Using VSim to Model Wafer Etching Processes for Micro Electronics

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Background

- Silicon wafer is 10-20 cm in diameter and a few mm thick
- A plasma is generated which reacts with the wafer thus etching a desire pattern
- How VSim can be used to model this problem:
  - model many of the reactions which occurs in the plasma and at the plasma/wafer interface
  - Dielectrics can be placed in the simulation to determine how to create a uniform sheath across the wafer
- Desired Outcome: Create a uniform sheath across the length of the wafer so that the ions impact uniformly.

What is VSim?

- VSim is the entire computational engine, visualization setup, post-processing and data visualization package
  - Computational engine is called Vorpal
- VSim is a multi-physics, fully kinetic, electromagnetic particle in cell simulation
  - Multi-physics - plasma physics + associated physics (such as reactions with neutrals, secondary emission from boundaries, and many other processes)
  - Fully kinetic : all plasma processes can be captured (in principal)
    - In practice, some time scales are too long to use a PIC code
    - Other conditions also arise that make PIC impractical, e.g. the need for many particles per cell
    - Electrons and ions treated kinetically
  - Electromagnetic – Maxwell's equations are solved at each time step using the plasma current and charge density as source terms (in addition to BC's and external source terms)
    - Electrostatic is a special case in which only the E-field is solved for because self-consistent B-field is very small

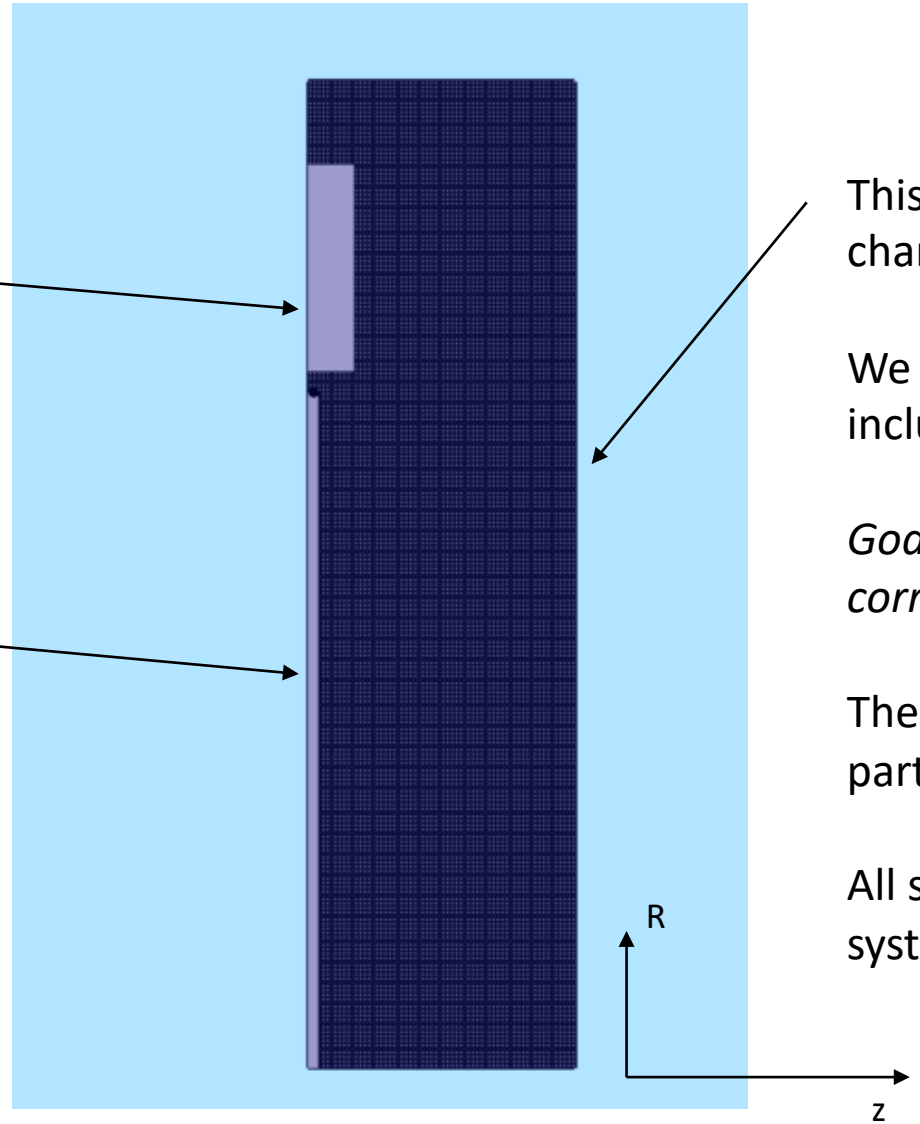
Advantages of VSim for Modeling Wafer Processing Simulations

- VSim computes the fully self-consistent electric field
  - Electrons and ions are both kinetic so sheath solved for correctly
- This sheath electric field is directly responsible for accelerating ions into wafer
  - This ion acceleration is directly responsible for etching process
  - *But correct ion acceleration depends on the correctly computed sheath electric field*
- When a plasma interacts with any surface (including the wafer) a sheath naturally forms.
  - Sheath oscillates between 10-100 electron Debye Lengths (λ_D)
  - Therefore, it is essential to resolve λ_D in order to get electric field correct near wafer
- **VSim naturally captures all sheath dynamics**
  - Any fluid model needs to determine what needs to be included to compute the sheath correctly (such as a pressure term, correct collision rates, etc.)
  - No ad-hoc methods are needed in VSim
- VSim includes many collisional processes and secondary electron emission

Overview of Setup

Focus Ring

Silicon Wafer



This boundary is in the middle of many plasma chambers

We simulate the region near the wafer and do not include the whole chamber

Goal is to capture the detailed sheath dynamics correctly

Therefore, need BC that smoothly injects new particles and models the potential correctly

All simulations done in 2D cylindrical coordinate system

Video Showing Potential and Ion Dynamics

Modeling Edge Effects in Wafer Processing Using VSim

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Explanation of Simulation Setup

- The simulation domain includes the near-wafer region
- As a result, need a way to smoothly inject plasma species at upper boundary
  - VSim has a nice emission boundary condition which places the particles correctly in the boundary cell
  - But we still need a way to specify the velocity correctly.

Explanation of Boundary Conditions

- We have injected particles at a boundary to model small part of a much larger plasma
- If particle injection not done correctly, a sheath often builds at injection boundary
  - But this sheath would be artificial and we have found a way to eliminate the sheath
- We will show that the following quantities are conserved at the injection boundary:
  - Density
  - Flux
  - Temperature
- Also, we show that no sheath forms if injection done correctly

Injection Method

- The simulation is initialized with a distribution function given by $f(\vec{v})$.
  - Distribution function is spatially uniform
- We assume $f(\vec{v})$ is a drifting Maxwellian in –z direction and no drift in r and phi directions
  - Plasma is initially charge neutral and no net current ($v_{dx\mathrm{i}} = v_{dx\mathrm{e}}$ and $q_{\mathrm{e}} = -q_{\mathrm{i}}$)
- Bohm's criteria states the following:
  - No sheath will form if $v_{di} = \sqrt{\frac{T_e}{M_i}}$ = Ion Sound speed
  - This is the initial drift speed we choose for the plasma along with the injection speed (for both species) at the boundary opposite the wafer

Choosing Initial Particle Velocity

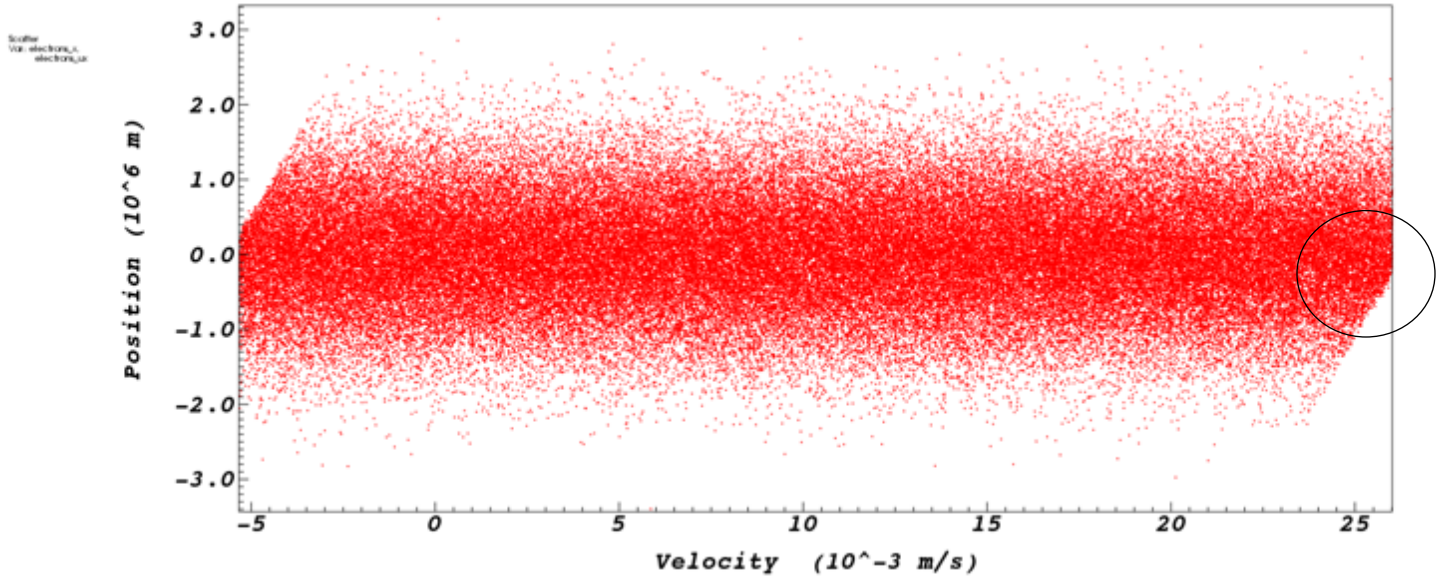
- In a PIC code, particle velocity is chosen via cumulative distribution function:

$$R = \frac{\int_{-\infty}^{v_x} f(v'_x) dv'_x}{\int_{-\infty}^{\infty} f(v'_x) dv'_x}$$

- R is random number between 0 and 1. This equation is inverted for each R and v_x is determined
- If R is uniformly chosen between 0 and 1, then the likeliest chosen value of v_x occurs where $f(v_x)$ peaks
- An analytic inversion exists which speeds up choosing particle velocity

Choosing Injected Particle Velocity

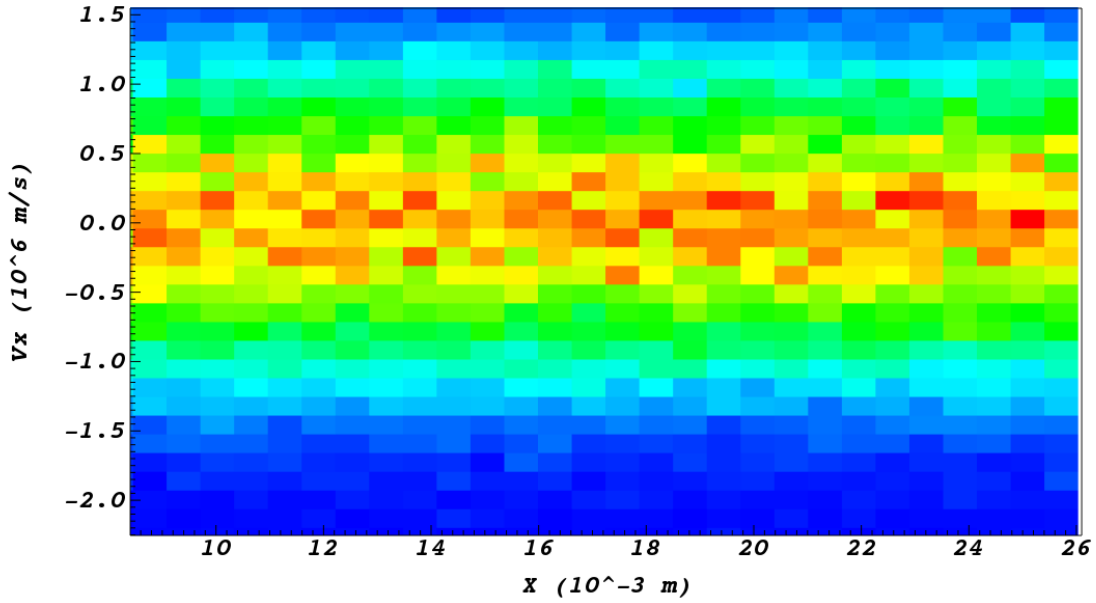
- To choose the correct distribution function for the injected particles, lets assume the initial distribution function is a non-drifting Maxwellian (though the results are general, this is simply for illustration)
- Lowest velocity particles (v=0) travel slowly away from the boundary as illustrated below:



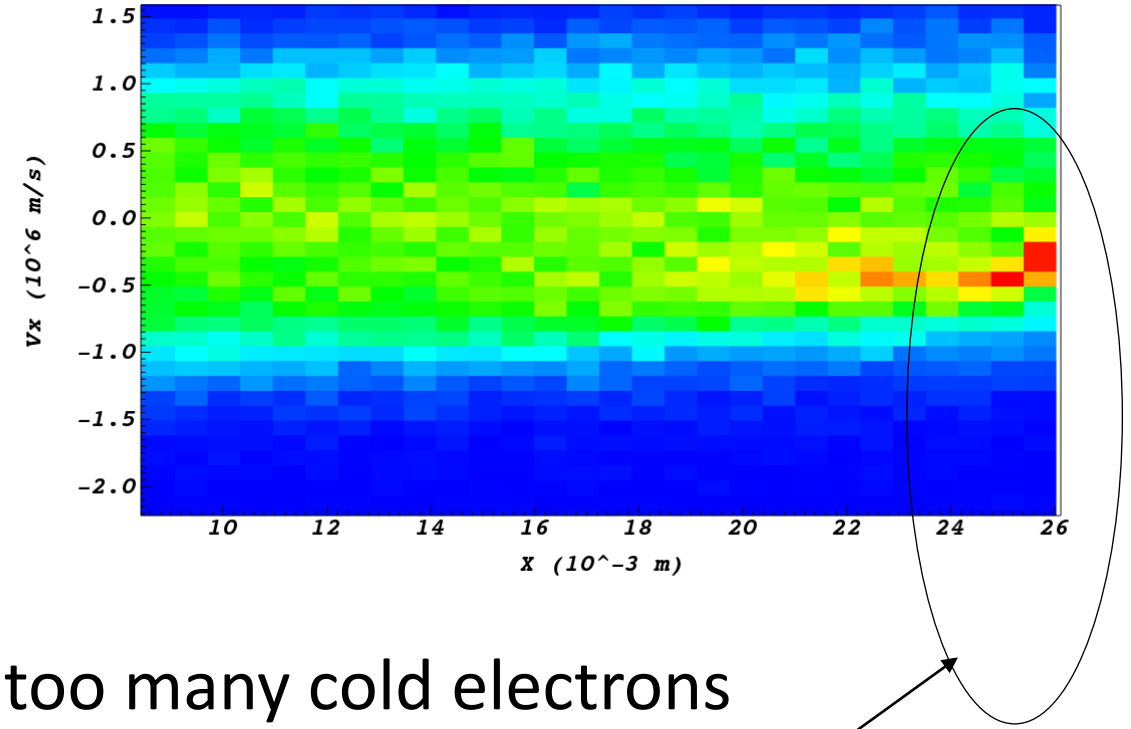
Injecting a Maxwellian would be incorrect since too many low-velocity particles would be injected.

Injection with Maxwellian is Wrong

Initial Phase Space



Evolved Phase Space



If injected with a Maxwellian, then too many cold electrons injected at boundary

Choosing Injected Particle Velocity

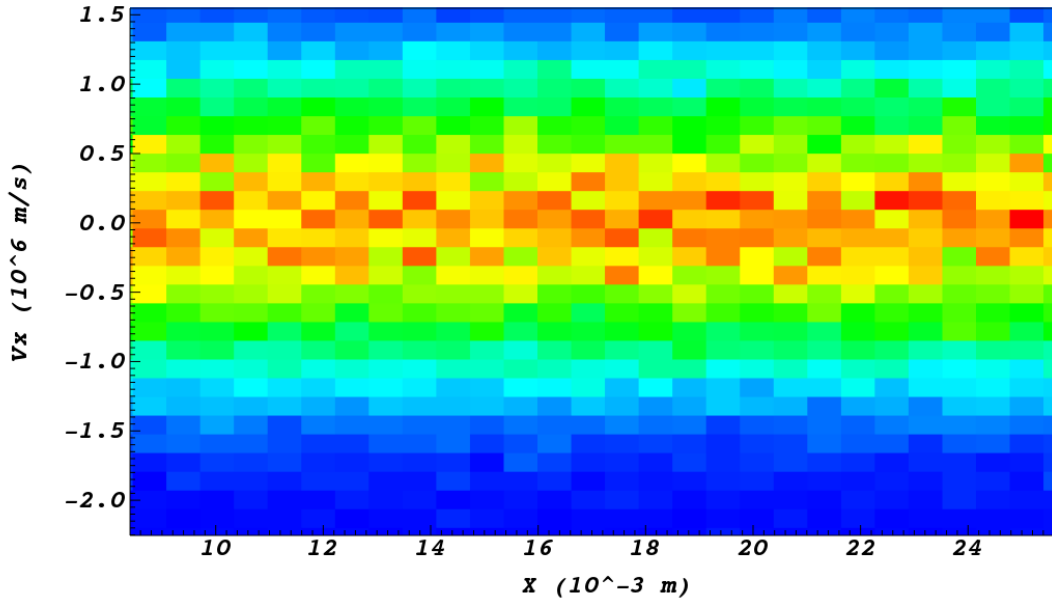
- The correct way to replace the initial distribution function is to match the flux leaving the boundary:

$$R = \frac{\int_{-\infty}^{v_x} v'_x f(v'_x) d\, v'_x}{\int_{-\infty}^{\infty} v'_x f(v'_x) dv'_x}$$

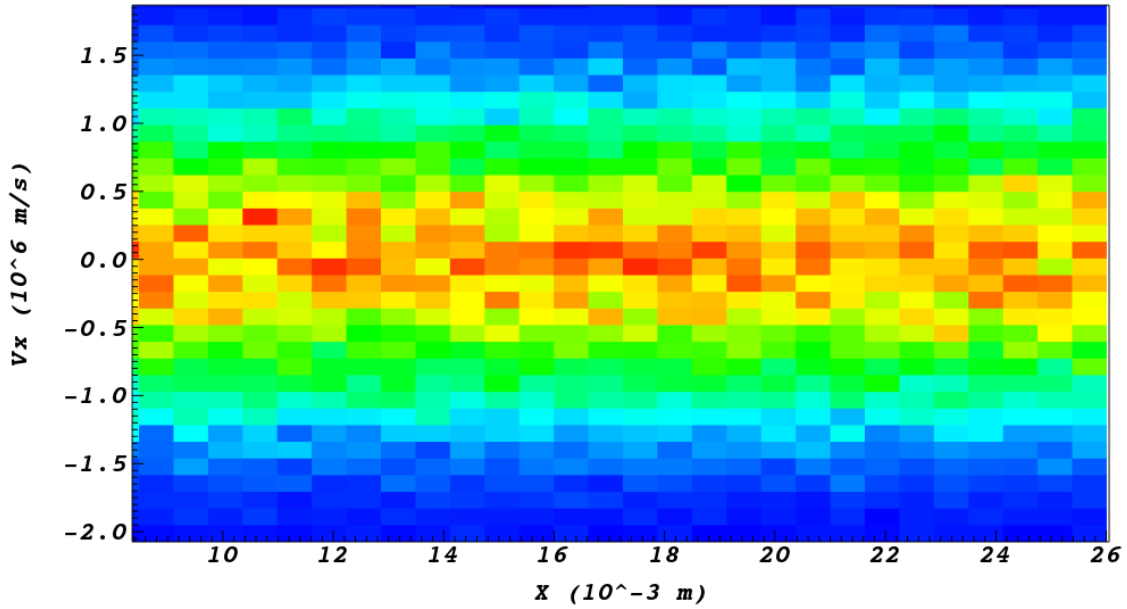
- Crux of the problem: The above equation can be inverted analytically if $f(v'_x)$ is a non drifting Maxwellian. Otherwise, must be inverted numerically

Injection with Flux-Conserving : $\boldsymbol{vf(v)}$

Initial Phase Space



Evolved Phase Space



Initial phase space is preserved with correct injection method

Therefore, need to inject with *vf(v)* NOT *f(v)*

Method of Inverting $\int vf(v)dv$

- We invert the cumulative distribution function using a semi-analytic method called Rejection-Sampling Theory
- Recall that $\int vf(v)dv$ is integrable if $f(v)$ is a non-drifting Maxwellian
- Steps to applying Rejection-Sampling method
  - Define $\tilde{g}(v) > g(v)$ such that $\int v\tilde{f}(v)dv = \int \tilde{g}(v)dv$ is invertible
- $\tilde{g}(v) = \frac{v}{v_{th}^2}\exp\left(-\frac{v^2}{2v_{th}^2}\right)$ → $\tilde{g}(v)$ is integrable
- Solution to cumulative distribution function is: Choose a random number ξ between [0,1).
- $\xi = \int_0^v dv' \frac{v'}{v_{th}^2}\exp\left(-\frac{v'^2}{2v_{th}^2}\right)$
- $v = v_{th}\sqrt{-2\ln(1-\xi)}$

Method of Inverting $\int vf(v)dv$

- $g(v) = vf(v) = \frac{v}{v_{th}^2}\exp\left(-\frac{(v-v_d)^2}{2v_{th}^2}\right)$

$\tilde{g}(v) > g(v)$

$$\tilde{g}(v) = A\frac{v}{v_{th}^2}\exp\left(-\frac{v^2}{2\sigma^2}\right) > \frac{v}{v_{th}^2}\exp\left(-\frac{(v-v_d)^2}{2v_{th}^2}\right)$$

- Choose A and σ based on the following:

$$A = \exp(|v_d|/v_{th})$$

$$\sigma^2 = \frac{v_{th}^2}{1-\alpha^2} = \left(1+\frac{|v_d|}{2v_{th}}\right)v_{th}^2$$

Method of Inverting $\int \boldsymbol{vf(v)dv}$

- Pick a velocity based on analytic solution from $\hat{g}(v)$
  - Pick ξ uniformly in [0,1)
  - $v = \sigma\sqrt{-2\ln(1-\xi)}$
  - Choose a different random number R
  - Define the following: $\zeta = R * A\frac{v}{v_{th}^2}\exp\left(-\frac{v^2}{2\sigma^2}\right)$
  - If $\zeta < \frac{v}{v_{th}^2}\exp\left(-\frac{(v-v_d)^2}{2v_{th}^2}\right)$ then load particle

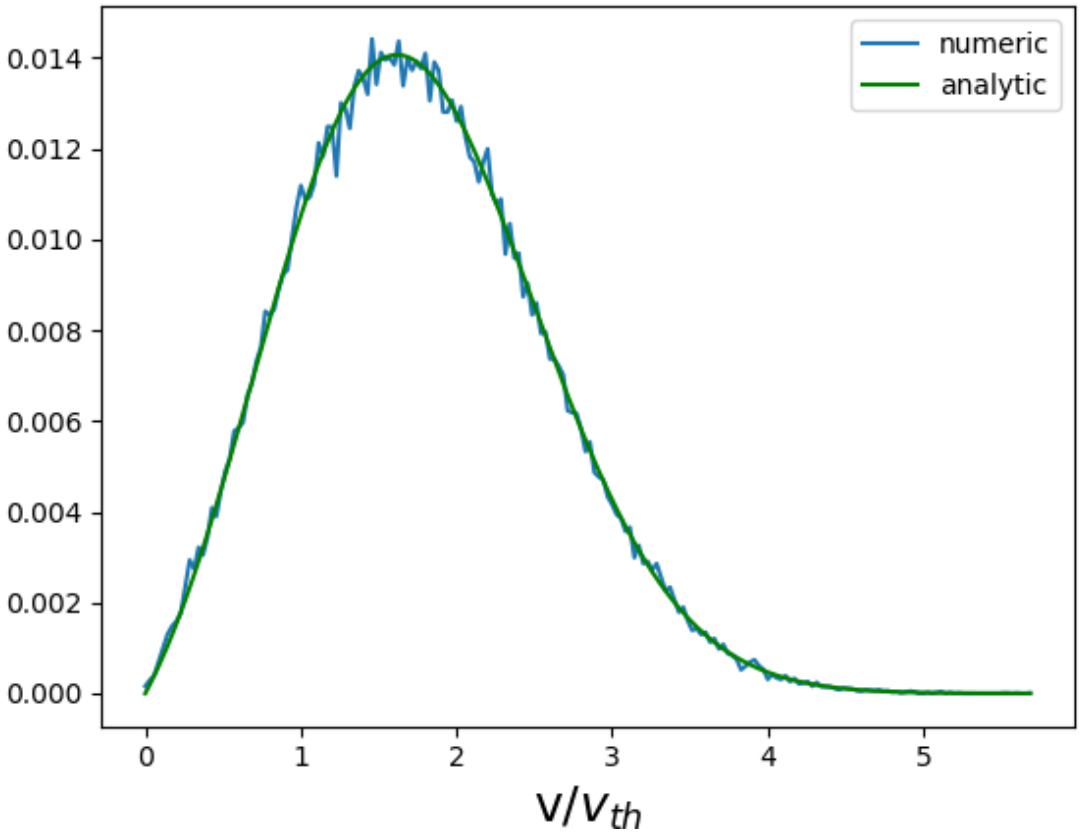
Same v

All of these steps are carried out in the python script that comes with the example: waferImpact.py

Else, loop through algorithm again

Example and benchmarking

- Assume the following: $V_d = V_{th}$
- ~150,000 points were sampled.
- Distribution function filled with 100,000 points
- More sampled points needed as V_d increases



Gas and plasma species

- Electrons and Ar+ ions
  - Te = 3 eV
  - Ti = 1 eV
  - Both drifting towards wafer with a speed of $1.5Cs = 1.5\sqrt{\frac{T_e}{M_i}}$
- Some simulations include a Ar neutral background with the following properties
  - Pressure ~ 0.15 Torr
  - Temperature : 300 K
- Some simulations also include Secondary electron emission from dielectrics

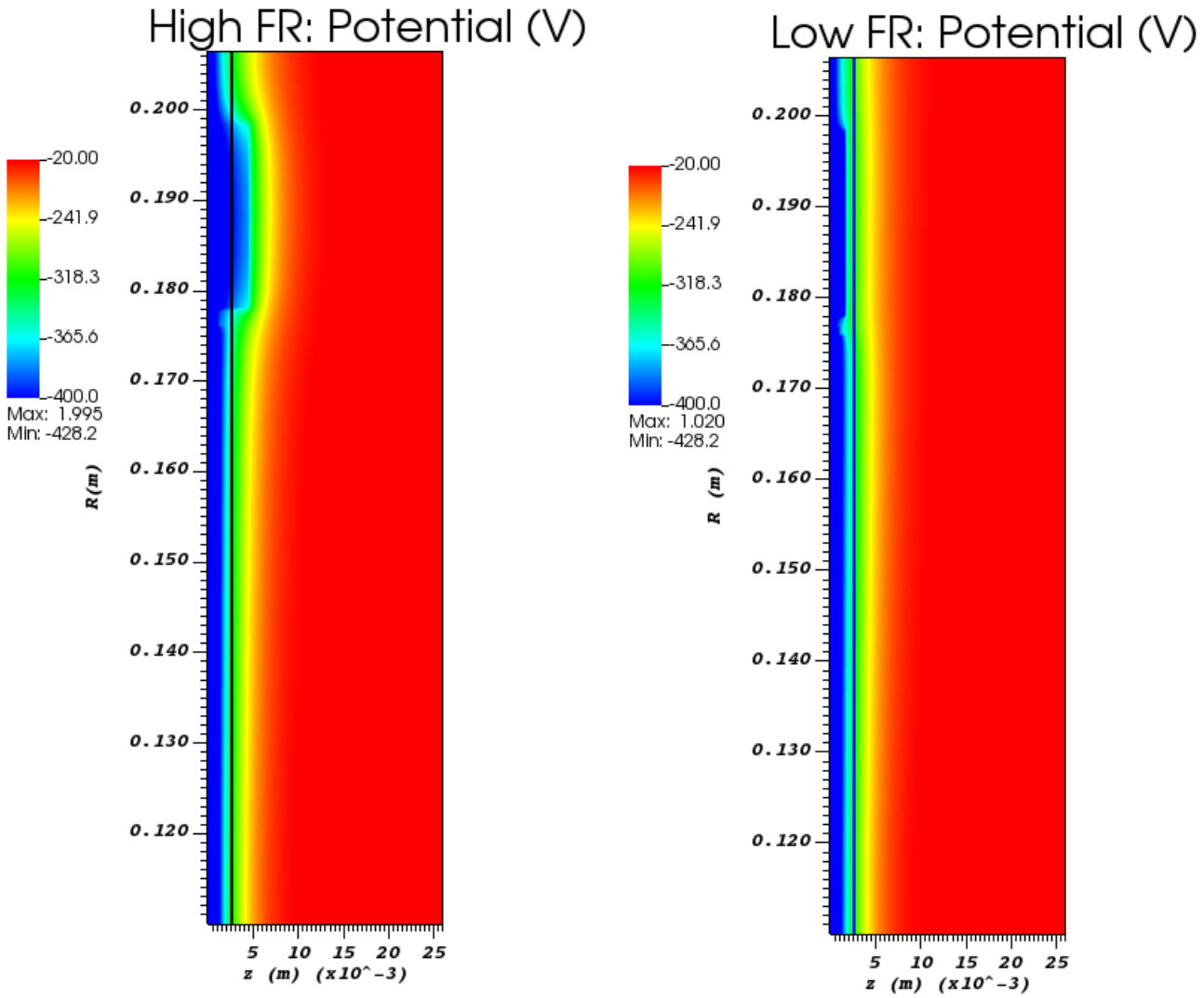
Angular Energy Distribution Function

- Four different simulations have been performed
  - Ion Angular Energy Distribution are compared to determine role of various part of the physics such as:
    - Inclusion of collisions with background neutral population
    - Inclusion of secondary emission off of dielectrics
    - Height of Focus Ring
- VSim includes the capability of including many different types of collisions. In this model we have included 3:
  - Ionization collisions
  - Elastic collisions
  - 11.83 eV excitation collision (this one had the largest cross section)

Secondary Emission

- In addition to collisions, VSim can model secondary emission off of dielectrics and conductors
- In our model, we include two types of secondaries.
  - Electrons and ions that accumulate on the surface
  - Secondary electrons that are emitted due to the impact of electrons and ions
- Using VSim, you can model how these secondaries affect the IAED.

Role of Focus Ring



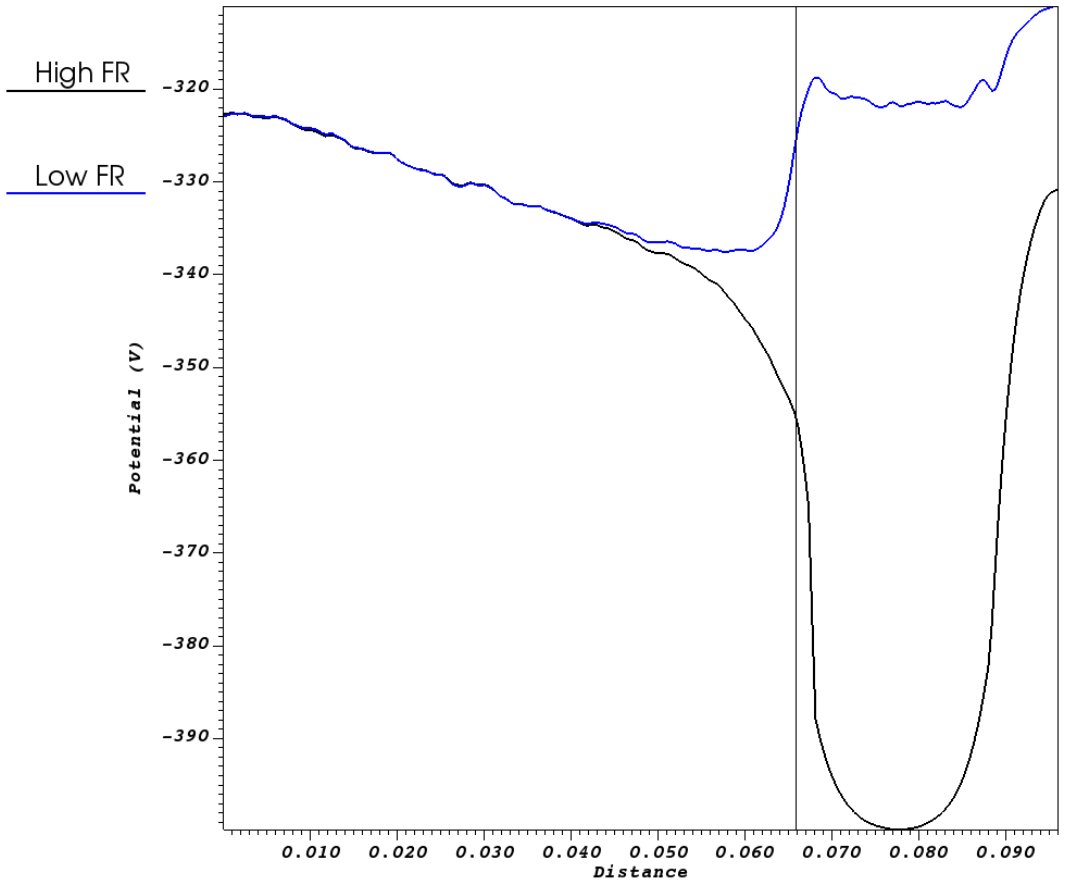
Color contour plots of potential at RF cycle ~ 14 (time step 9600).

Impact on sheath near wafer is difficult to discern

Cutouts are needed

NOTE: All data analysis done in Visit, which is free!!

Role of FR on Sheath Potential

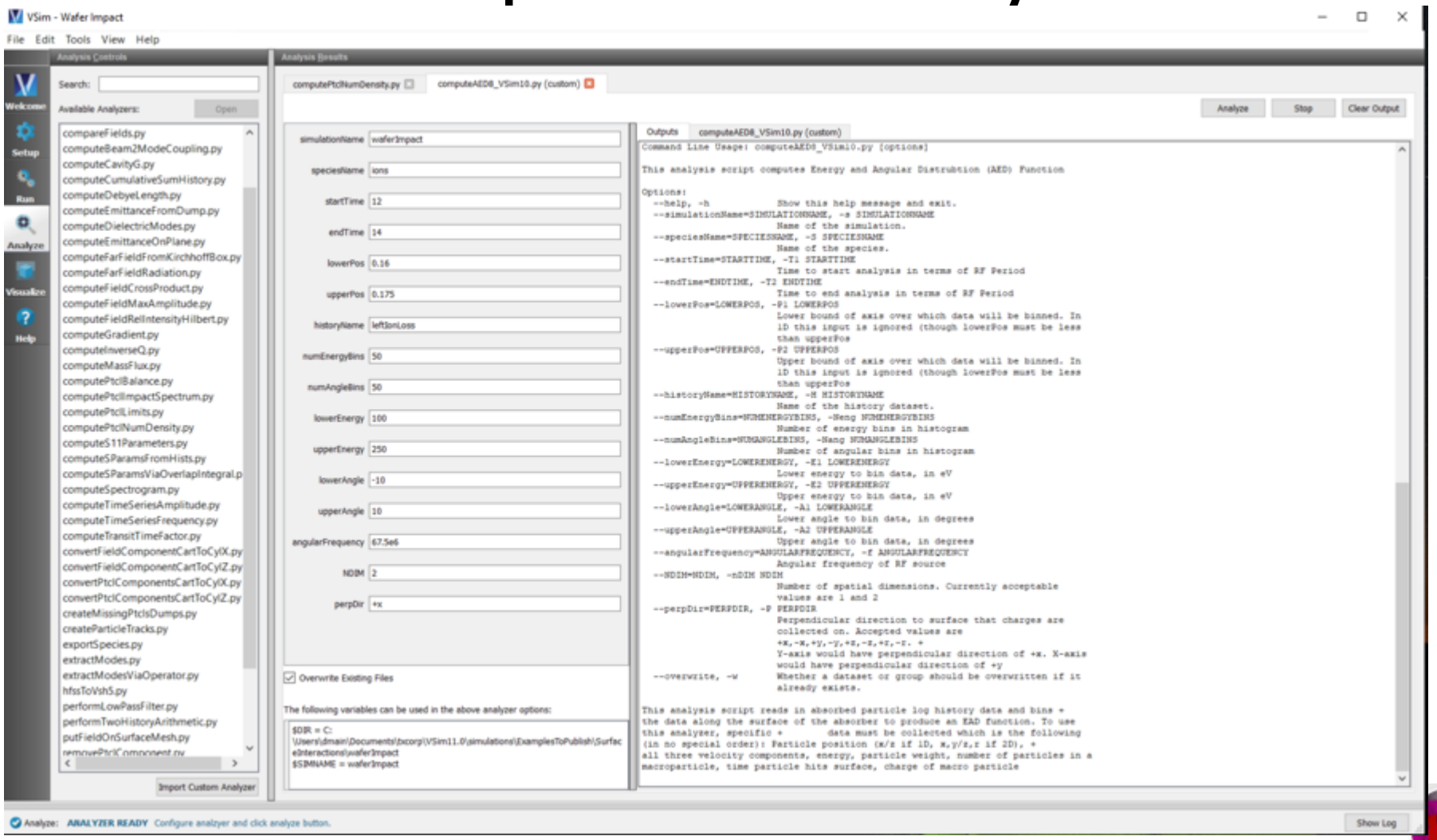


The higher FR causes greater inhomogeneity in the potential near the wafer edge (indicated by the vertical line)

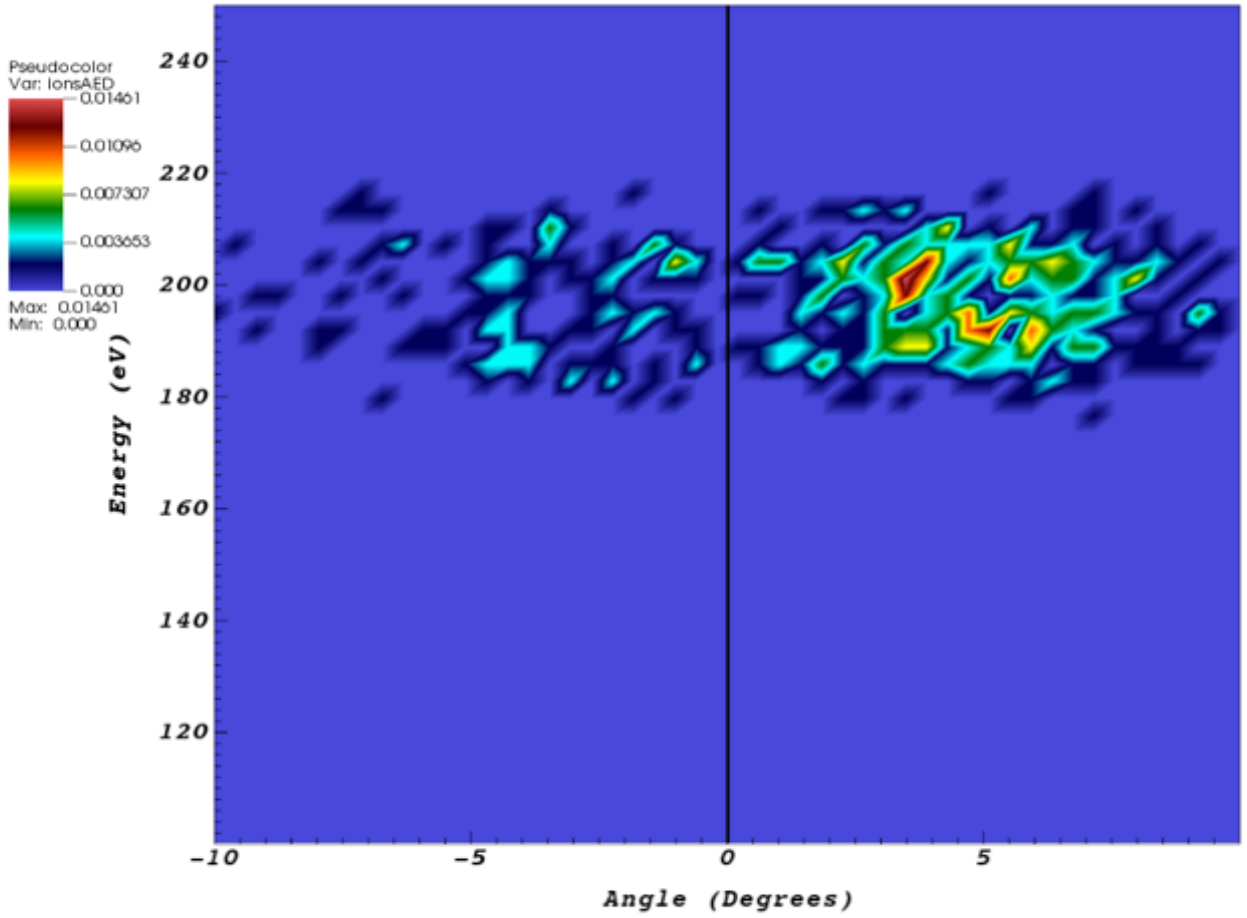
Angular Energy Distribution Function

- We built a new analyzer for these sorts of simulations
- Requires collecting the correct data along the wafer which includes the following:
  - Particle position
  - Particle velocity (all three components)
  - Particle energy
  - Weight of Particle
  - Particle charge
  - Time particle hits surface
  - Number of particles in macro particle
- All of this data is collected at each time step.
- The analyzer then bins the data along the surface and in time
- The analyzer then computes the angle and energy it hits the surface and bins the data using a 2D histogram function in Python.
- All of this can be done in VSim

Snapshot of Analyzer



Ion AED High Focus Ring



Data are binned between RF cycles 12 And 14 at last 1.5 cm of wafer (near FR)

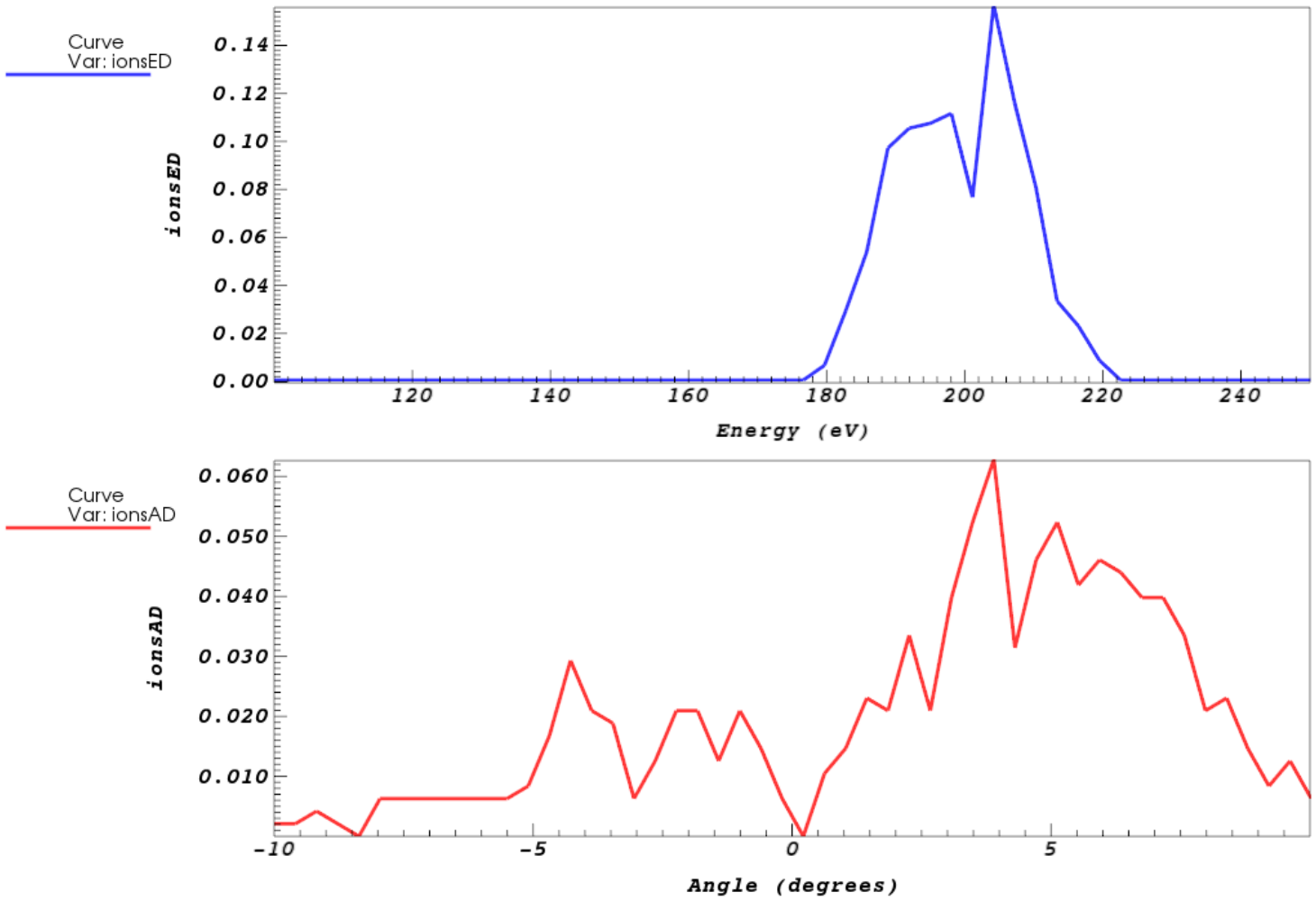
An obvious asymmetry is observed

Integrating along angle yields energy distribution

Integrating along energy yields angular distribution

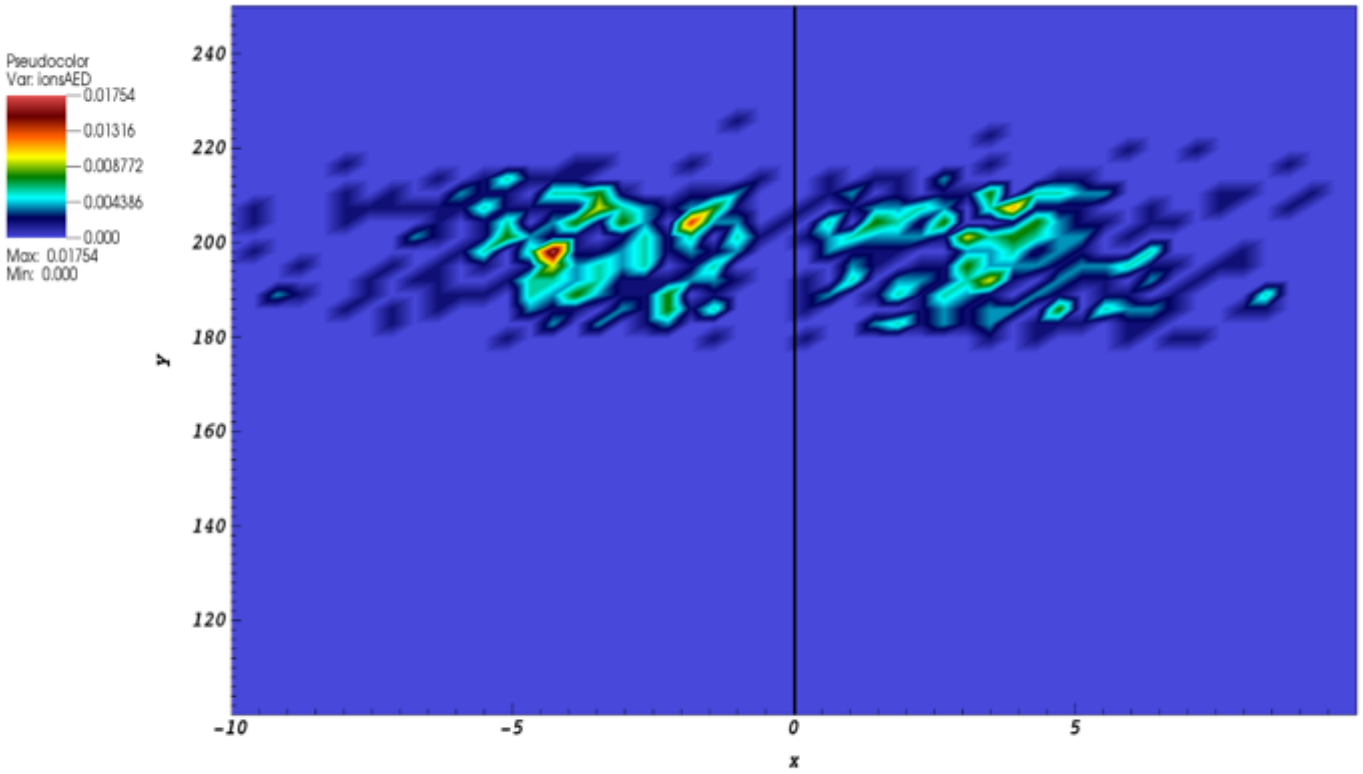
Both of these are also computed

1D Angular and Energy Distribution Functions: High FR



The asymmetry is also obvious in the 1D plot

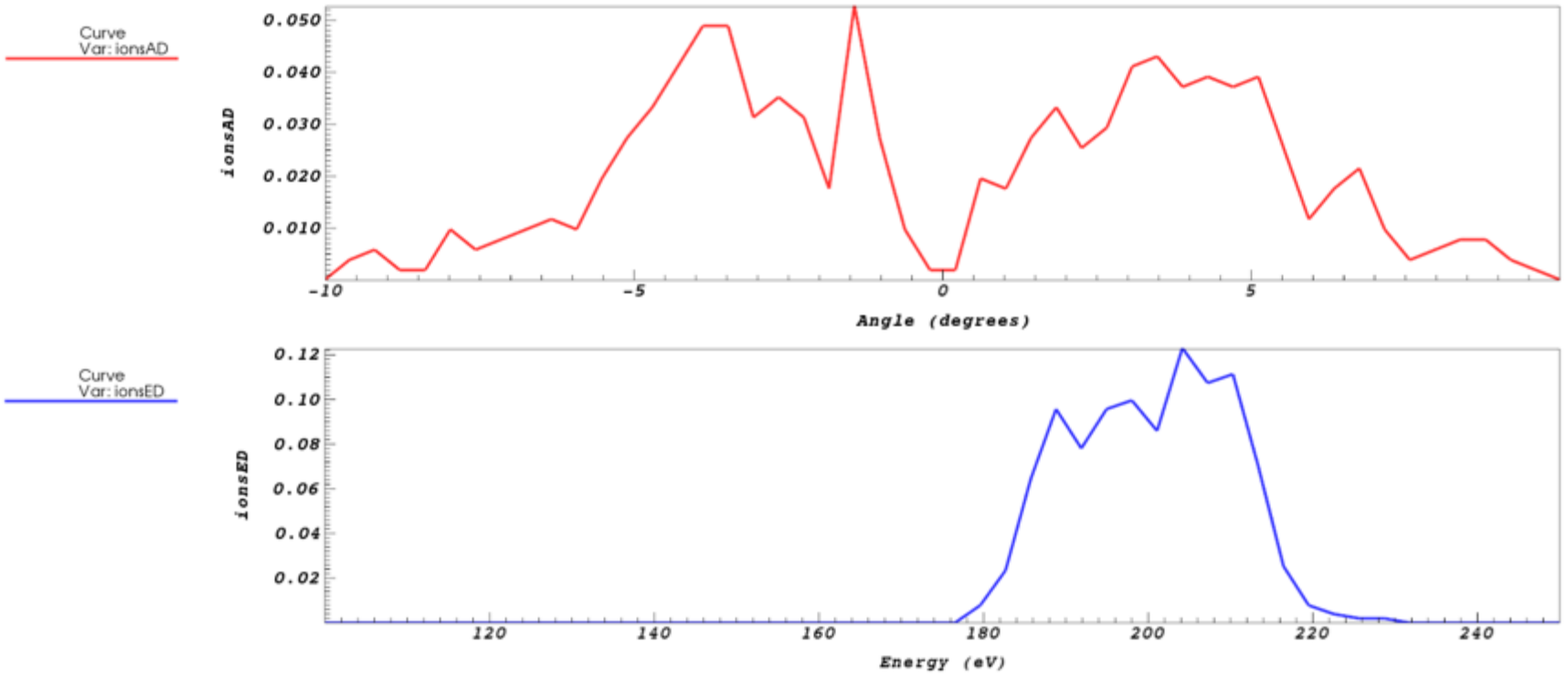
Ion AED Low Focus Ring



Same binning in time and space as before

A more symmetric distribution is now seen

1D Angular and Energy Distribution Functions: Low FR

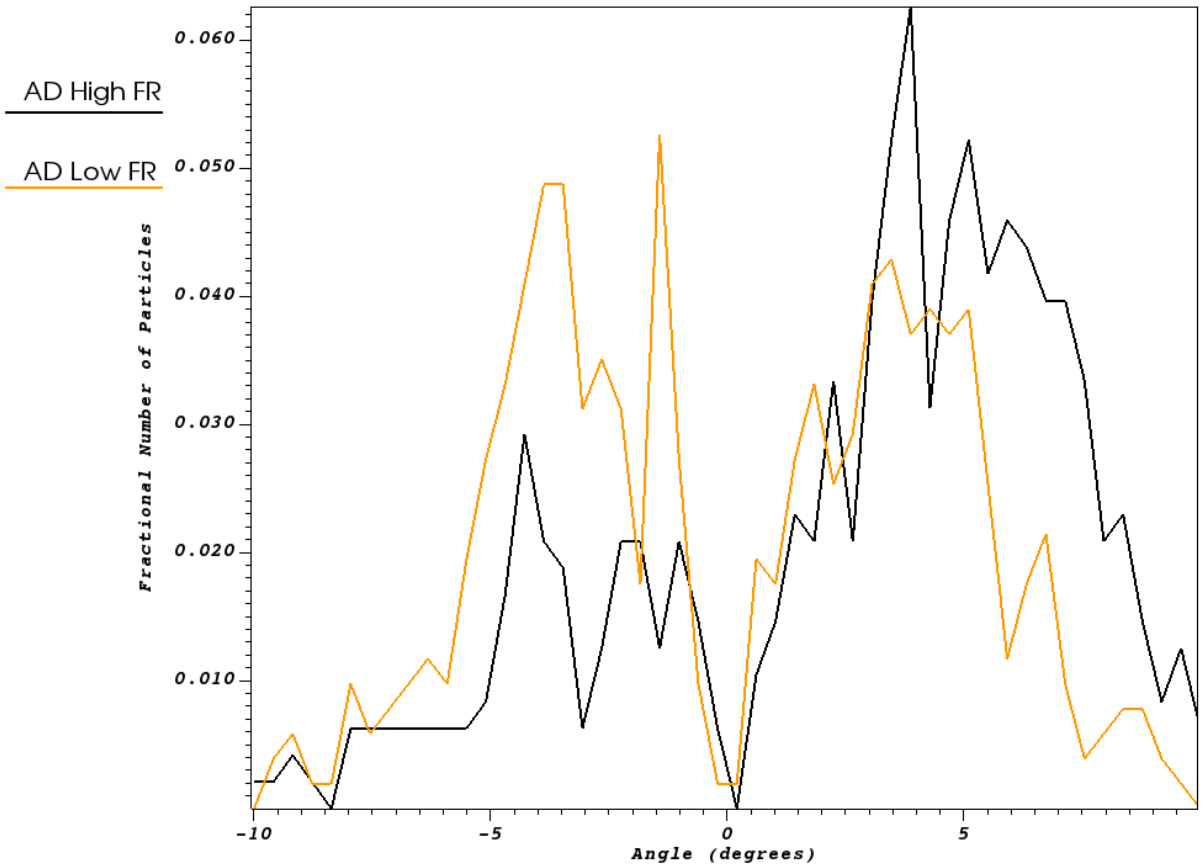


Angle

We now see a more Symmetric AD

Energy

Comparison of Low and High FR



Clearly there is an optimal height for the FR.

This optimal height can be found through multiple simulations with VSim

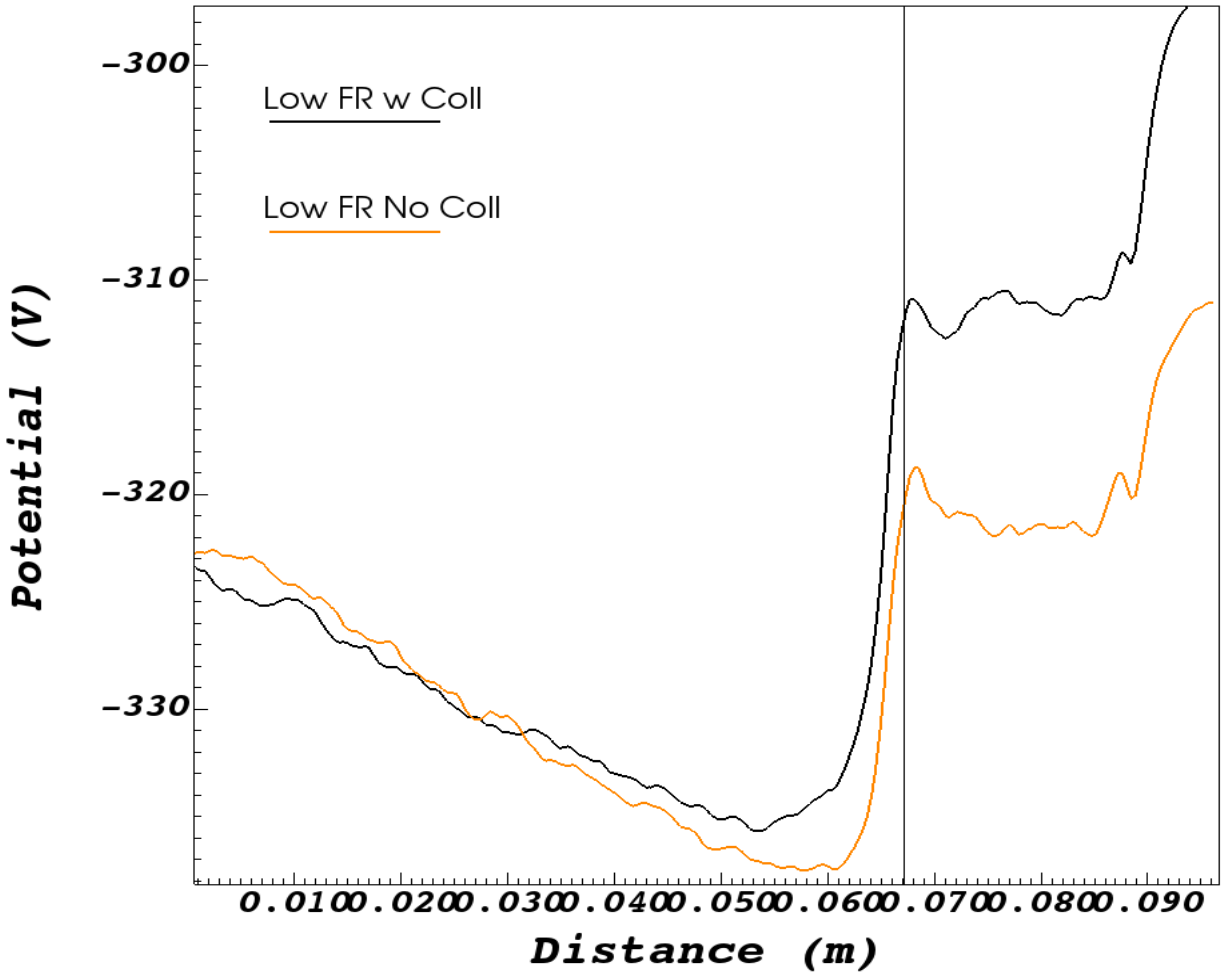
Role of Collisions

- We have added the following collisions:
  - Impact Ionization
  - Excitation (we chose the one with the largest cross section
  - Elastic Collisions
- Background neutral pressure ~ 0.15 Torr
- Arbitrary background densities can be used
- A few caveats
  - DX < MPF
  - DT < Collision Period
  - If collisions result on lots of new particles, very useful to use managed weights

A Word on Managed Weights

- In VSim, if lots of new particles are created due to ionization collisions, then this will slow down the simulation
- Managed weights allows particles to combine particles while conserving charge, density, fluxes, momentum, etc
- However, if there's not enough particles in a cell, the simulation will be very noisy.
  - So, you can also split particles to reduce noise if there are not enough particles to resolve the physics.

Comparing Run With and Without Collisions

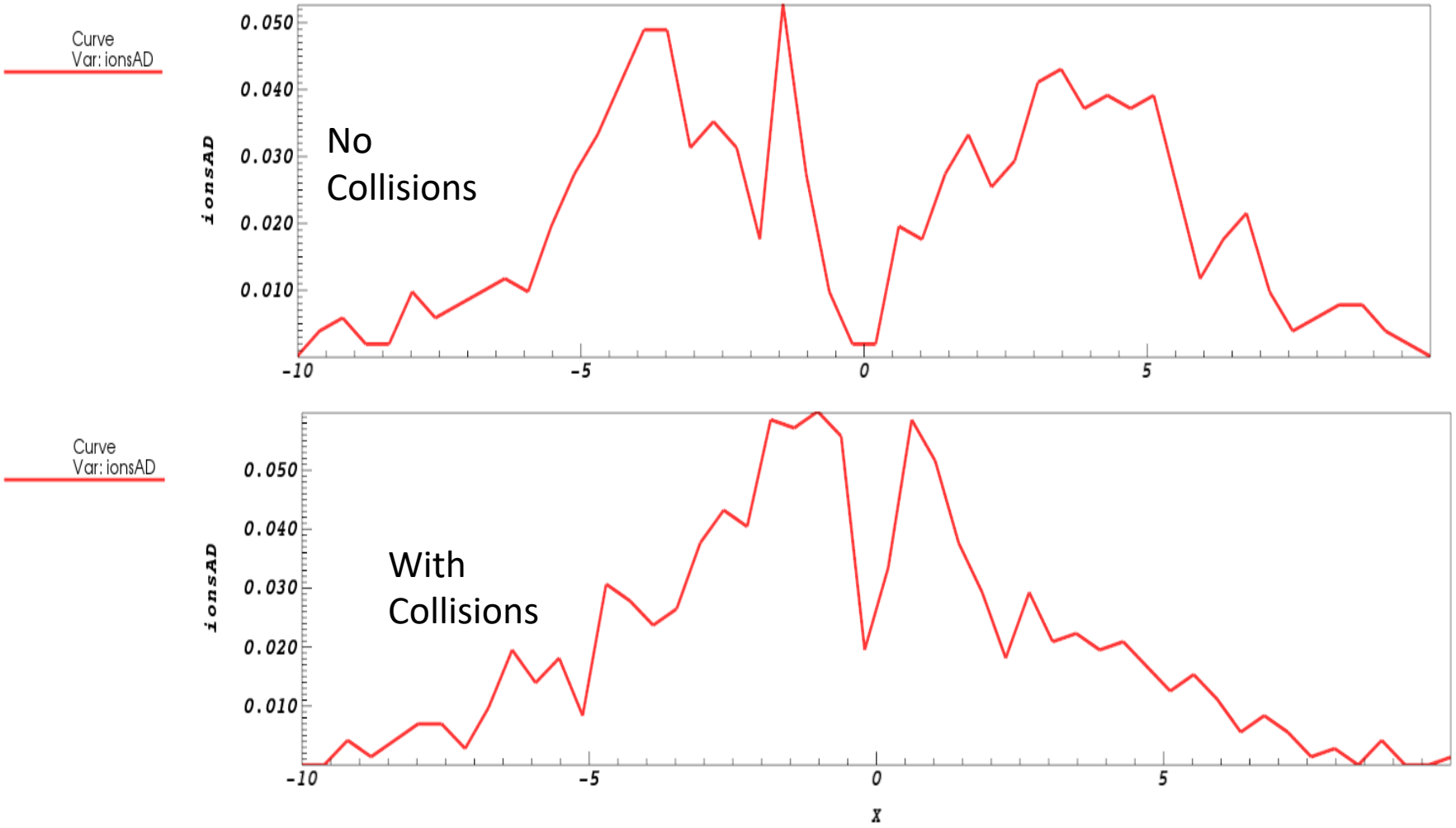


Plot of potential along wafer within sheath

Aside from an offset, the two plots look very similar

So potential doesn't tell us much

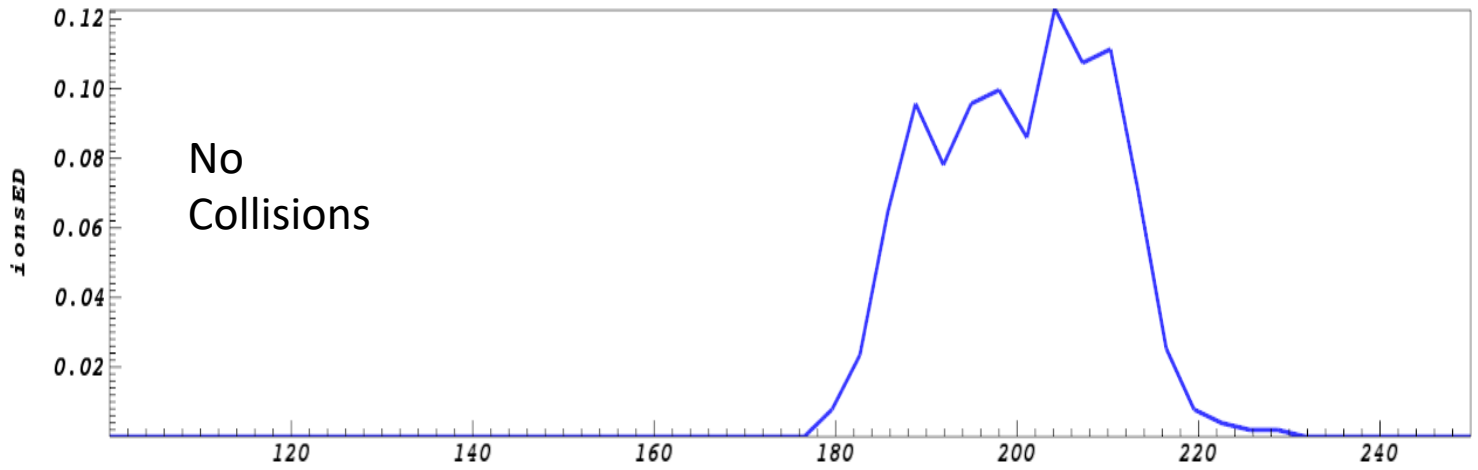
Compare AD plots

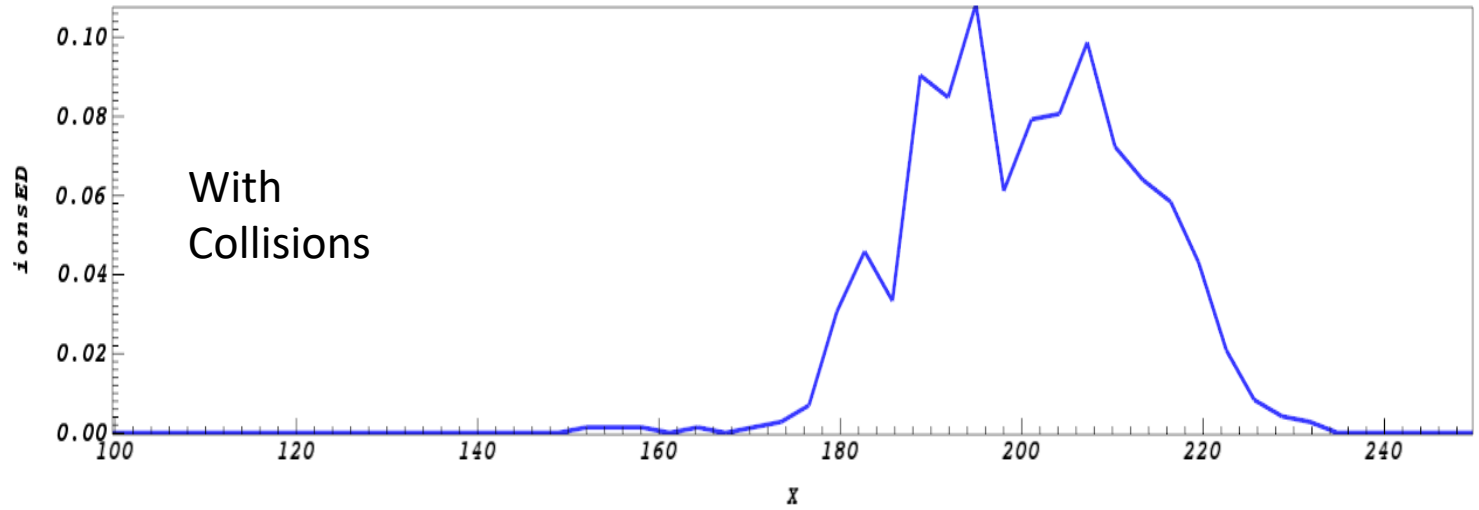


Collisions play an important role

Collisions fill in the AD so that more ions impact at a 90^{o} Angle (0^{o} w.r.t. surface normal)

Compare ED plots





Little Energy is lost due to collisions

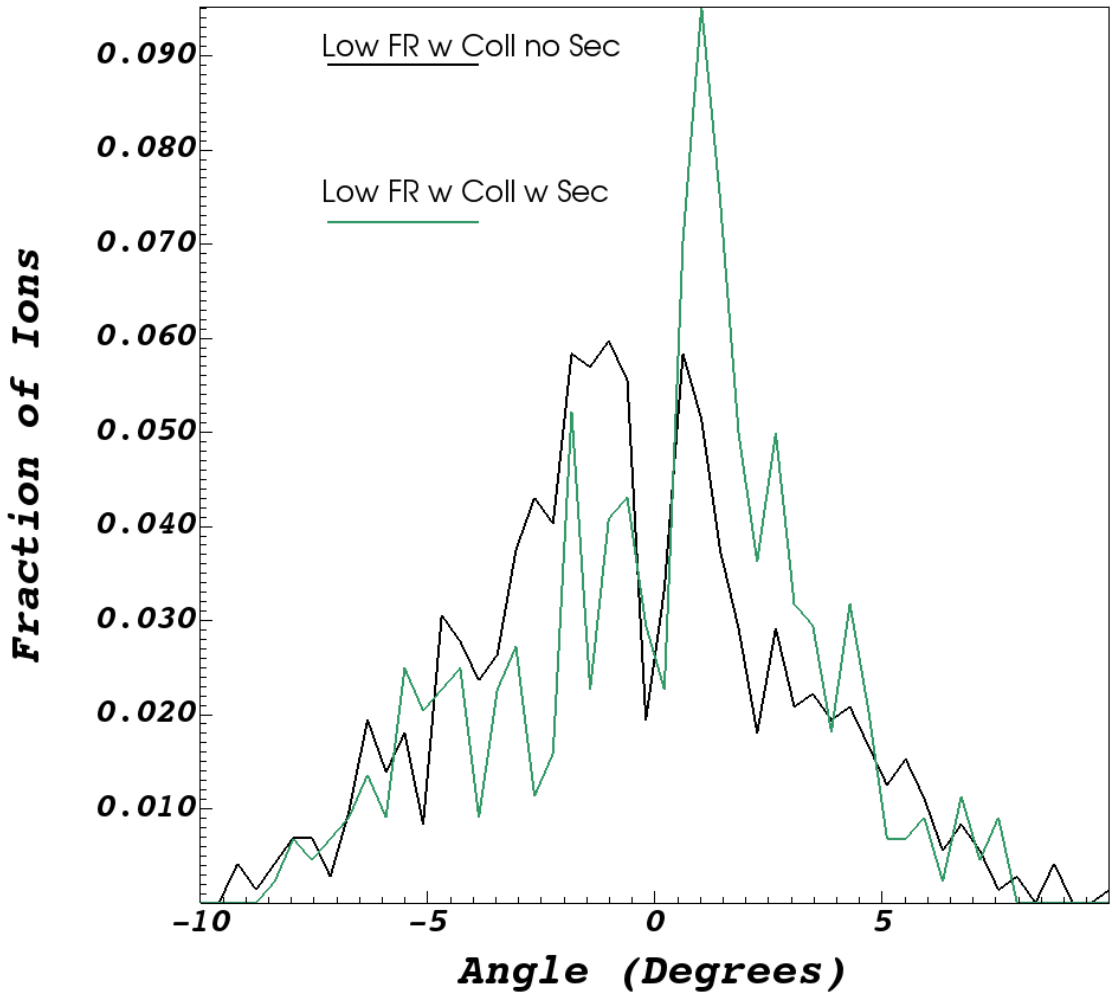
Keep in mind that the dominant collisional process is elastic which is energy conserving

At higher neutral densities we might see more energy lost

Now add Secondaries from Wafer and FR

- To model secondaries, I split both ions and electrons in to two equally dense population
- One population would accumulate on to the wafer and FR
- The other population, when striking the wafer or FR, could produce a secondary electron with a 30% probability

What Role do Secondaries Play?



We see that secondaries cause the AD to become asymmetric

Vsim can include sophisticated secondary emission models that allow the user to put in emission as a function of energy

Conclusion

- In this talk, I have discussed how VSim can be used to aid in the design of your wafer processing chamber
- VSim can be used in the following areas
  - Role of surrounding dielectrics in determining the homogeneity of ions impacting the wafer
  - Role of reactions
  - Determining optimum neutral pressure
  - Role of secondary electrons and how to account for or subtract out their effect

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