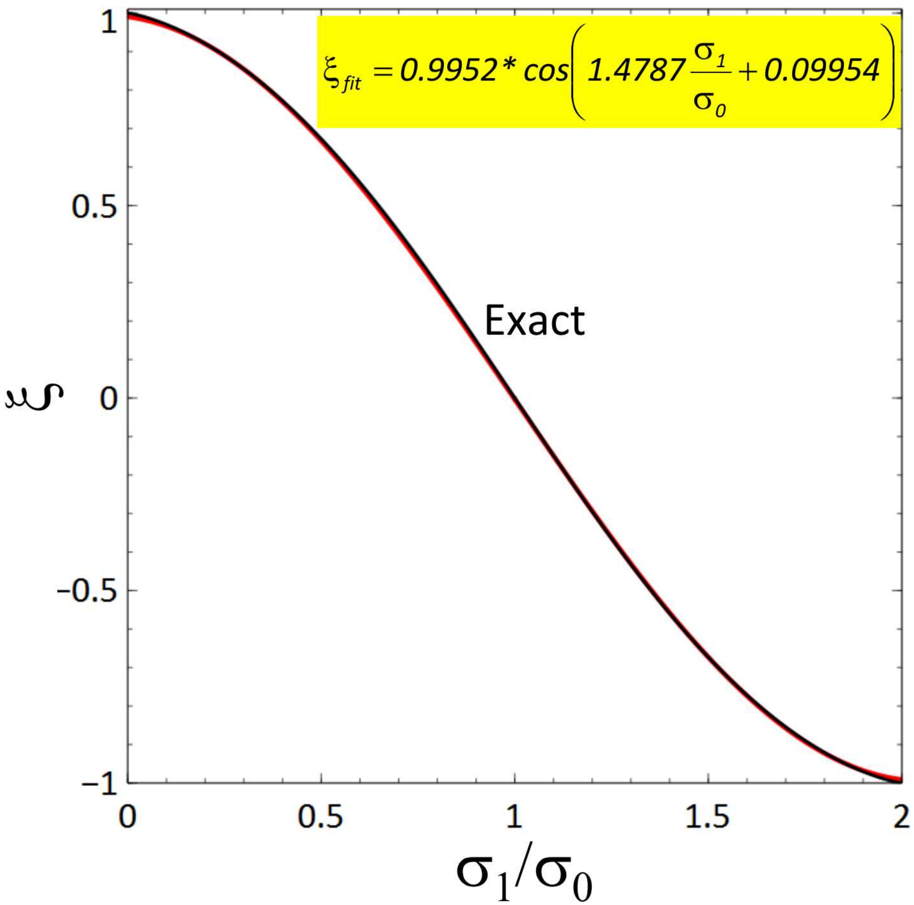
- The chosen form also matches the 2nd moment!

$$\frac{\sigma_2}{\sigma_0} = \int_{-\pi}^{\pi} \left[1 - P_2(\cos\theta)\right] \left(\frac{1}{\sigma_0} \frac{d\sigma}{d\Omega} \right) 2\pi \sin\theta d\theta$$
$$= \frac{3}{4} \frac{\left(1-\xi^2\right)}{\xi^3} \left[2 \ln \frac{1+\xi}{1+\xi} - 4\xi \right]$$



A. Okhrimovskyy, A. Bogaerts, R. Gijbels, Electron anisotropic scattering in gases: a formula for Monte Carlo simulations, Phys. Rev. E 65 (2002) 037402.

The screening parameter can be determined from a simple fit



- The screening parameter $\xi(\varepsilon)$ can be determined for any gas from $\sigma_1(\varepsilon)/\sigma_0(\varepsilon)$
- ξ_{fit} provides a good approximation for ξ and greatly simplifies inversion

$$\xi_{fit} = 0.9952 * \cos(1.4787 * \frac{\sigma_1}{\sigma_0} + 0.09554)$$

MCSwarm Algorithm

Collisions are modeled as a Poisson process

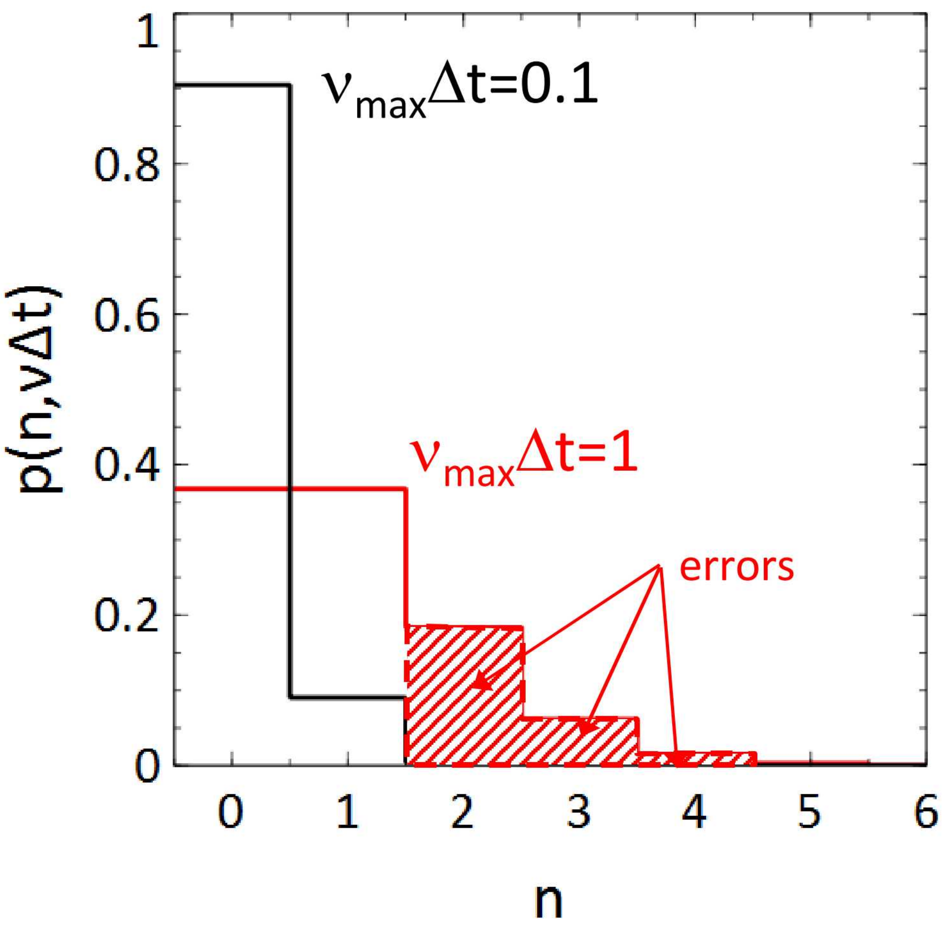
- Independent increments (the number of collisions in different time intervals are independent of each other)
- Stationary increments (the probability distribution of the number of occurrences counted in any time interval only depends on the length of the interval)
- The collision probability is given by Poisson distribution

$$P(n, \nu\Delta t) = e^{-\nu\Delta t}(\nu\Delta t)^n/n!$$

- No counted occurrences are simultaneous.

MCSwarm assumes no more than one collision in Δt

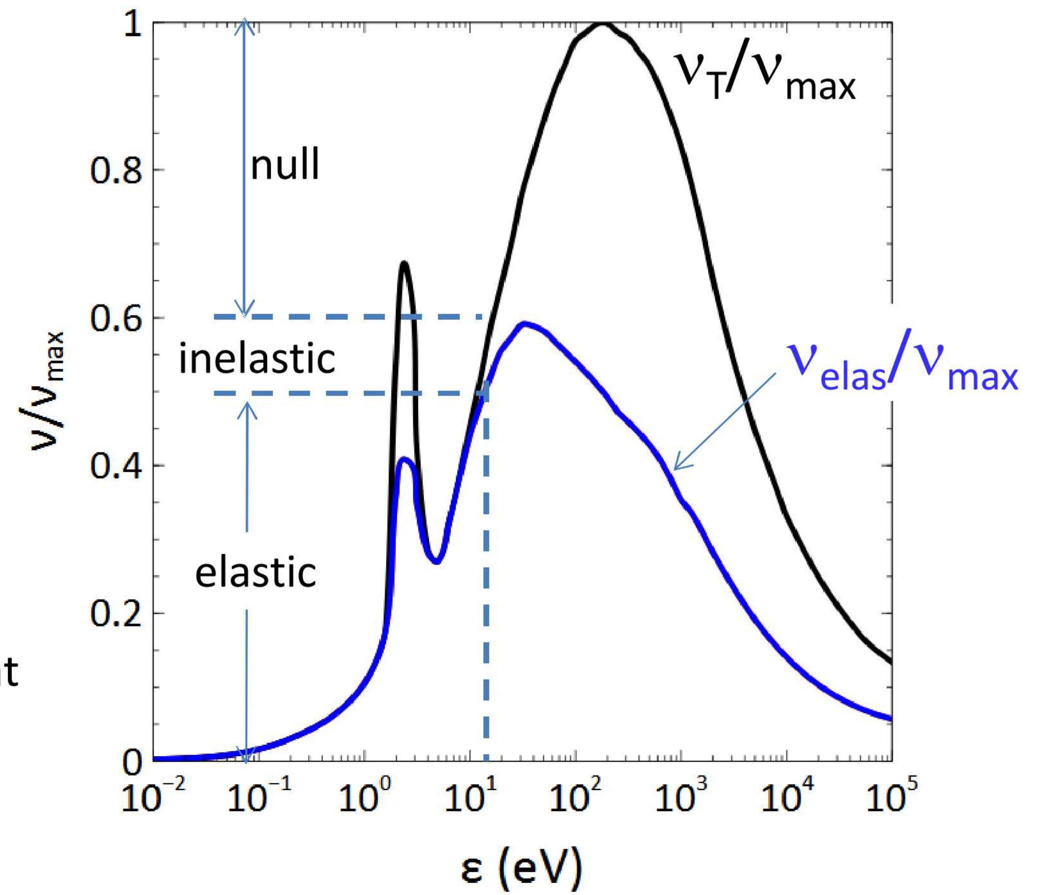
- $\nu_{max} = \max(\nu(E))$
- Errors occur if more than one collision occurs in Δt
- Errors are minimized by choosing $\nu_{max}\Delta t \leq 0.1$ (error < 0.5%)
- Collisions are applied if $[1-P(0,\nu_{max}\Delta t)] < R$ (R=random(0,1])



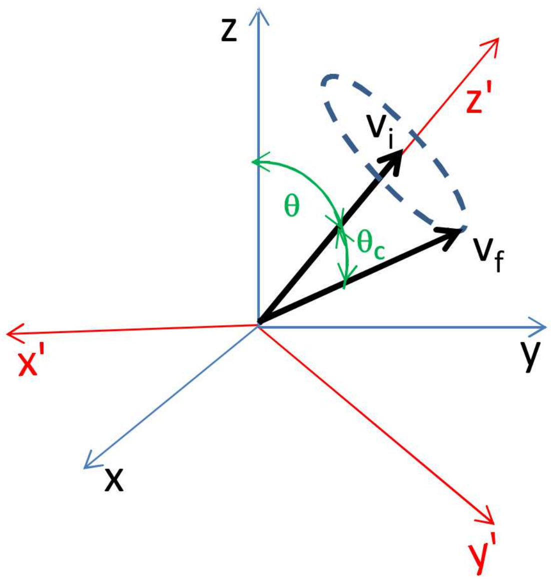
The null-collision method simplifies the collision algorithm

- A null collision is introduced to make collision frequency independent of energy
- Collision type is chosen by random number R

$\nu_T/\nu_{max} < R < 1$	null event
$\nu_{elas}/\nu_{max} < R < \nu_T/\nu_{max}$	inelastic event
$0 < R < \nu_{elas}/\nu_{max}$	elastic event



Kinematics of the collision process



$$v_f = \underline{\underline{R}}^{-1}\underline{\underline{C}}\,\underline{\underline{R}} \cdot \overrightarrow{v_i}$$

- Rotate coordinate system so that z-axis of the new coordinate system is aligned with particle velocity

$$\overrightarrow{v_i'} = \underline{\underline{R}} \cdot \overrightarrow{v_i} = \begin{bmatrix} \cos\theta\cos\phi & \cos\theta\sin\phi & -\sin\theta \\ -\sin\phi & \cos\phi & 0 \\ \sin\theta\cos\phi & \sin\theta\sin\phi & \cos\theta \end{bmatrix} \cdot \overrightarrow{v_i}$$

- Sample differential cross section to get scattered angle θ_c and rotate *v'* according to

$$\overrightarrow{v_f'} = \underline{\underline{C}} \cdot \overrightarrow{v_i'} = \begin{bmatrix} \cos\theta_c\cos\phi_c & -\sin\phi_c & \sin\theta_c\cos\phi_c \\ \cos\theta_c\sin\phi_c & \cos\phi_c & \sin\theta_c\sin\phi_c \\ -\sin\theta_c & 0 & \cos\theta_c \end{bmatrix} \cdot \overrightarrow{v_i'}$$

- Rotate back into lab frame ($R^{-1}=R^T$)

$$v_f = \underline{\underline{R}}^{-1}\overrightarrow{v_f'}$$

Energy loss during collisions

- Elastic collisions with molecules of mass M at rest

$$\varepsilon_f = \varepsilon_i \left(1 - \frac{2m}{M} (1 - \cos\theta_c) \right)$$

- Inelastic collisions with bound electrons with threshold energy ε^*

$$\varepsilon_f = \varepsilon_i - \varepsilon^*$$

- Energy is shared between primary (ε_i) and secondary electron (ε_{sec}) in ionizing collisions†

$$\varepsilon_f = \varepsilon_i - \varepsilon_{ion} - \varepsilon_{sec}$$

$$\varepsilon_{sec} = B \tan\left\{ R \left[a\tan\left(\frac{\varepsilon_i - \varepsilon^*}{B} \right) \right] \right\}$$

(B=15.6 eV for N_2 and 12.2 for O_2 and R is a random number between 0 and 1)

†C.B. Opal, W.K. Peterson, E.C. Beaty, *Measurements of secondary-electron spectra produced by electron impact ionization of a number of simple gases*, J. Chem. Phys. 55 (8) (1971) 4100–4106.

Between collisions, particles move in electric and magnetic fields

$$\frac{d\vec{p}}{dt} = -e\left(\vec{E} + \frac{\vec{p}\times\vec{B}}{\gamma mc}\right)$$

- The Lorentz force equation is updated with a second-order Boris pusher

$$\frac{\vec{p}_{n+\frac{1}{2}} - \vec{p}_{n-\frac{1}{2}}}{\Delta t} = -e\left(\vec{E} + \frac{\vec{p}_{n+\frac{1}{2}} + \vec{p}_{n-\frac{1}{2}}}{2\gamma_n mc}\times\vec{B}\right)$$

Define $\vec{p}^{+}$ *and* $\vec{p}^{-}$ *by*

$$\vec{p}^{+} = \vec{p}_{n+\frac{1}{2}} - e\vec{E}\Delta t/2\ ,\quad \vec{p}^{-} = \vec{p}_{n-\frac{1}{2}} + e\vec{E}\Delta t/2$$

$$\vec{p}^{+} - \vec{p}^{-} = (\vec{p}^{+} + \vec{p}^{-})\times e\vec{B}\Delta t/2\gamma_n mc$$

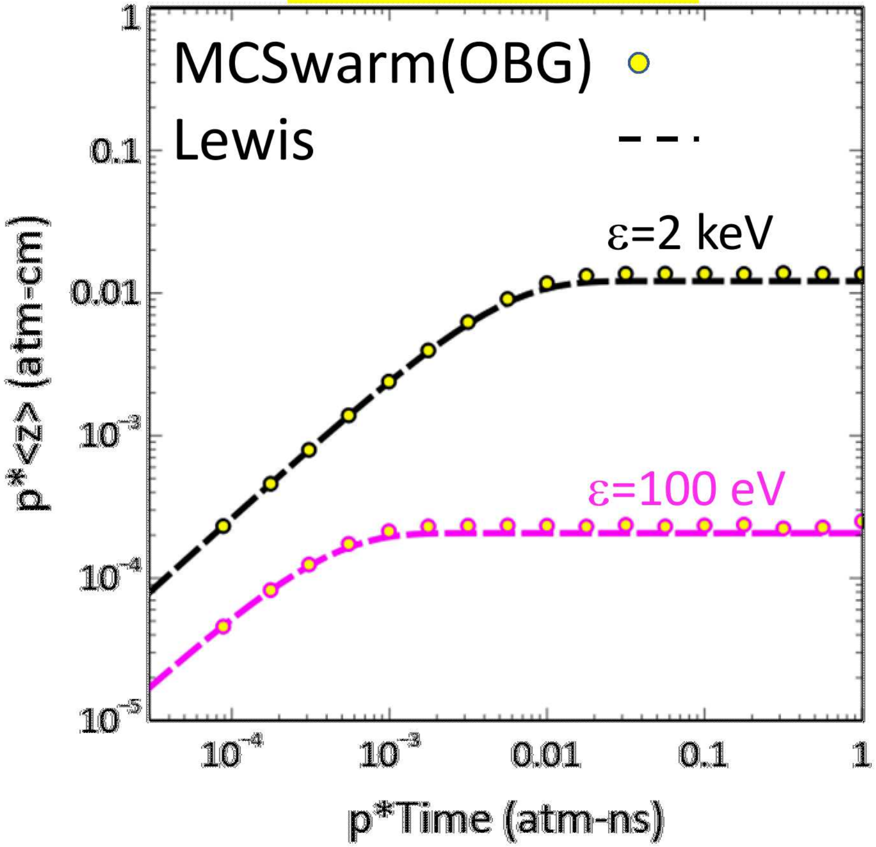
The solution can be written as

$$\vec{p}^{+} = \vec{p}^{-} + \vec{p}'\times\vec{s}\ \ \text{with}\ \ \vec{p}' = \vec{p}^{-} + \vec{p}^{-}\times\vec{b}\ ,\ \vec{b} = \frac{e\vec{B}\Delta t}{2\gamma_n mc},\ \vec{s} = \frac{2\vec{b}}{(1+b^{2})}$$

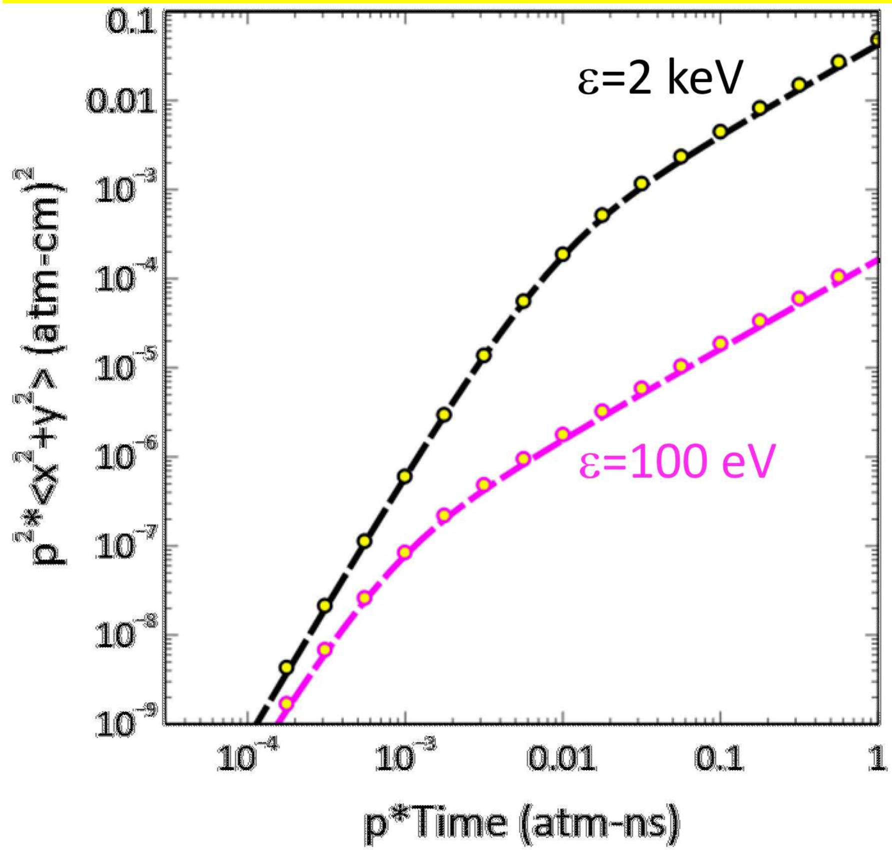
Verification of MCSwarm algorithms

MCSwarm reproduces the exact solutions of Lewis for elastic scattering

$$\langle z \rangle = \frac{(1 - e^{-vt/(N\sigma_1)})}{N\sigma_1}$$



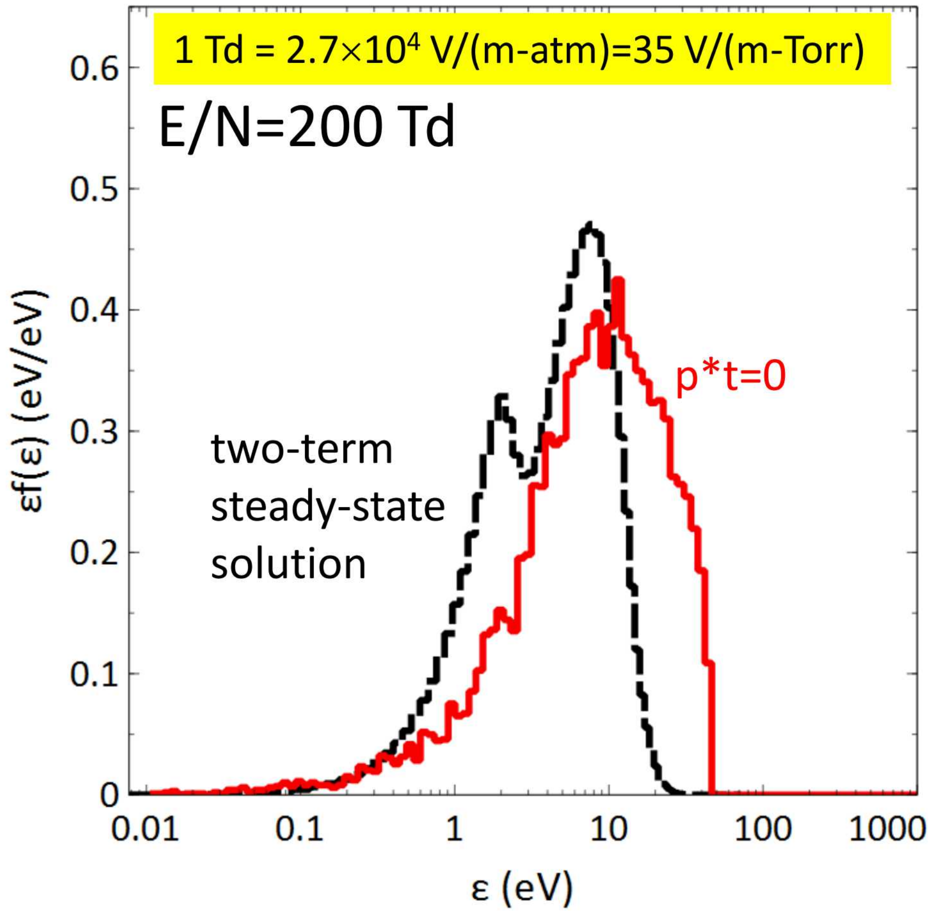
$$\langle x^2 + y^2 \rangle = \frac{4}{3}\int_0^{vt} d\xi (1 - e^{-\xi/(N\sigma_1)}) \int_0^{\xi} du (1 - e^{-u/(N\sigma_2)}) e^{u/(N\sigma_1)}$$



* H. W. Lewis, *Multiple scattering in an infinite medium*, Phys. Rev. **78** (1950), 529.

The time-dependent eedf approaches the 2-term steady state solution

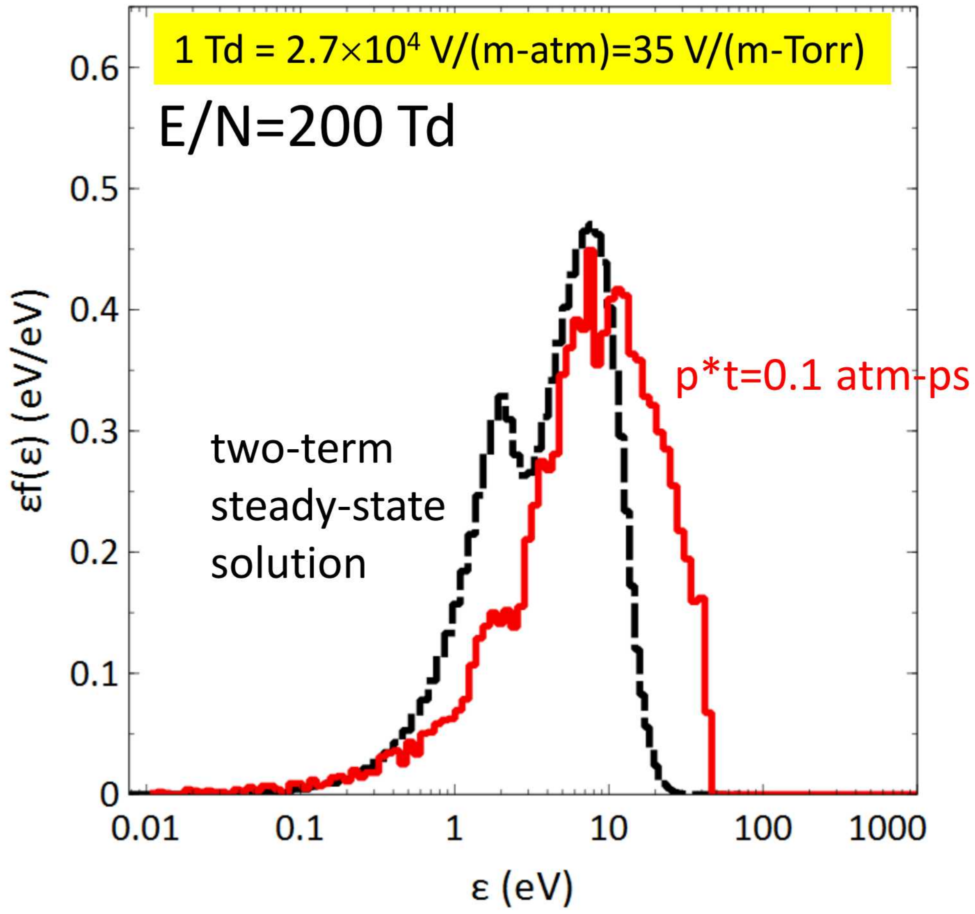
- Initial condition is the distribution of secondaries created by 100 eV beam of electrons
- The time-dependent eedf provides the time-dependent transport coefficients



The time-dependent eedf approaches the 2-term steady state solution

- Initial condition is the distribution of secondaries created by 100 eV beam of electrons

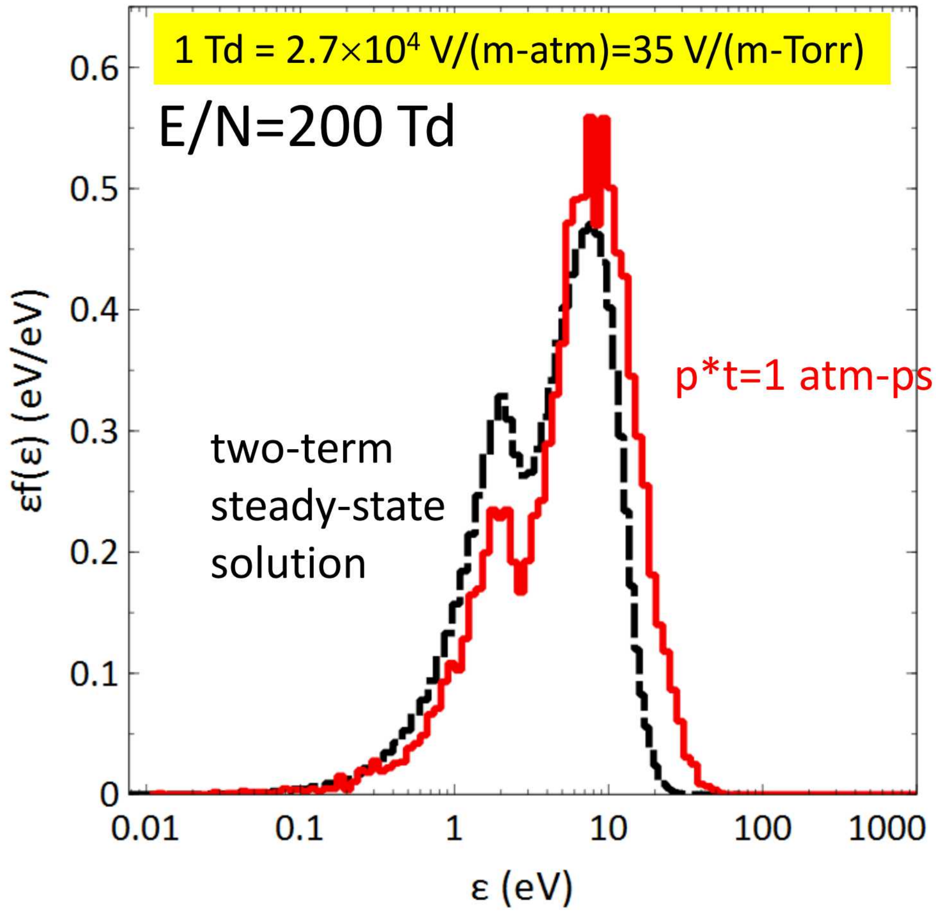
- The time-dependent eedf provides the time-dependent transport coefficients



The time-dependent eedf approaches the 2-term steady state solution

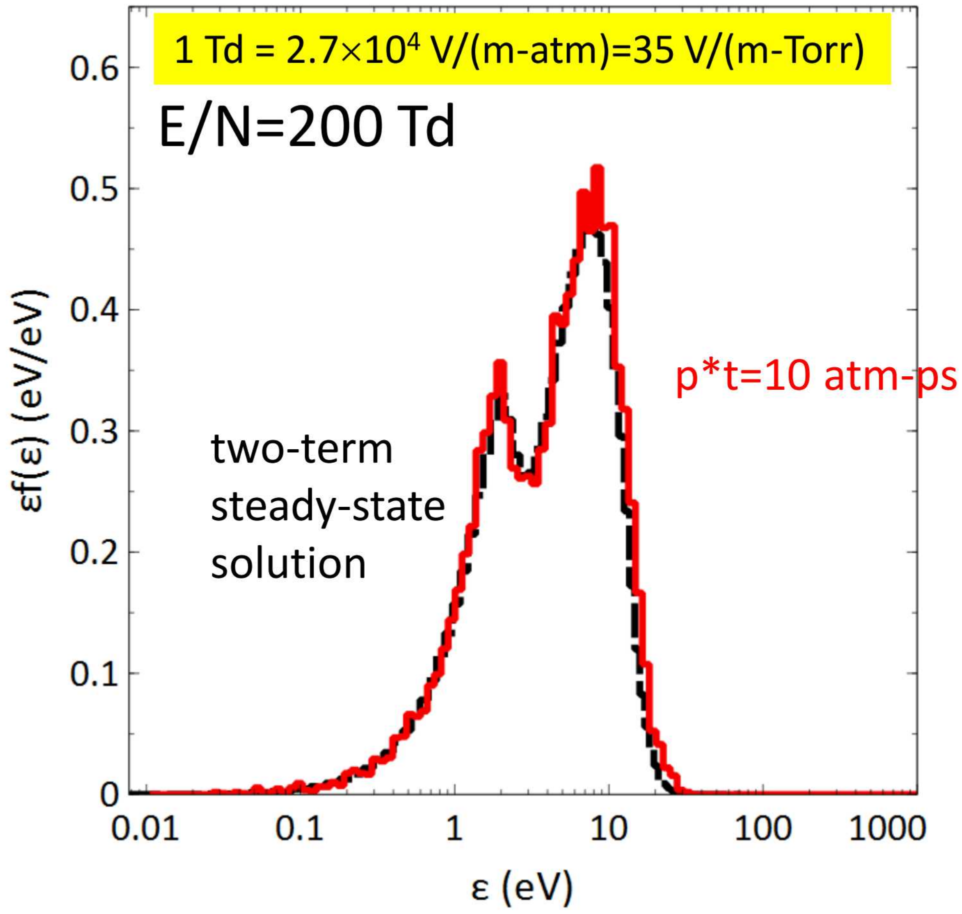
- Initial condition is the distribution of secondaries created by 100 eV beam of electrons

- The time-dependent eedf provides the time-dependent transport coefficients



The time-dependent eedf approaches the 2-term steady state solution

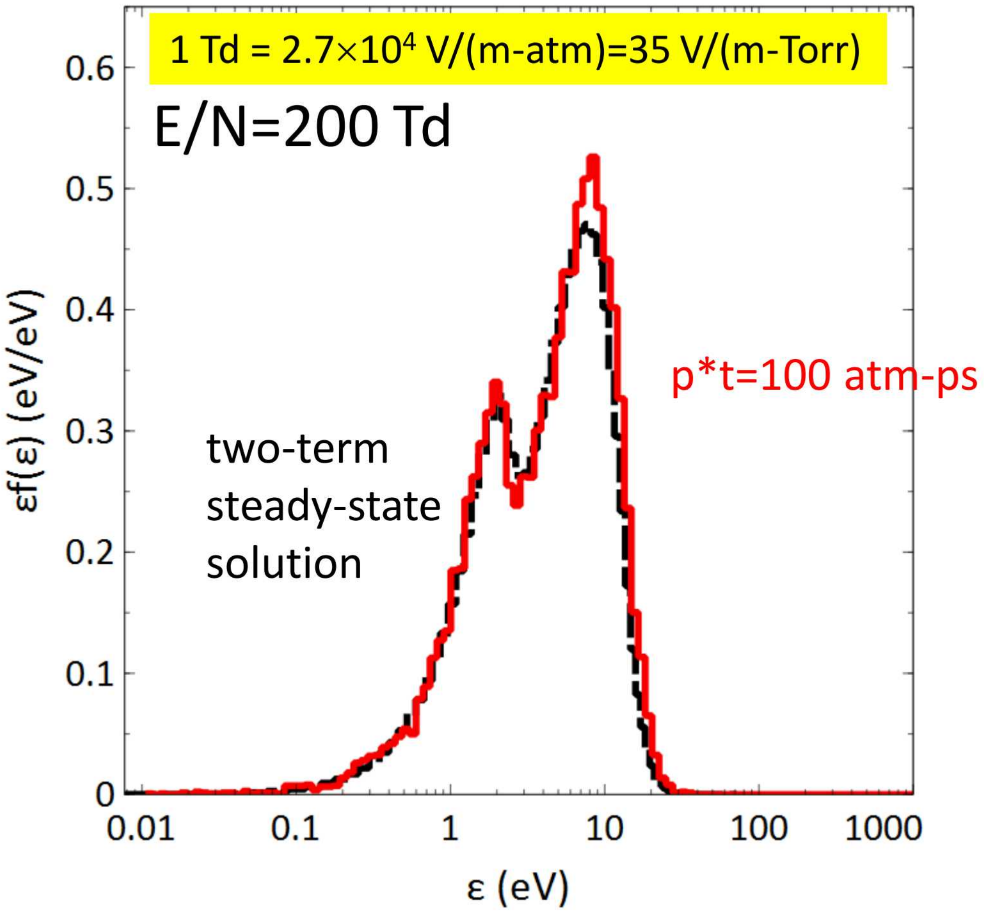
- Initial condition is the distribution of secondaries created by 100 eV beam of electrons
- The time-dependent eedf provides the time-dependent transport coefficients



The time-dependent eedf approaches the 2-term steady state solution

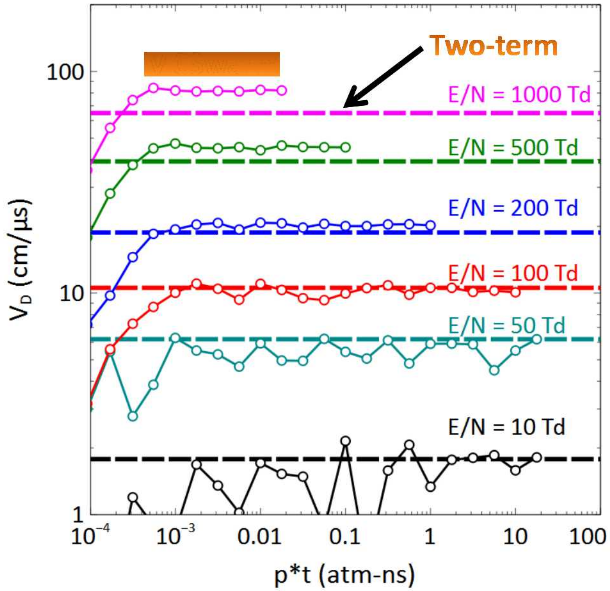
- Initial condition is the distribution of secondaries created by 100 eV beam of electrons

- The time-dependent eedf provides the time-dependent transport coefficients

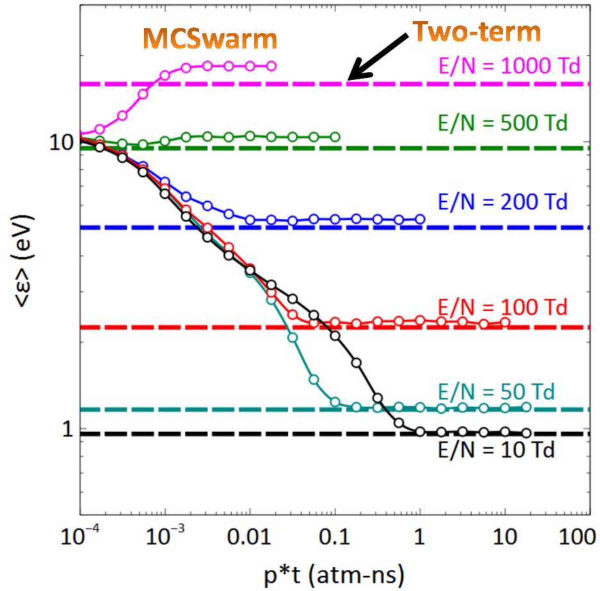


MCSwarm moments are in good agreement with two-term solution for low values of E/N~~gas~~

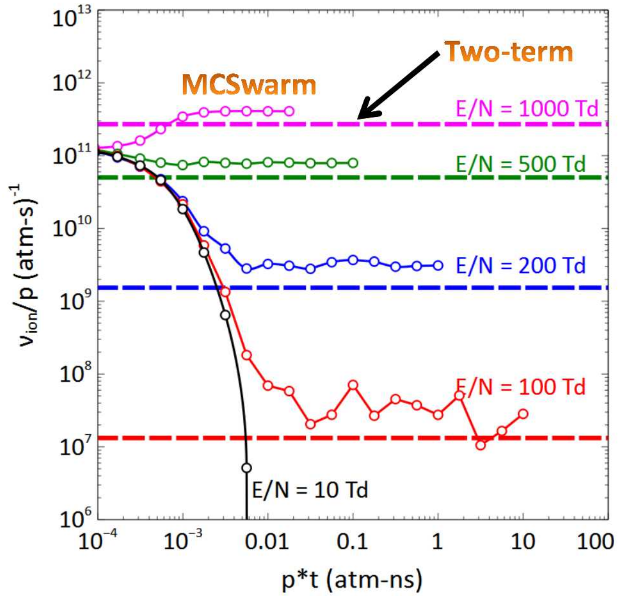
Drift velocity along E-field



Average energy



Ionization rate

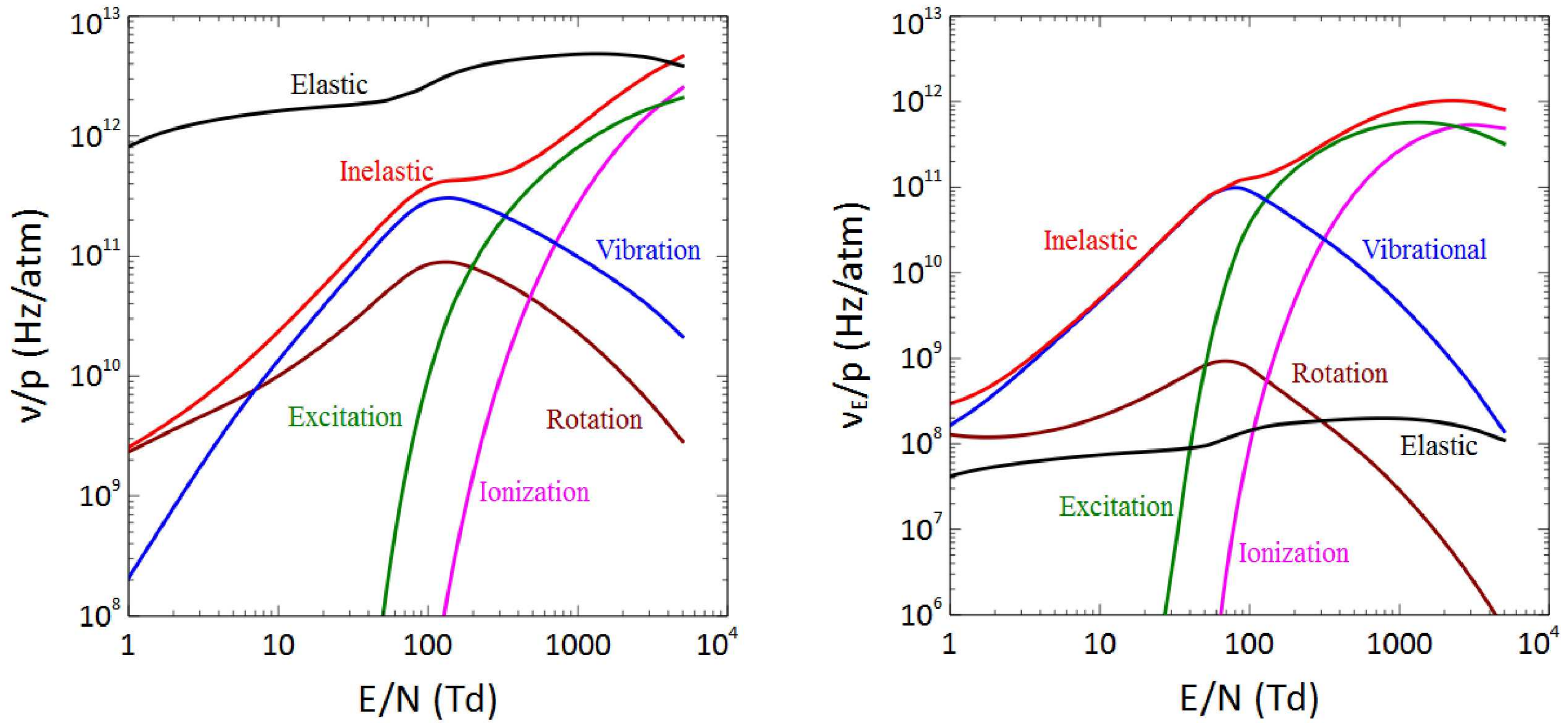


- MCSwarm more accurate than two-term code because it includes the effects of higher-order terms
- Velocity along E-field equilibrates quickly while average energy and energy-dependent ionization rate take longer

*Two-term solutions from Bolsig+ is downloadable from http://www.bolsig.laplace.univ-tlse.fr/download.php

Elastic collisions dominate momentum transfer while inelastic collisions dominate energy loss

Collision frequencies (left) and energy equilibration rates (right) averaged over the eedf



- Large gains in computational speed could be achieved if elastic collisions could be sampled less frequently

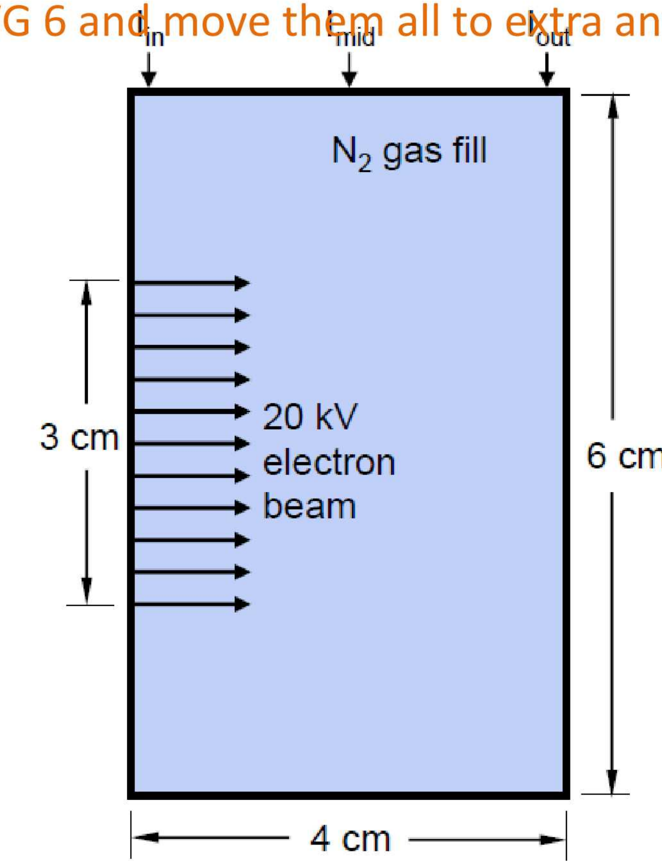
(From T.D. Pointon, 2014 Gaseous electronics conf.)

A test problem illustrates some basic features of cavity SGEMP

Is MCSwarm used for these computations?
How can you tell its doing a good job?
Otherwise, why not move all to extras.
If MCSwarm was used, give Pointon a bullet on VG 6 and move them all to extra anyway.

- 2D, N_2-filled box
  - Gap in x: d = 4 cm
  - Width in y: w = 6 cm, w_{emit} = 3 cm
- W_0 = 20 kV mono-energetic beam
  - emitted normal to box wall
- Space-charge limited current for these parameters: $J_{sl} \cong 1.9$ A/cm^2
  - $J_{sl} \cong \frac{4\varepsilon_0}{9}\left(\frac{2e}{m_e}\right)^{1/2}\frac{W_0^{3/2}}{(d/2)^2}\left(1+\frac{d}{2\pi w_{emit}}\right)$
- Actually inject 10 A/cm^2 ~ $5J_{sl}$
- Current diagnostics
  - I_{in}, I_{mid}, I_{out} B-dots at y-max wall
  - I_e current into the x-max wall

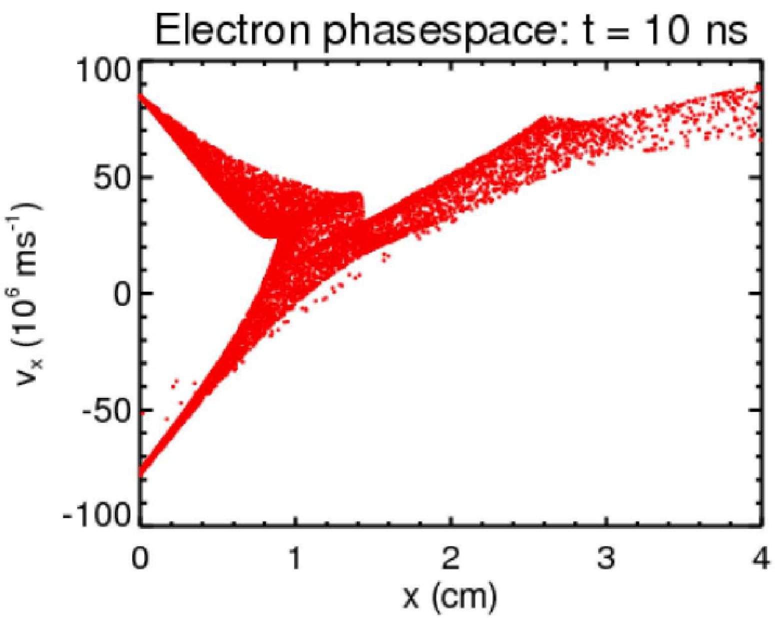
Problem Geometry

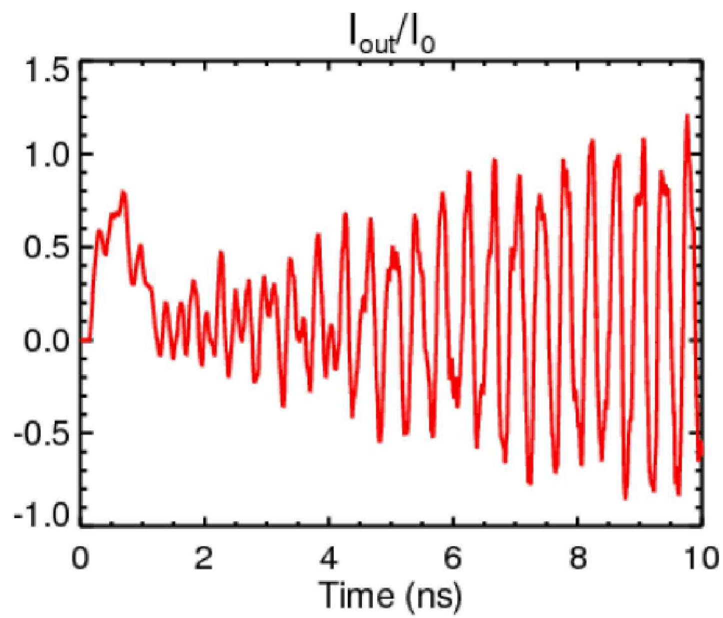


Sandia National Laboratories

(From T.D. Pointon, 2014 Gaseous electronics conf.)

In vacuum, there are virtual cathode oscillations of the beam



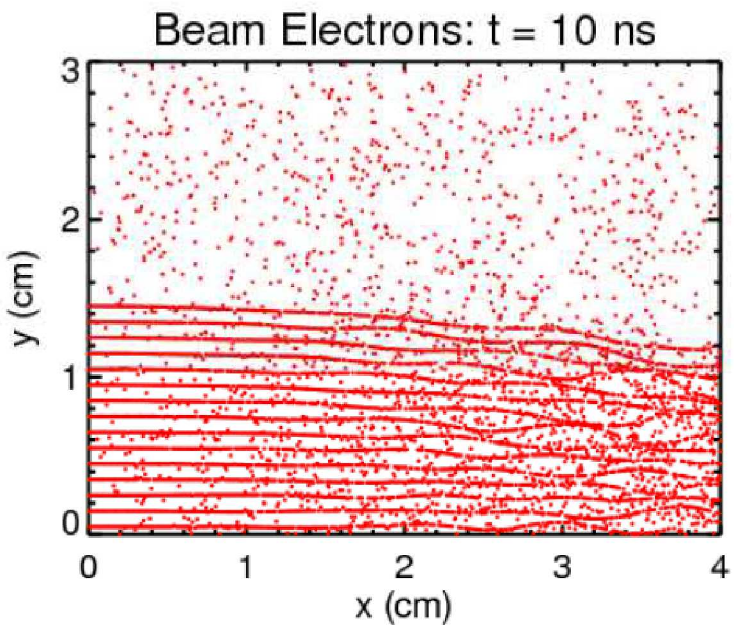


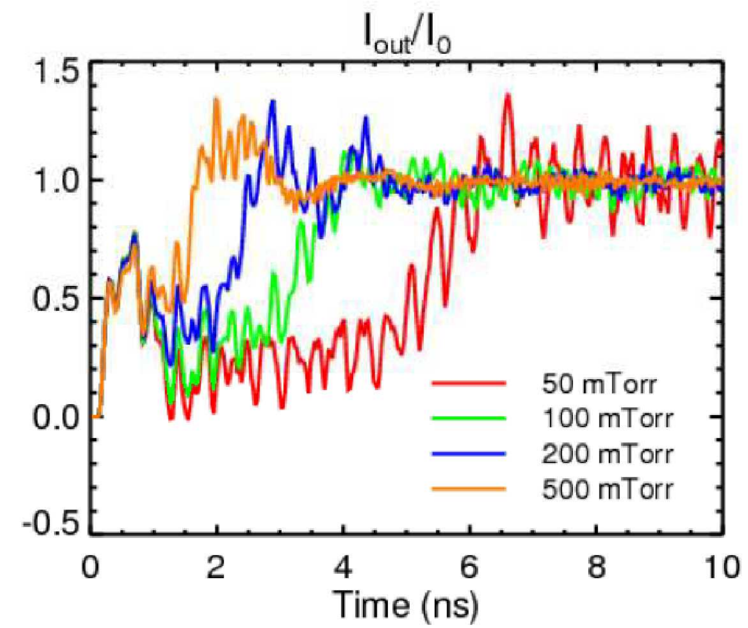
- No steady-state solution: way above the space-charge limit
  - Primary oscillation frequency is 2.5 GHz (nominal transit time = 0.49 ns)
- About 10% of the emitted current is transmitted across the gap

Sandia National Laboratories

(From T.D. Pointon, 2014 Gaseous electronics conf.)

The transmitted beam current increases with pressure up to P ~ 1 Torr



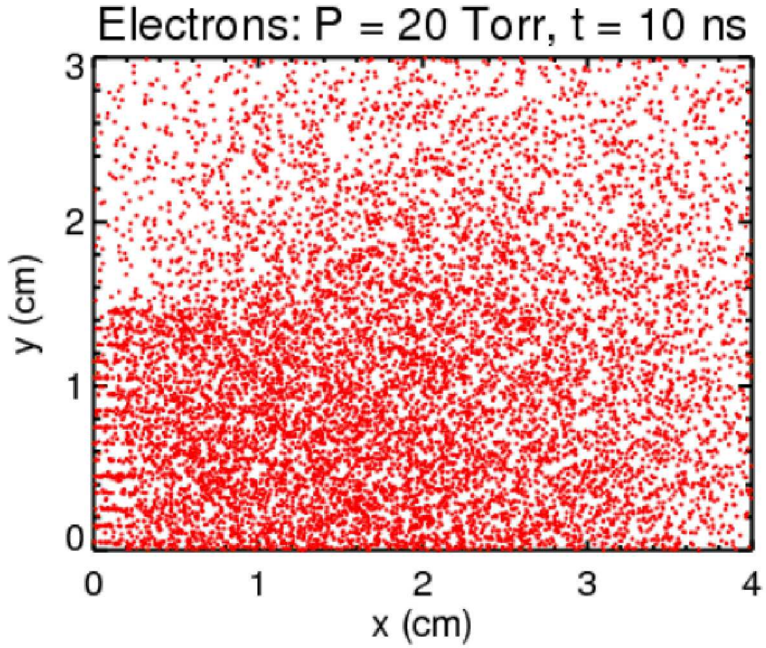


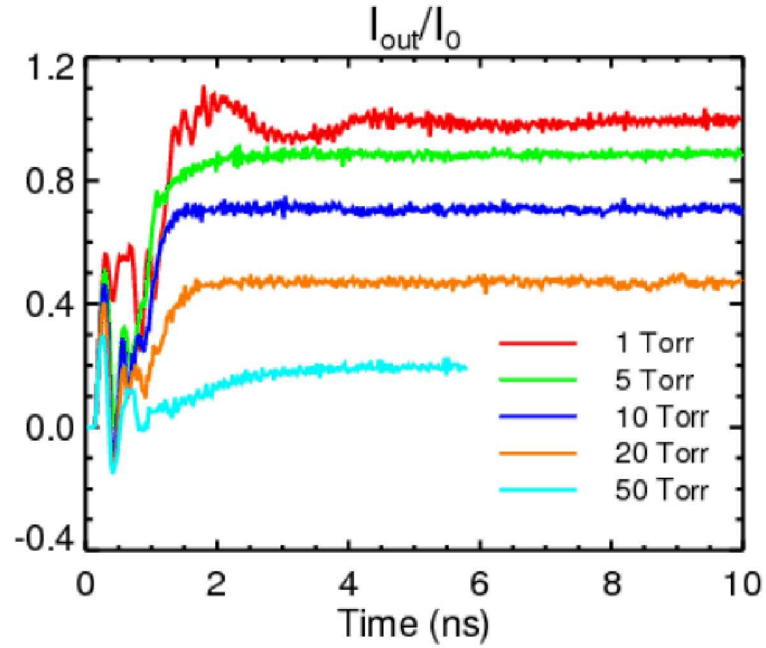
- As the pressure increases:
  - Time required to build up a space-charge neutralizing plasma decreases
  - Amplitude of virtual cathode oscillations decrease
- Small fraction of the electrons are scattered to $y = y_{max}$ wall

Sandia National Laboratories

(From T.D. Pointon, 2014 Gaseous electronics conf.)

The transmitted beam current decreases with pressure above P ~ 1 Torr





- Scattering of the beam electrons now dominates
  - An increasing fraction of the electrons hit the $y = y_{max}$ wall

Sandia National Laboratories

Experiments and code validation

Today's x-ray simulators do not produce the correct x-ray environment

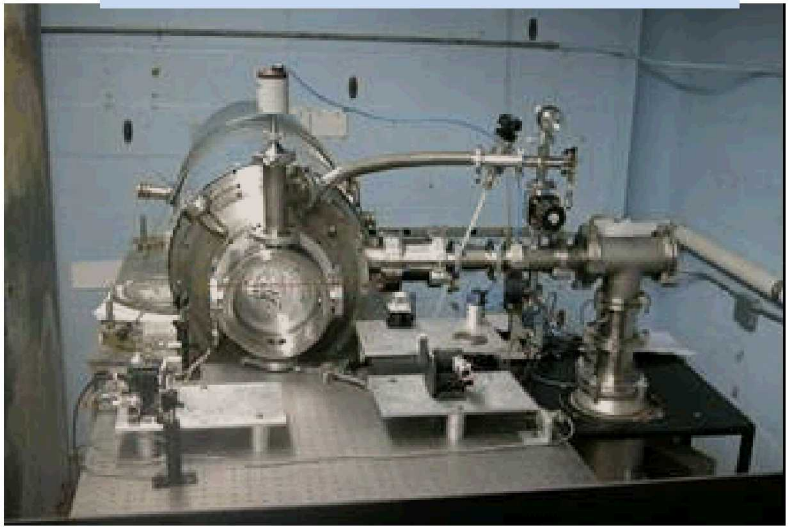
- Z and NIF are powerful x-ray sources but produce a maximum of 13 keV photons (i.e. the spectrum is too soft)
- Bremsstrahlung sources such as the high-fidelity reflex triode produce the right energy photons but fluences are several orders of magnitude below threat levels
- Investments in x-ray simulator R&D is continuing to improve simulator fidelity but that progress will take time and money
- Integrated cavity SGEMP experiments on Z and NIF are expensive and involve a complex array of physics phenomena that make the results difficult to unravel

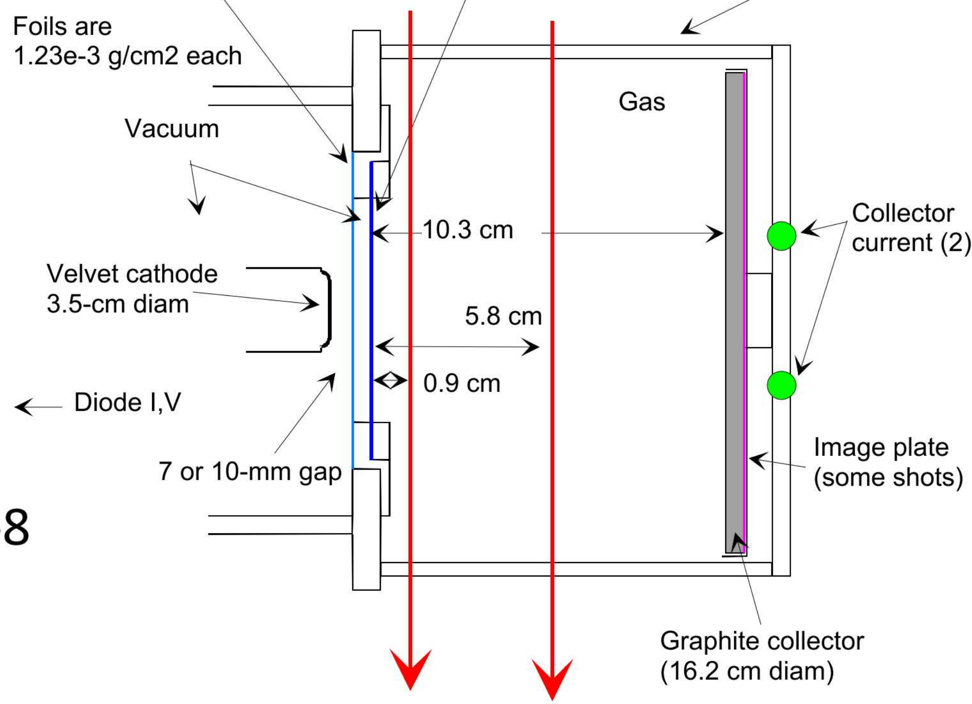
We are addressing an important part of the SGEMP problem

- Gas Chemistry
  - Direct e-beam injection into gas for gas-chemistry code validation (variation with pressure, e-beam energy, and current density)
- Electron-surface interactions
  - Ions sputtering from surfaces can greatly affect net current
  - Outgassing and plasma formation
  - Electron backscattering
- Photon-surface interactions
  - Photoelectron production

Small facilities have produced threat-level e-beams for validating gas-chemistry

70-kV beam into test cell for SGEMP

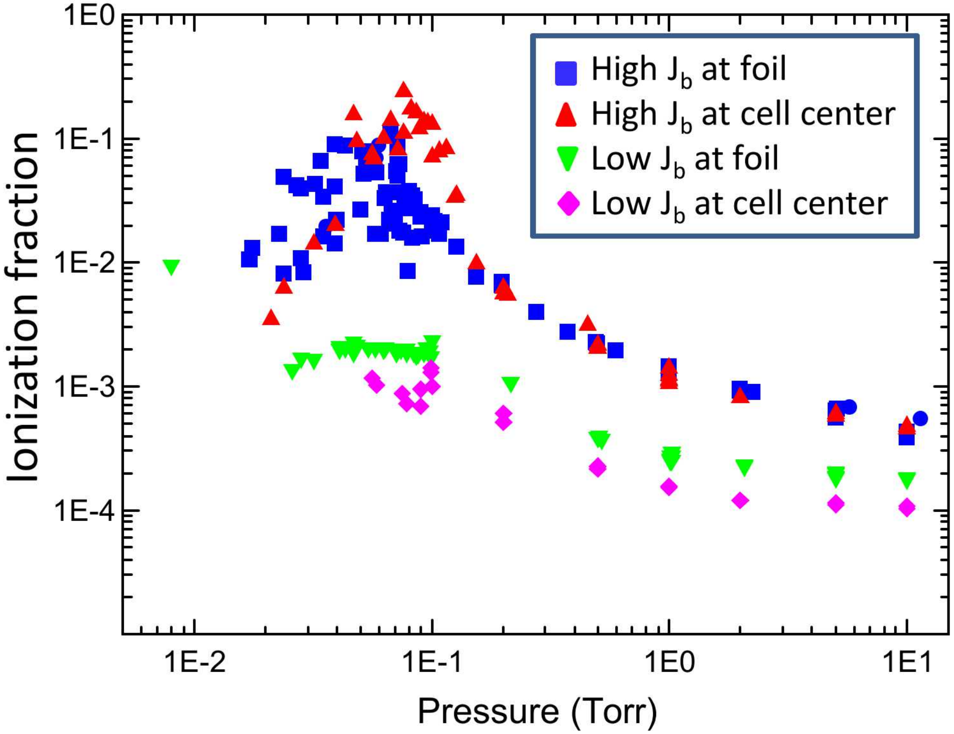




- 3 year experimental program 2005-8
  - 70 kV, 1-4 kA, 70 ns, 10-300 A/cm^2
  - Versatile, very high shot rate
- A pulser could be built to tailor to specific threat spectrum

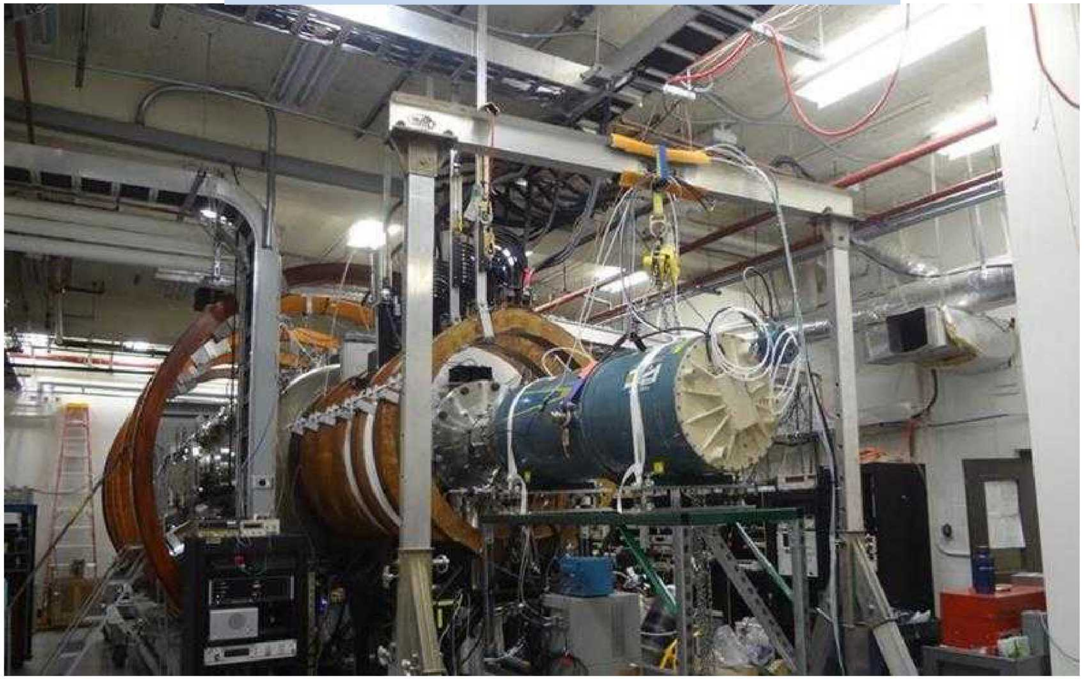
The NRL data has shown that MCSwarm is not good for high ionization fractions

- Swarm approximation is not good for high current density because the gas is no longer weakly ionized
- The effects of electron-electron collisions and reverse reactions become important at large n_e/N_{gas}
- High current density data shows the need for a more complex gas chemistry model (Justin)



Small facilities produce threat-level e-beams for validating gas-chemistry

200-kV beam into space chamber

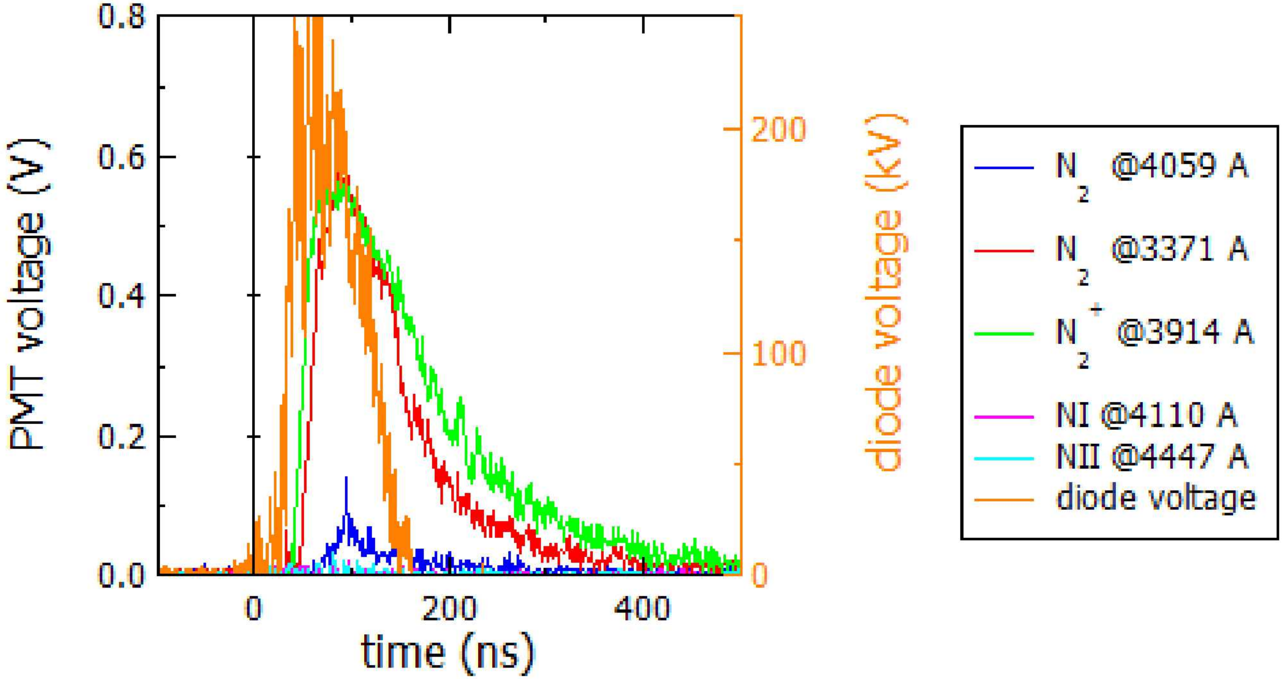


- A feasibility study was completed in 2014 with additional funds in 2015
  - 200 kV, 6 kA, 70 ns, 10's A/cm^2
  - Beam injected into 0.1 Torr air along 200-G axial field for 7 meters
  - Beam 1 meter from wall in main chamber

Experiments shows useful data can be obtained from direct electron beam injection into NRL space chamber

- Good propagation observed over 7 meters
- Ample light for spectroscopic measurements
- Beam and plasma are far from boundaries

PMT signals in large chamber, 465 cm from injection



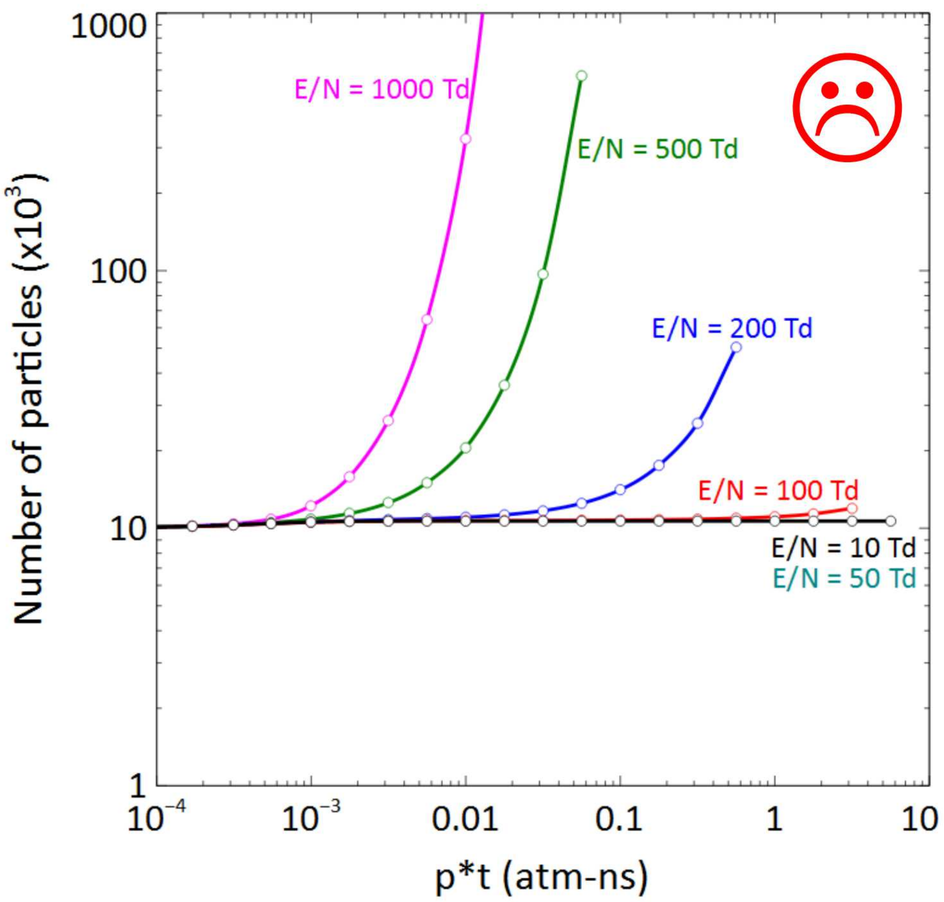
Improvements to MCSwarm

Limitations of and improvements to the MCSwarm code

- Particle count increases exponentially. Limit the number of particles produced.
- Errors introduced when $\nu\Delta t > 0.1$. Multiple-scattering distributions can relax this restraint.
- Ionization rate determined by electrons in the tail of the distribution where there are relatively few particles. Bias the eedf to produce more particles in the tail.
- Develop a time-dependent 2-term solution to the Boltzmann equation. Benchmarking for MCSwarm and other applications (Justin)
- Inner-shell ionizations not included. Could be a large energy sink for beam electrons (K-shell binding energy~400 eV) – Auger electrons are a source of high-energy (~400 eV) secondaries

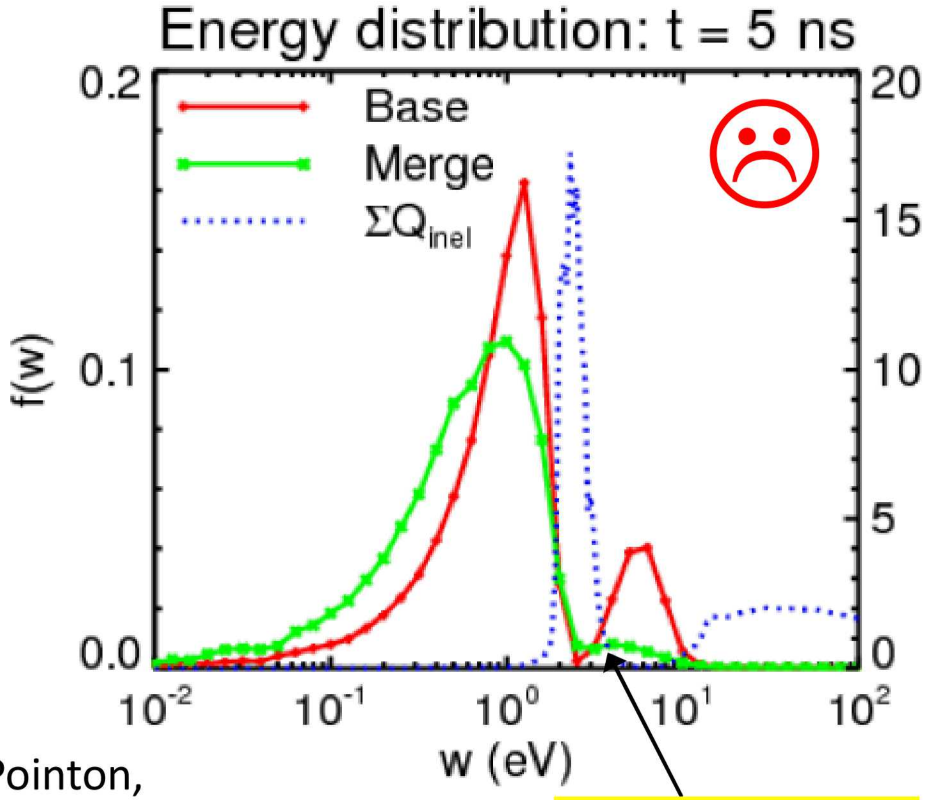
The particle count increases exponentially for large electric field

- Emphasis and Quicksilver have implemented an adaptive particle management algorithm to deal with this problem
- When particle count gets too large the particles are reweighted so that as many moments of the distribution as possible are preserved
- An alternate method follows exponential growth without an increase in particle count



Particle merging introduces undesired changes in the eedf

- The merging technique tends to cool the distribution
- Changes in the eedf above 10 eV have a profound affect on the ionization rate
- Need to take another look at particle management



(From T.D. Pointon,
2014 Gaseous electronics conf.)

This difference
Is troublesome

Exponential increase in the number of particles can be alleviated

- The Boltzmann equation with ionizing collisions in an electric field causes the eedf (f) to grow exponentially
  - MCSwarm is based on *f* which causes particle number to increase exponentially

$$\frac{\partial f}{\partial t}+\vec{v}\cdot\frac{\partial f}{\partial \vec{x}}+\vec{a}\cdot\frac{\partial f}{\partial \vec{v}}=C[f]$$

- Multiply Boltzmann equation by $e^{-\nu^* t}$ and define $F= e^{-\nu^* t} f$

$$\frac{\partial F}{\partial t}+\vec{v}\cdot\frac{\partial F}{\partial \vec{x}}+\vec{a}\cdot\frac{\partial F}{\partial \vec{v}}=C[F]-\nu^* F\equiv C'[F]$$

  - A Monte Carlo code based on the Boltzmann equation for F would not cause the particle number to increase exponentially
  - The Monte-Carlo representation for $C'[F]= C[F]- \nu^* F$ is to remove a particle for F and replace it with one from C[F] at the frequency ν^*

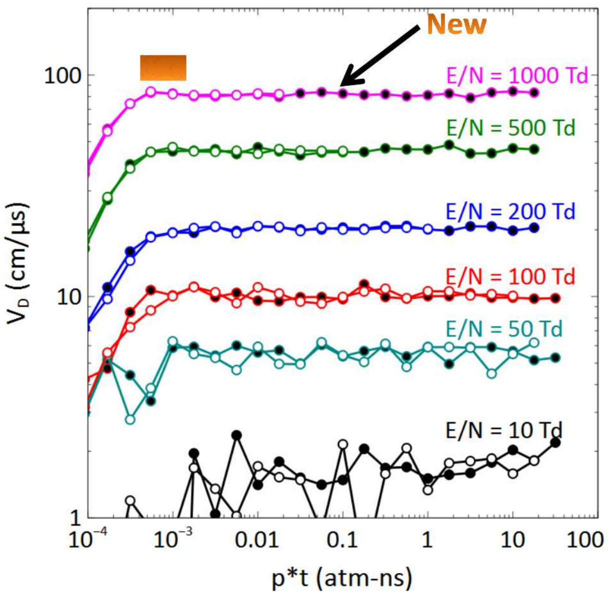
A Monte-Carlo representation of F preserves moments and particle number

- At every ionizing collision, add a secondary particle according to the differential ionization cross section $\sigma_i(\varepsilon_s,\varepsilon)$ and then remove a random particle from the existing particles and replace it with the newly created secondary.
- The number of simulation particles remains constant but their weights increase exponentially
- Moments are preserved

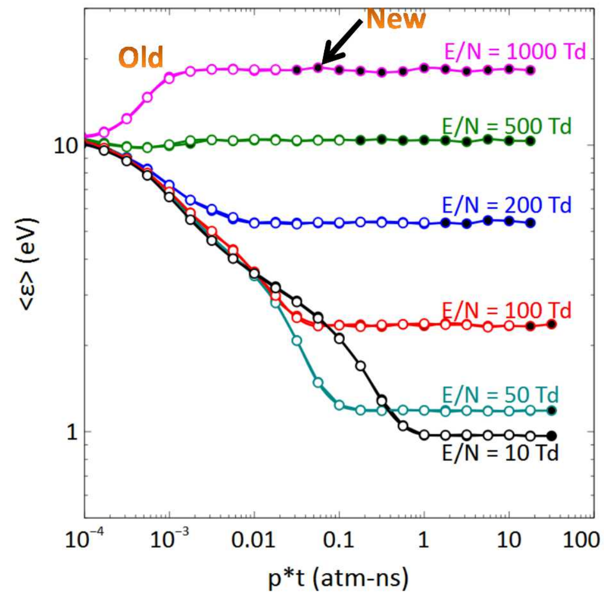
$$\langle g \rangle = \frac{\int g(\varepsilon) f\, d\varepsilon}{\int f\, d\varepsilon} = \frac{\int g(\varepsilon) F\, d\varepsilon}{\int F\, d\varepsilon}$$

The new algorithm avoids exponential growth and agrees with MCSwarm

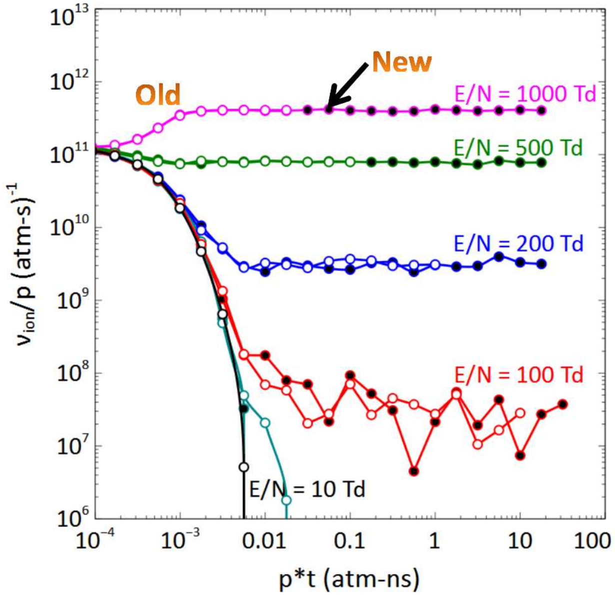
Drift velocity



Average energy

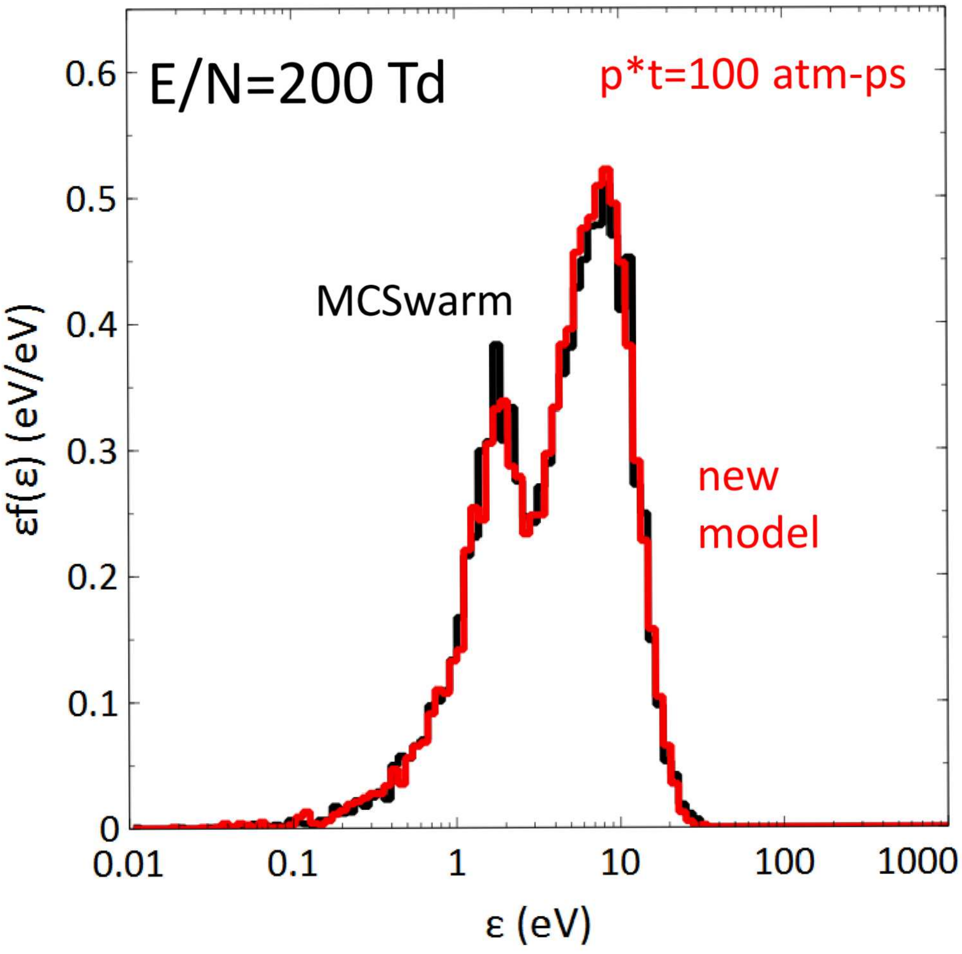


Ionization rate



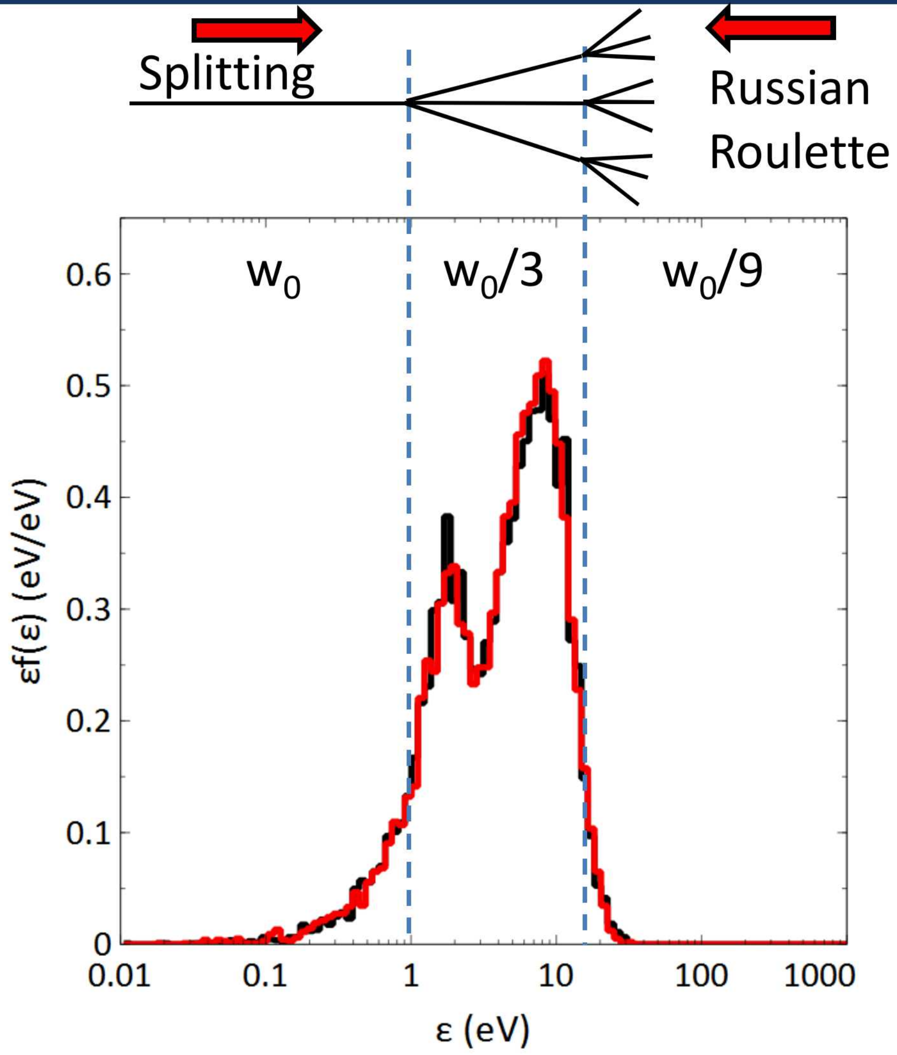
- This is a factor of >1000 speedup for large E/N
- An algorithm for applying this to a list of unequally weighted particles is needed for coupling with PIC

The time evolution of the eedf's for the two models are in good agreement



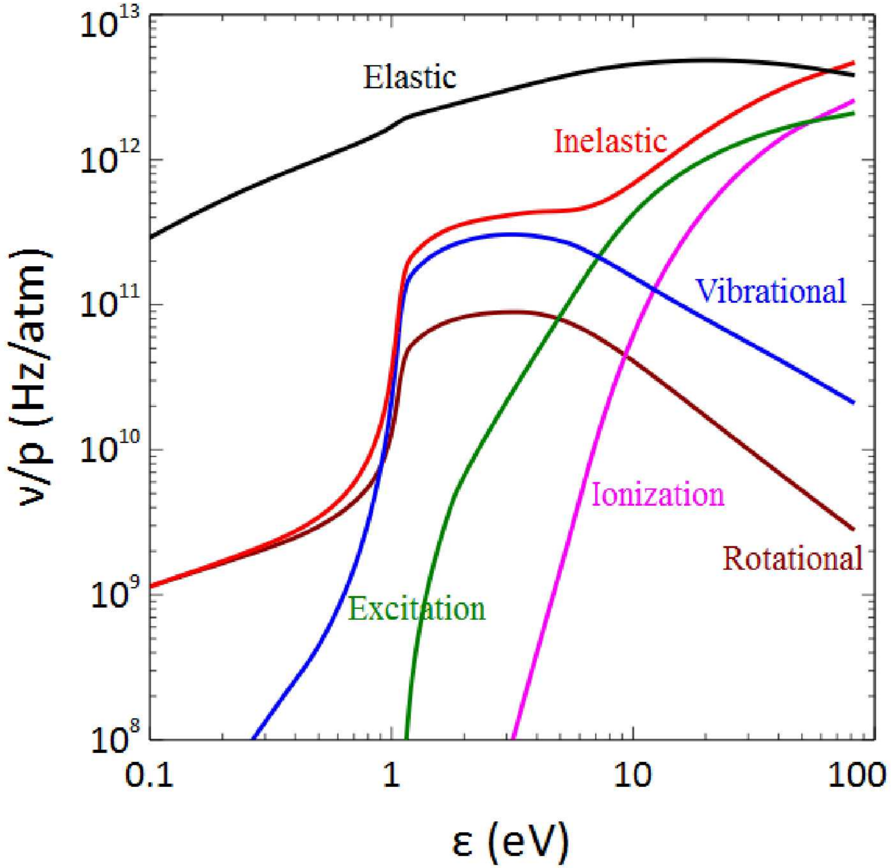
Energy splitting can put more particles in the tail of the eedf

- Energy splitting and Russian roulette is a method of biasing Monte-Carlo calculations so that more particles are in the tail
- As electrons gain energy they split into multiple particles with reduced weight
- As electrons lose energy they are removed from the simulation by Russian roulette. Surviving electrons are given a larger weight



Recall that the number of elastic collisions dominates at low-energy

- MCSwarm spends 10-100 times more time sampling elastic collisions
- Big reduction in run time could be realized if elastic and inelastic collisions are sampled at the same rate



Big reductions in run time if elastic scattering could be done less frequently

- This require a multiple scattering distribution which can be written as the sum over the number of collisions

$$f(\varepsilon,\Omega,\Delta t) = \left[p(N=0,\nu\Delta t)F_0(\Omega) + p(N=1,\nu\Delta t)F_1(\Omega) + p(N=2,\nu\Delta t)F_2(\Omega) + \ldots\right]$$

$$= \sum_k \frac{e^{-\nu\Delta t}(\nu\Delta t)^k}{k!} F_k(\Omega)$$

  - the F_k are the angular distributions after exactly k scattering events

- MCSwarm keeps only k=0 and k=1 terms of this expansion

$$f(\varepsilon,\Omega,\Delta t) \cong [e^{-\nu\Delta t} F_0(\Omega) + \nu\Delta t\, e^{-\nu\Delta t} F_1(\Omega)]$$

$$F_0(\Omega) = \delta(1-\cos\theta)/2\pi\,, \quad F_1(\Omega) = \frac{1}{\sigma_0}\frac{d\sigma}{d\Omega}$$

} MCSwarm

- Relaxing restrictions of $\nu\Delta t$ requires terms $k \geq 2$ in the expansion

The $F_k(\Omega)$ can be calculated by repeated application of the scattering matrix

- The results of applying the scattering matrix k times can be written as

$$\vec{v}\,' = \underline{\underline{R_i}} \cdot \vec{v}_i$$

$$\vec{v}\,'_{kf} = (\underline{\underline{C_1}}\,\underline{\underline{C_2}}\,\underline{\underline{C_3}} \ldots \underline{\underline{C_k}}) \cdot \vec{v}\,' \equiv \underline{\underline{S_k}} \cdot \vec{v}\,'$$

$$\vec{v}_{kf} = \underline{\underline{R_i^{-1}}}\,\underline{\underline{S_k}}\,\underline{\underline{R_i}} \cdot \vec{v}_i$$

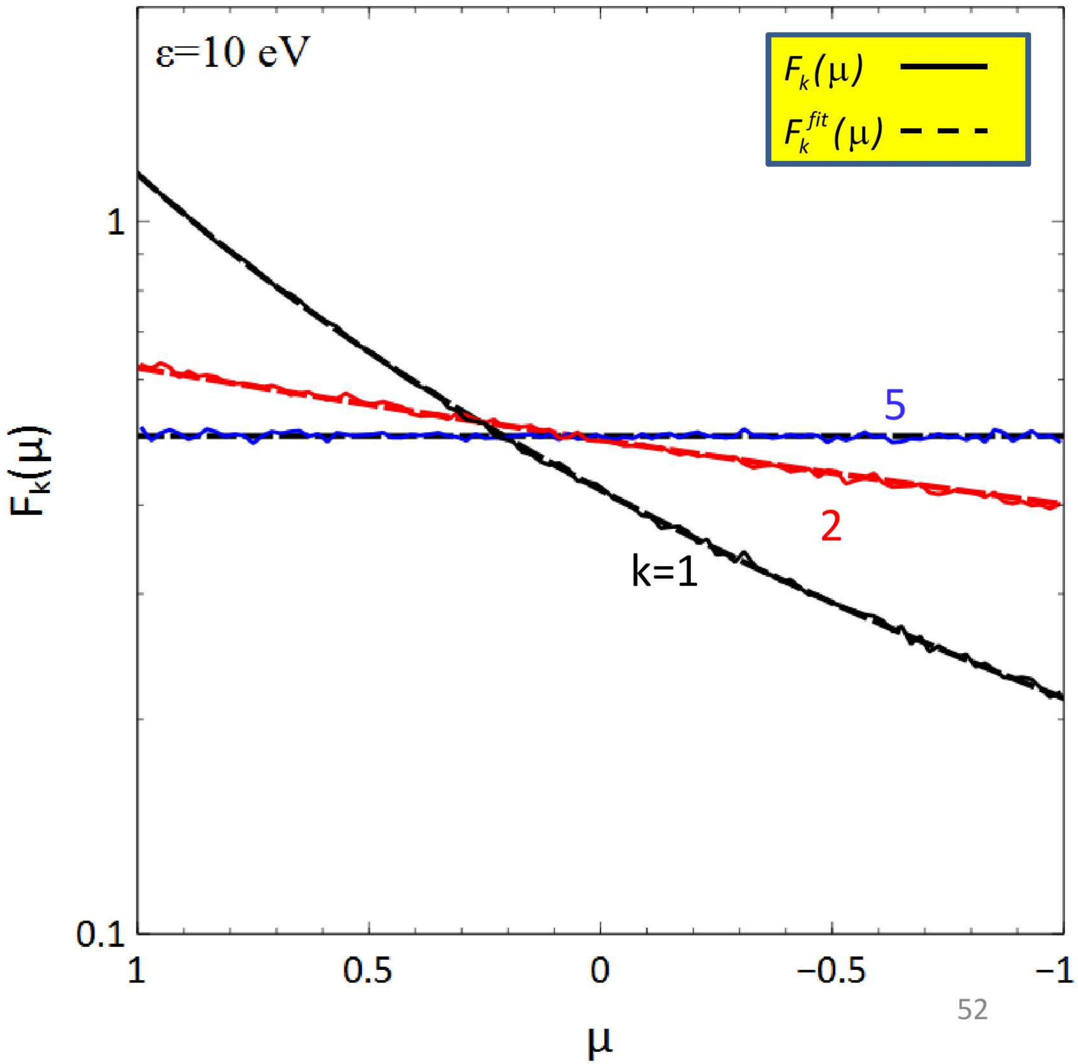
- The distributions F_k can be built by calculating the multiple scattering matrices, S_k, with many different random number sequences and constructing histograms

Multiple scattering distributions for N_2 gas for ε=10 eV

$$F_k^{fit}(\mu) = \frac{1}{2}\frac{\left(1-\xi_k^2\right)}{\left(1-\xi_k\mu\right)^2}$$

k	ξ_k
1	0.40
2	0.12
5	0.0

- F_k is isotropic for k>5
- Figuring out how to implement this for non-zero E and B fields still needs to be figured out



Current status of MCSwarm

- A stand-alone, parallel, class-based Python version now exists (Richardson and Swanekamp)
- A class-based C^{++} version is currently being tested – loosely based on the Python version (Richardson)
  - Improving the computational efficiency (i.e. H. Sugawara, *et al.*, J. Comput. Phys. **223** (2007) 298)
- We are working with Sandia and NRL to obtain permissions to release both the Python and C^{++} the codes as open source (Swanekamp and Richardson)
- An earlier Fortran version exists but has not had any new updates since ~2010
- More validation work will proceed in FY15 as funding permits
- Experiments on both Gamble II and the NRL space chamber began in FY 14 and will continue in FY15 – a golden opportunity for code verification
- A NIF SGEMP shot was taken in FY14 and another is planned in FY15

The chemistry becomes more complex as the ionization fraction increases

n_e/N_2: 10^{-5} → 10^{-3} → 10^{-1} → 1

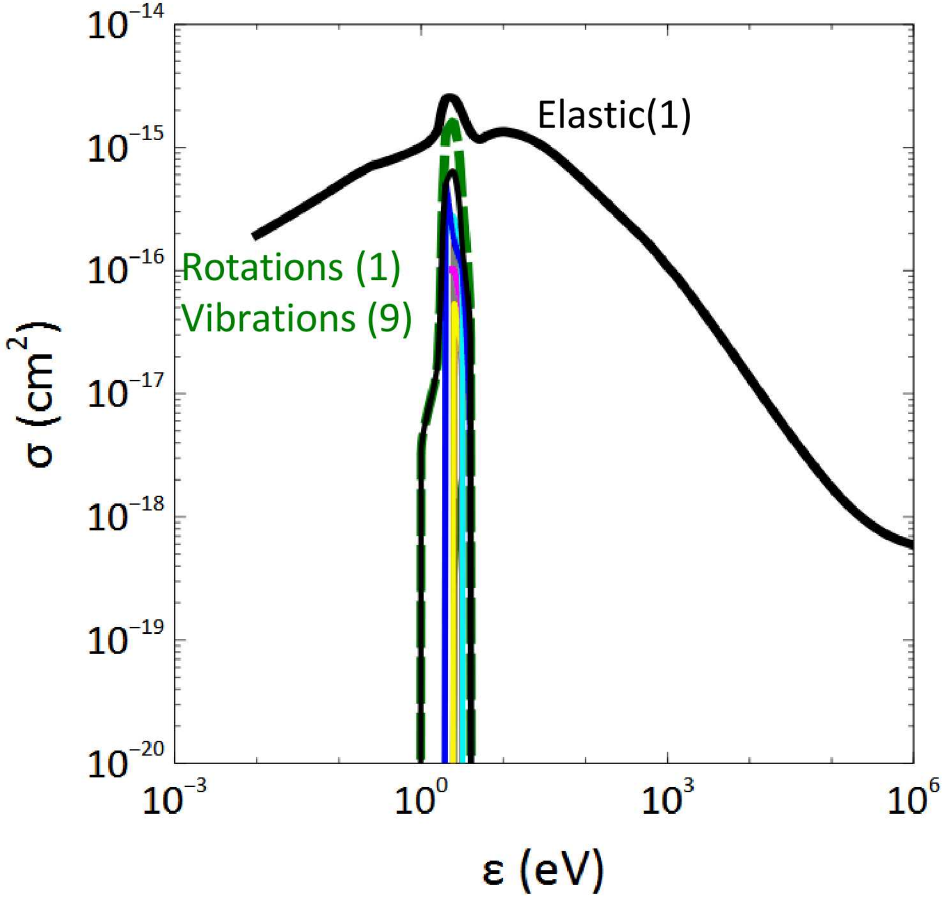
Thermal Excitation:	$N_2 + e \Rightarrow N_2^j + e$	• Weakly ionized, swarm
Avalanche Breakdown:	$N_2 + e \Rightarrow N_2^+ + 2e$	• Exponential Growth in n_e
Energy exchange between excited states:	$N_2^j + e \Rightarrow N_2^k + e$	• Some decay rates very long (metastable)
Ionization from excited state:	$N_2^j + e \Rightarrow N_2^+ + 2e$	• Lowers ionization threshold
Electron-Electron collisions:	$e + e \Rightarrow e + e$	• Hotter Maxwellian eedf
Dissociative Recombination:	$N_2^+ + e \Rightarrow 2N$	
Electron-Ion collisions:	$N_2^+ + e \Rightarrow N_2^+ + e$ $N^+ + e \Rightarrow N^+ + e$	• Changes Momentum transfer (V_D)
Ionization of atomic gas:	$N + e \Rightarrow N^+ + 2e$	• Multiply-ionized plasma

A code that includes these processes and has been implemented in LSP will be discussed by Justin Angus in the next talk

Extra VGs

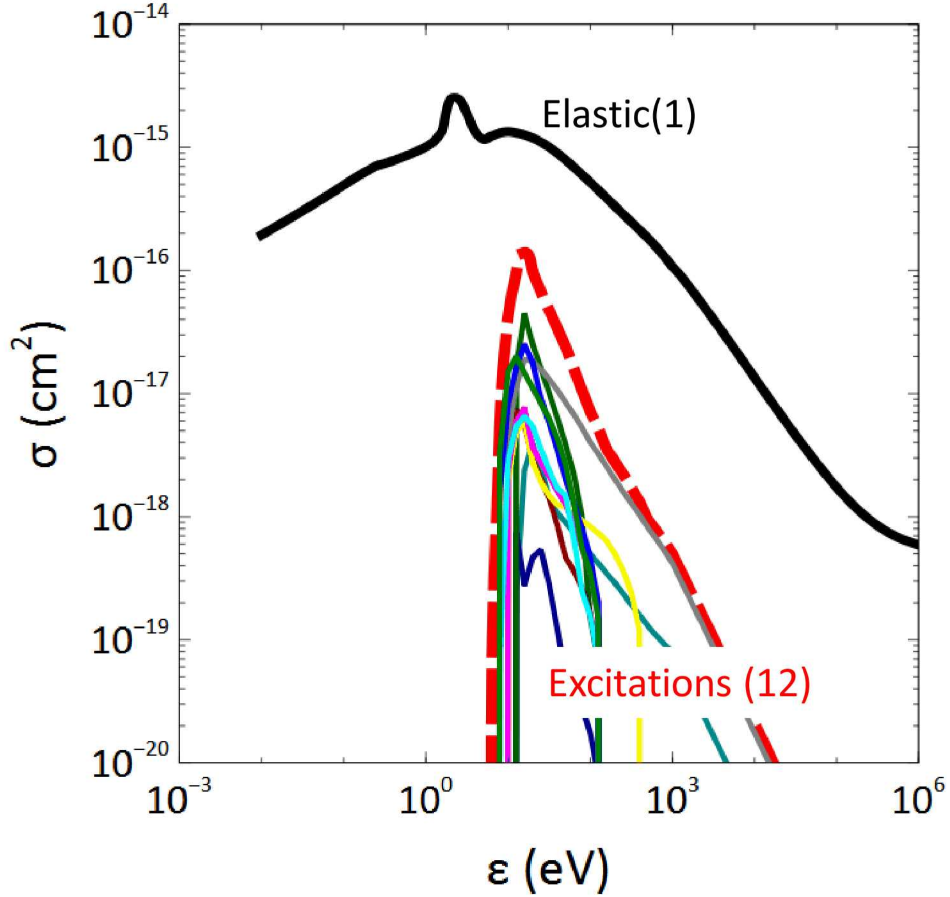
Neutral N_2 cross sections used in the MCSwarm avalanche model

All these reactions are important for accurate electron-energy distribution function f(ε) (eedf)



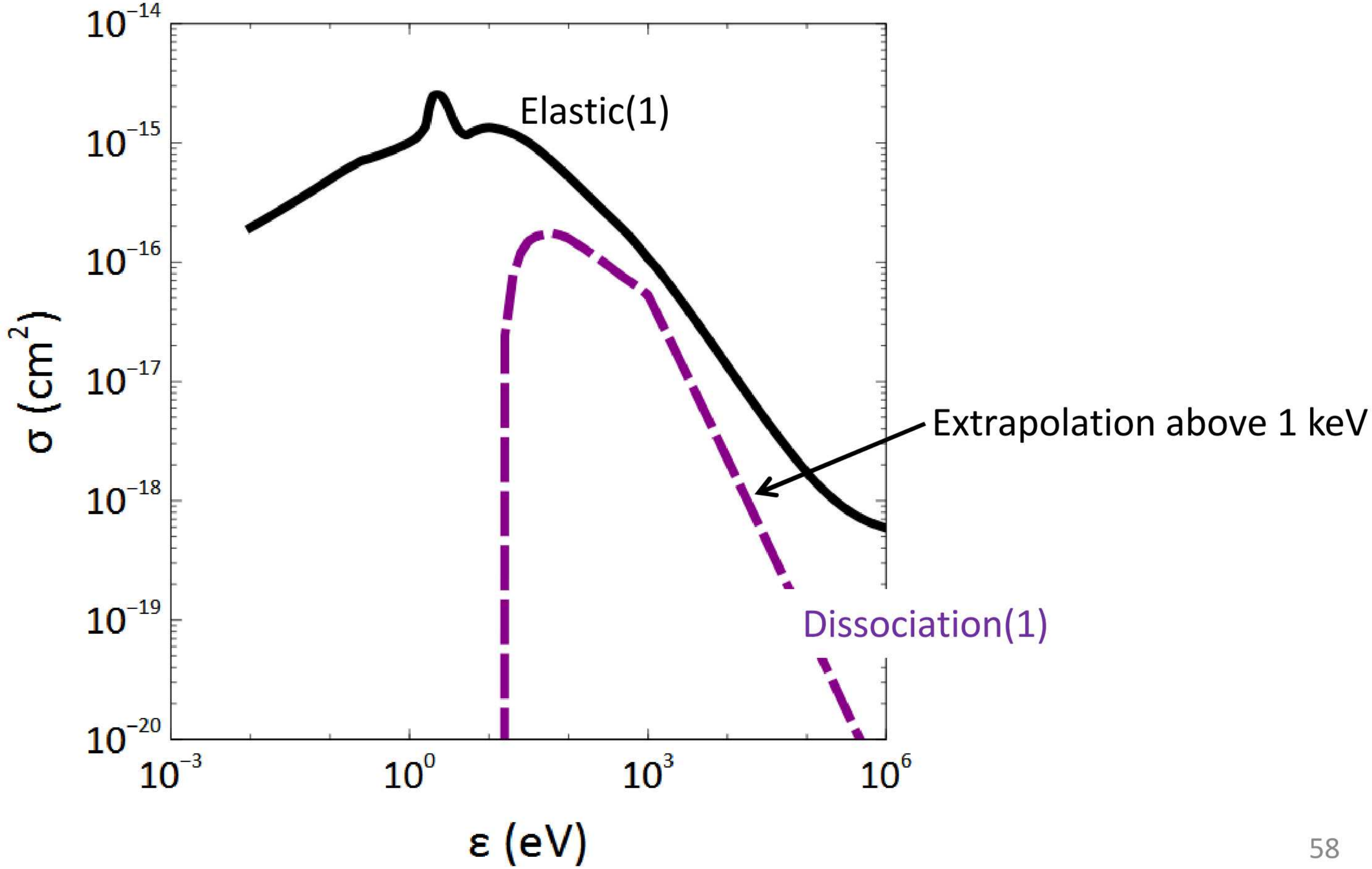
Neutral N_2 cross sections used in the MCSwarm avalanche model

All these reactions are important for accurate electron-energy distribution function f(ε) (eedf)



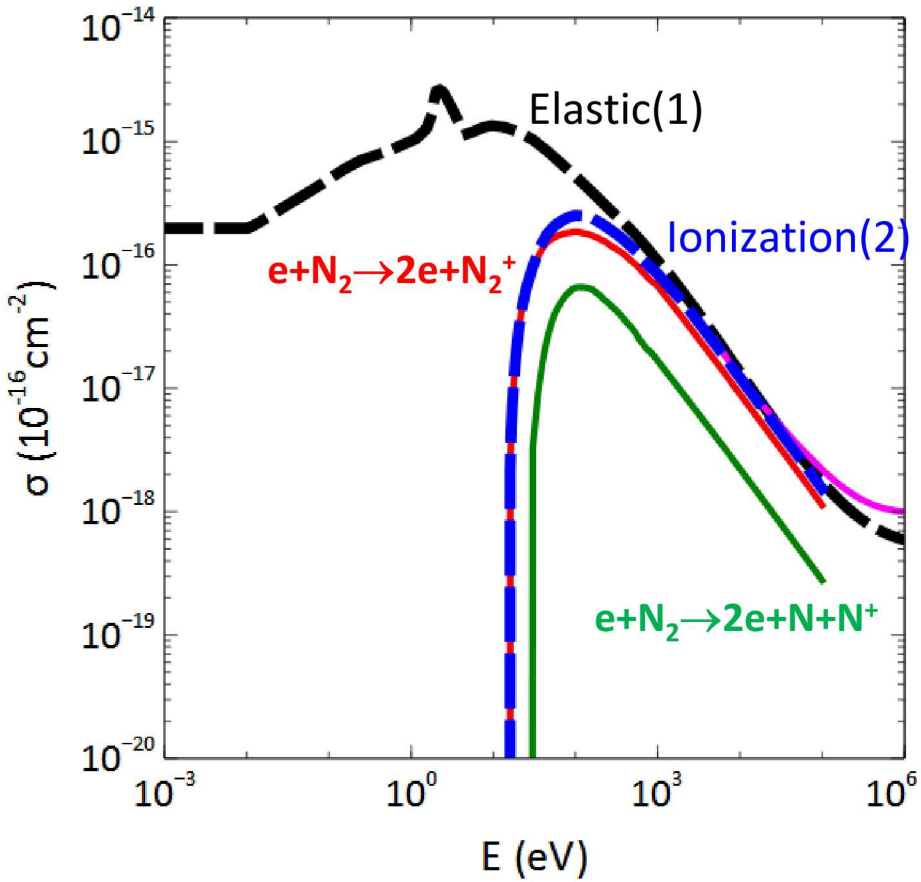
Neutral N_2 cross sections used in the MCSwarm avalanche model

All these reactions are important for accurate electron-energy distribution function f(ε) (eedf)

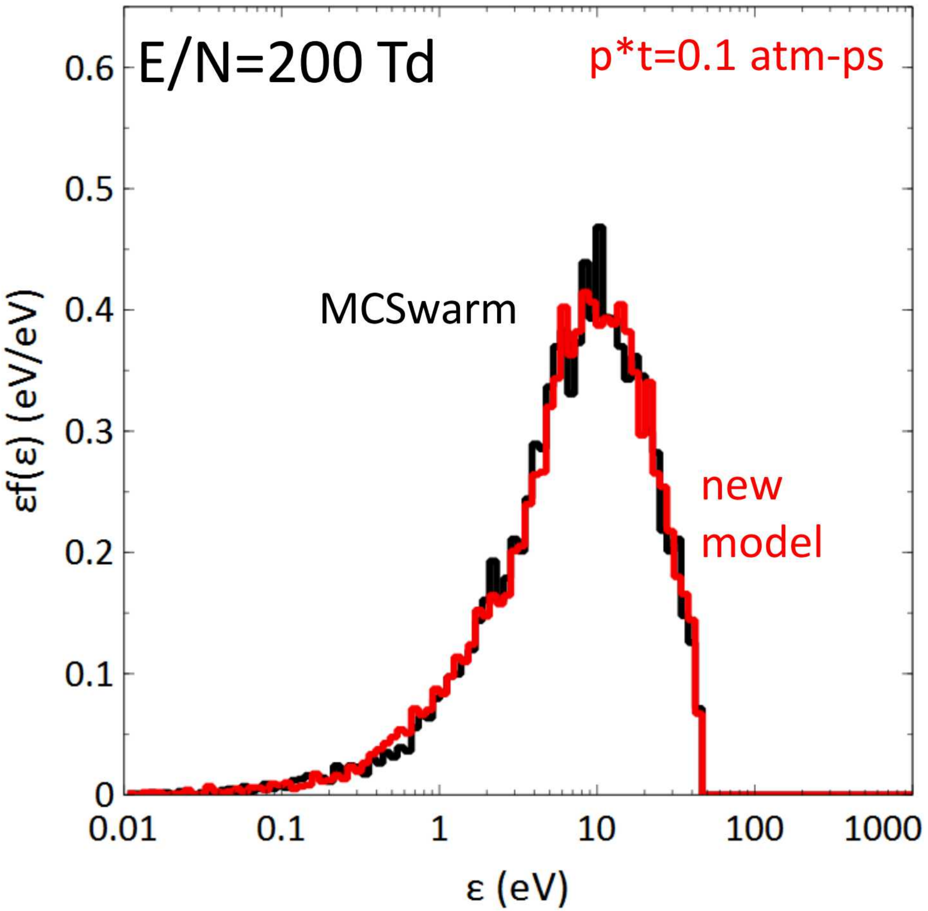


Neutral N_2 cross sections used in the MCSwarm avalanche model

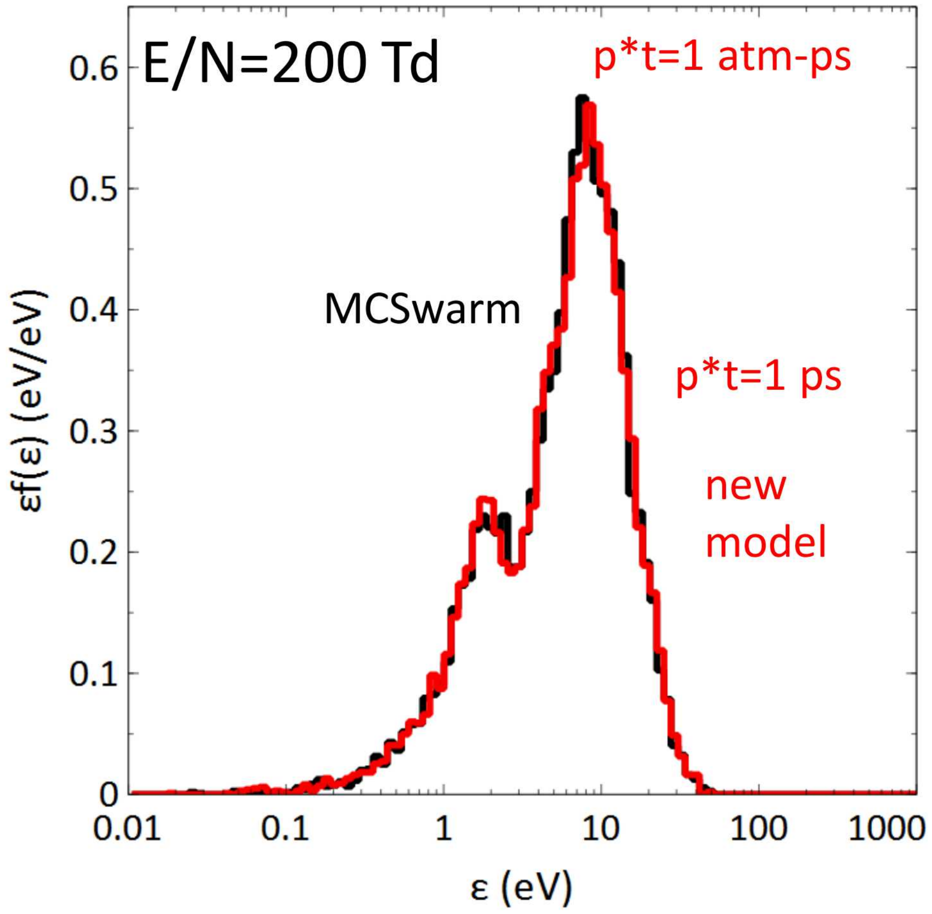
All these reactions are important for accurate electron-energy distribution function $f(\varepsilon)$ (eedf)



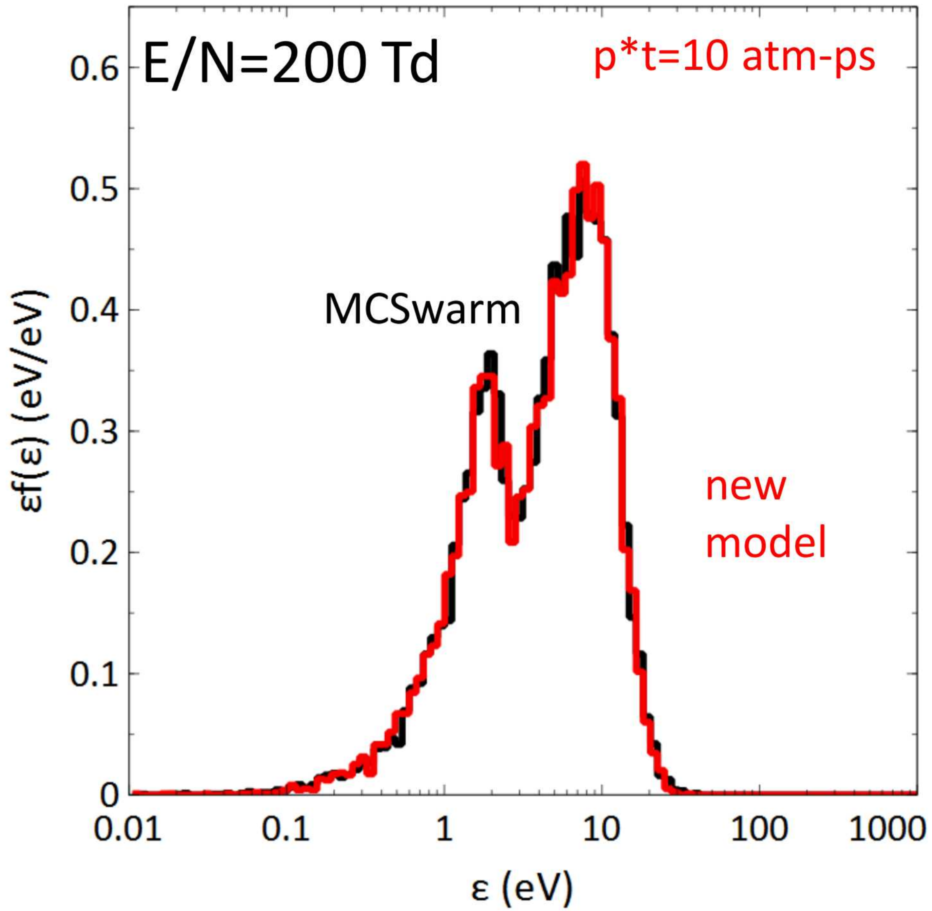
The eedf's of two models are in good agreement



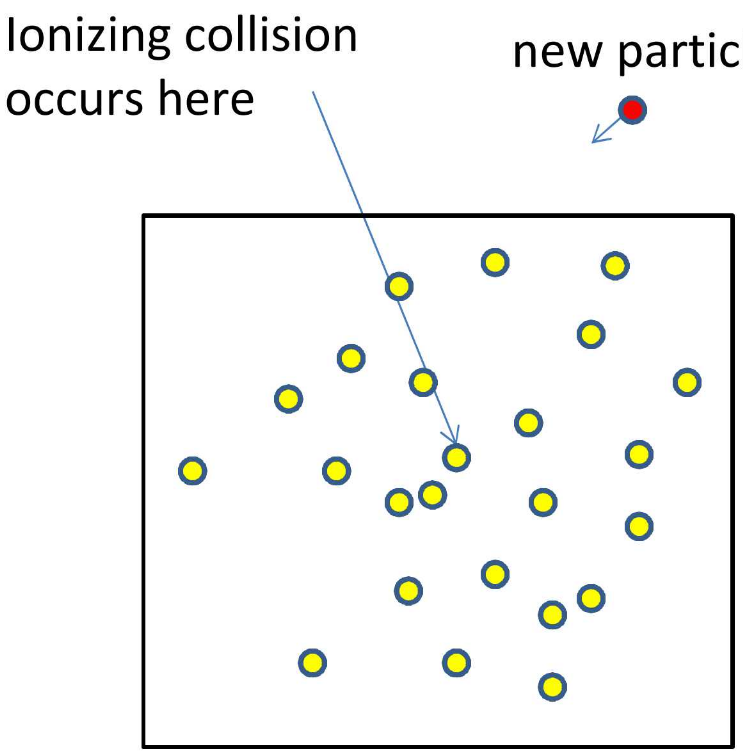
The eedf's of two models are in good agreement



The eedf's of two models are in good agreement

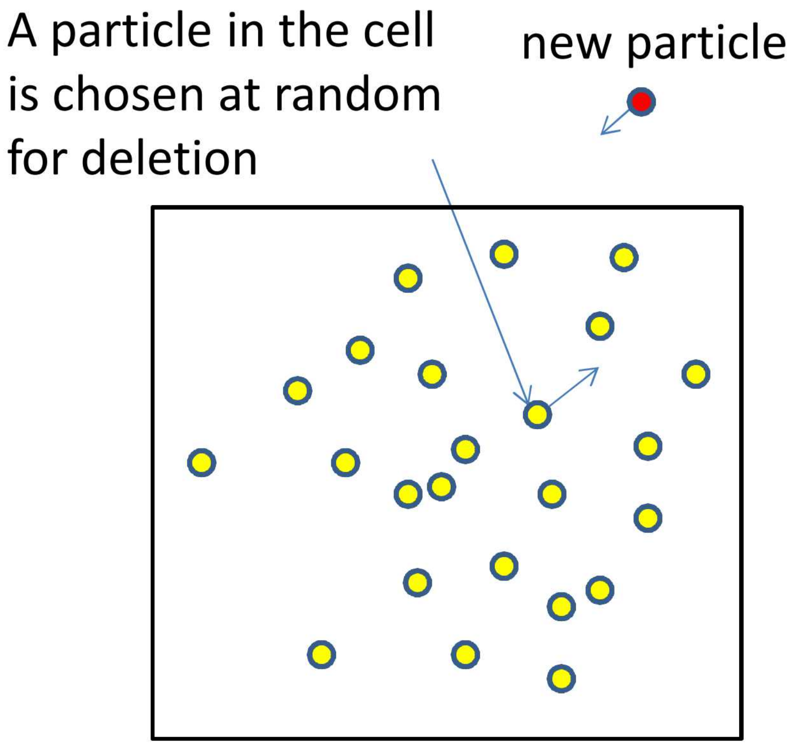


One way to implement this in PIC



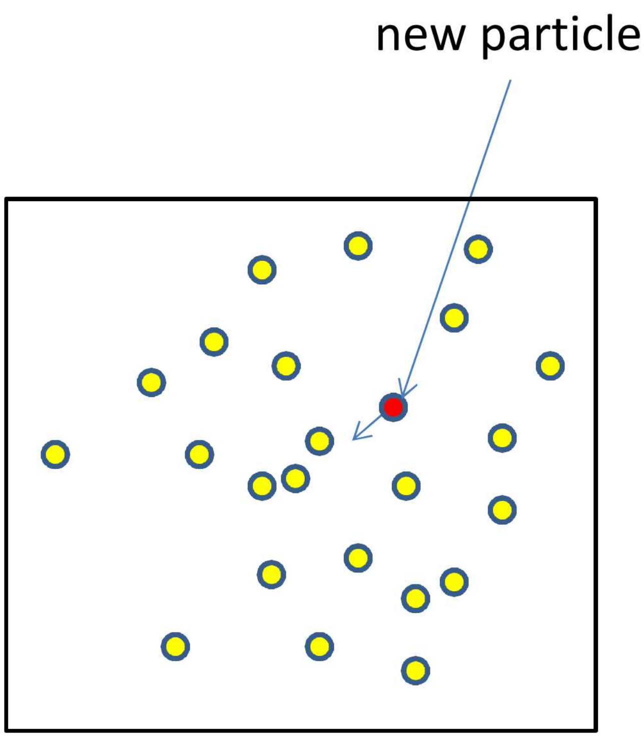
- When an ionizing collision occurs in a cell a new particle is created

One way to implement this in PIC



- When an ionizing collision occurs in a cell a new particle is created
- One of the existing particles in the cell is chosen at random for deletion

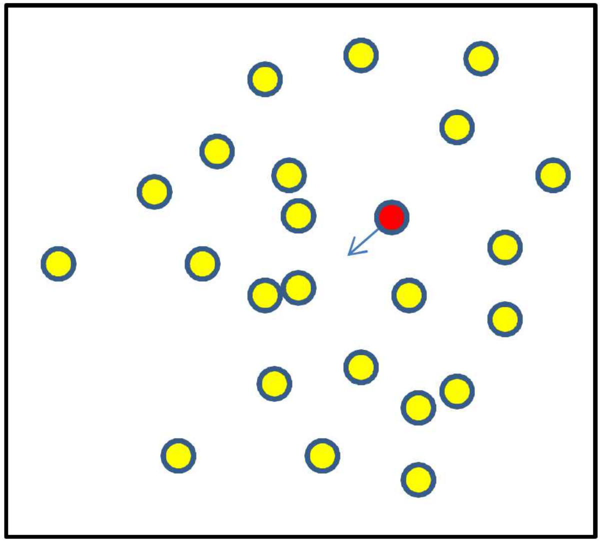
One way to implement this in PIC



- When an ionizing collision occurs in a cell a new particle is created
- One of the existing particles in the cell is chosen at random for deletion
- The newly created particle is swapped for the deleted one

One way to implement this in PIC

Increase particle weights



- When an ionizing collision occurs in a cell a new particle is created
- One of the existing particles in the cell is chosen at random for deletion
- The newly created particle is swapped for the deleted one
- Weights of existing particles is increased by (N+1)/N (equally weighted particles)
  - Particle weights increase with each ionizing collision not particle number