Description and Testing of the GITR Surface Model

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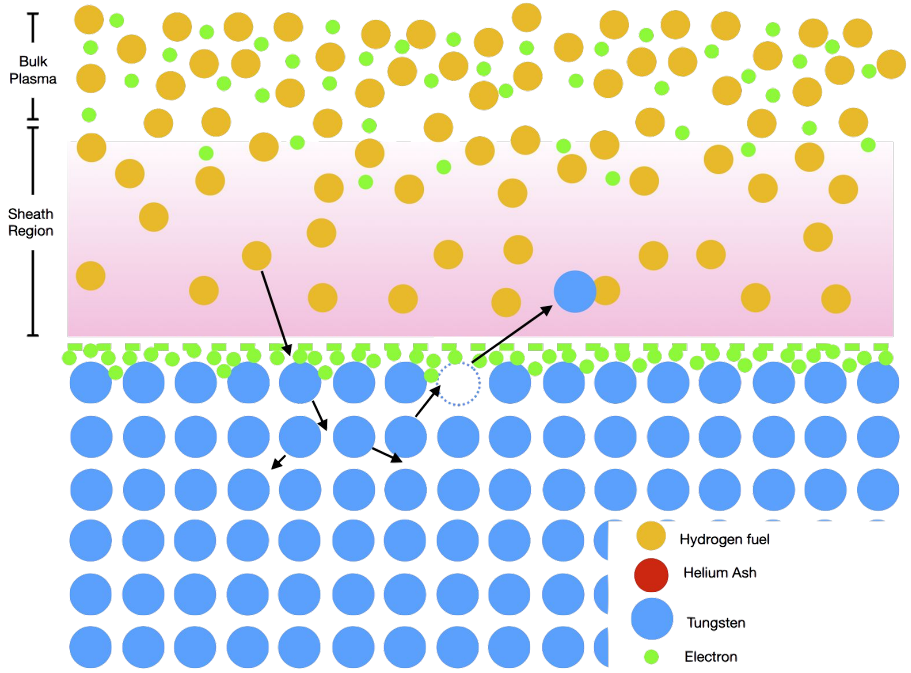
Tim Younkin

What do we mean by surface model?

- We mean what happens when at atom/ion hits the surface
  - Deposition
  - Sputtering
  - Reflection

Physical sputtering of wall material is the predominant source of impurities during steady-state plasmas



$$Y(Ion, Material, E_{impact}, \theta_{impact})$$

Sputtered atom energy and angular distributions of sputtered particles are dependent on material properties such as surface binding energy E_b

- Charged particle physical sputtering (hydrogen and impurities)
- Chemical sputtering
- Neutral particle sputtering (fast charge exchange)
- Evaporation of material from over-heating
- Desorption from the wall surface by ions, electrons, or photons
- Arcing and run-away electrons

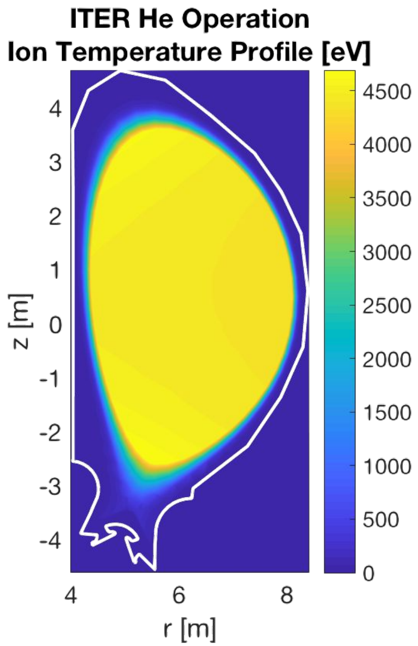
	Erosion Rate	Erosion per year	Lifetime (shots)
Gross Erosion	2 nm/s	6 cm	10,000
Net Erosion	0.3 nm/s	0.9 cm	60,000

Estimates are based on steady-state assumptions for 400s Q=10 ITER discharge.

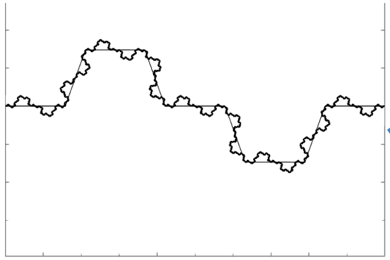
Joachim Roth. Recent analysis of key plasma wall interactions issues for ITER. Journal of Nuclear Materials 390–391 (2009) 1–9

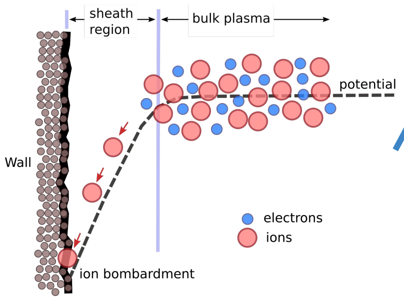
Varying Temporal and Spatial Scale Physics Create the Need for Integrated Physics Models

Bulk Plasma - Meter length scale, evolves on millisecond time scale. Averaged particle motion can be treated as a fluid.

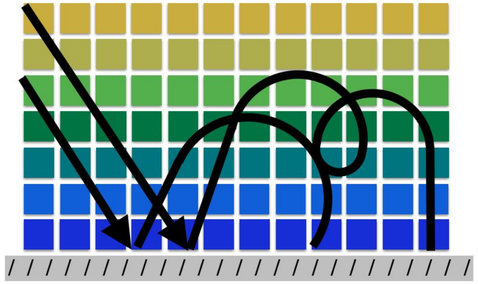


Ion-surface interaction - Sputtering, reflection, and implantation occur on the nm length scale and ns time scale.



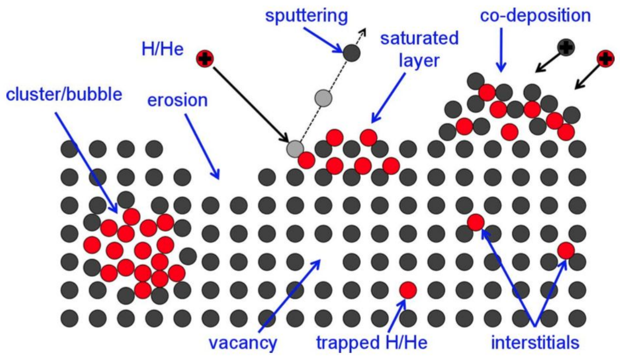


Sheath electric field structures - micron length scale, evolves on the sub-microsecond times.

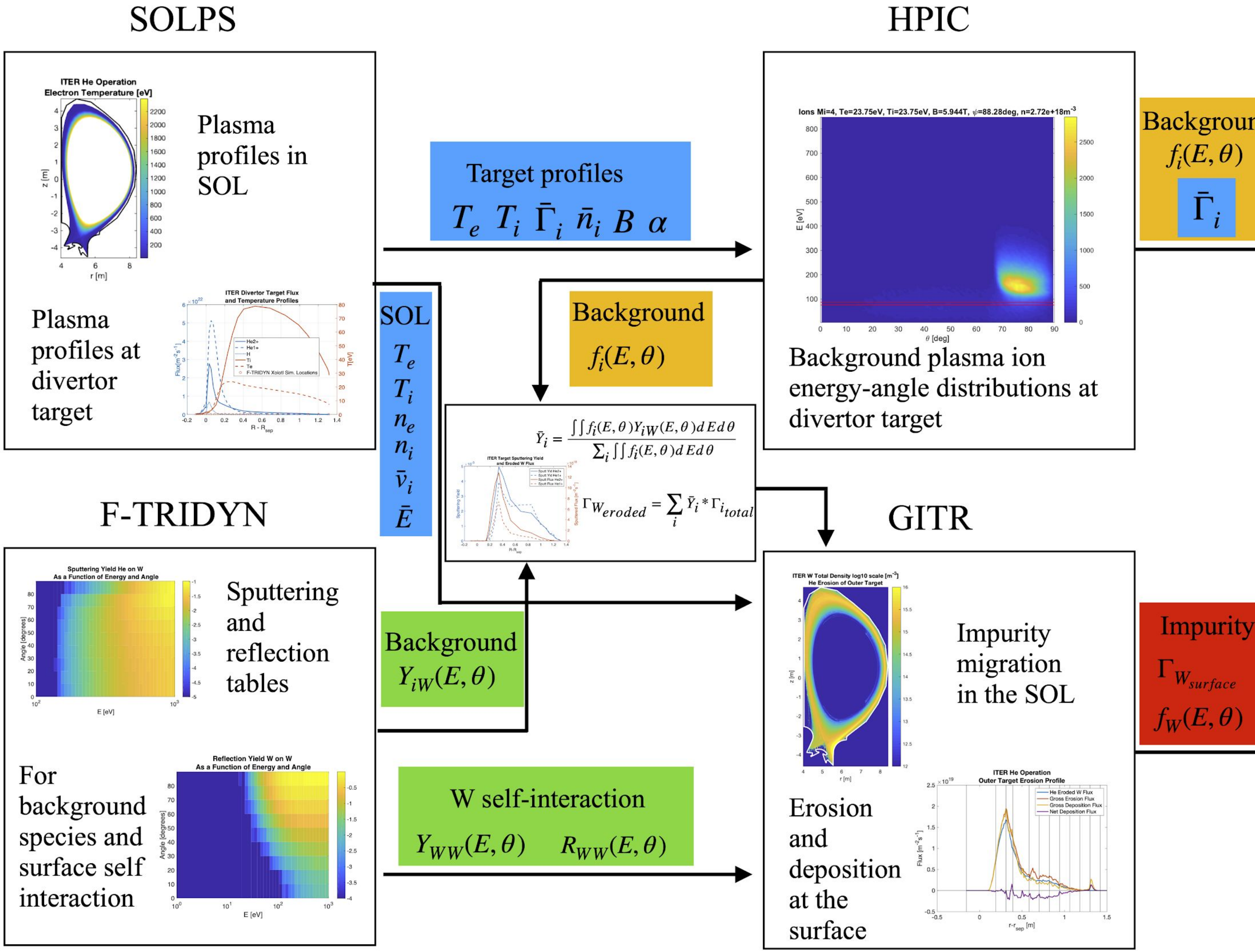


Surface sputtering, impurity migration, and redeposition - nanosecond to second migration times, nanometers to many meters.

Erosion and implantation of ions. Subsurface concentration formations and surface morphology evolution - nm to meters. from seconds to years



PSI Workflow



What is the current approach in GITR?

- Currently, GITR treats erosion due to the “background” plasma as a constant in time. This an input and gives a steady state flux “boundary condition” of eroded atoms.
- The material which is being eroded is the atom/impurity species which is tracked, which interacts with the surface of the same material.
- In mixed material systems we have treated impacts on materials different than the impurity species as 100% deposition (no sputtering or reflection).

Tracking eroded and reflected species uses a statistical/computational weighting approach

- GITR CPC paper example
- Y = 0.1, R = 0.5
- nP = 100 particles hit a surface, all which initially have weight 1
- 10 will sputter, 50 will reflect, 50 will gross deposit, 40 will net deposit
- We now represent the 10 sputtered particles as Y*nP/(Y+R) = 17 computational particles with weight (Y+R) = 0.6
- The 50 reflected particles are represented as R*nP/(Y+R) = 83 computational particles with weight (Y+R) = 0.6

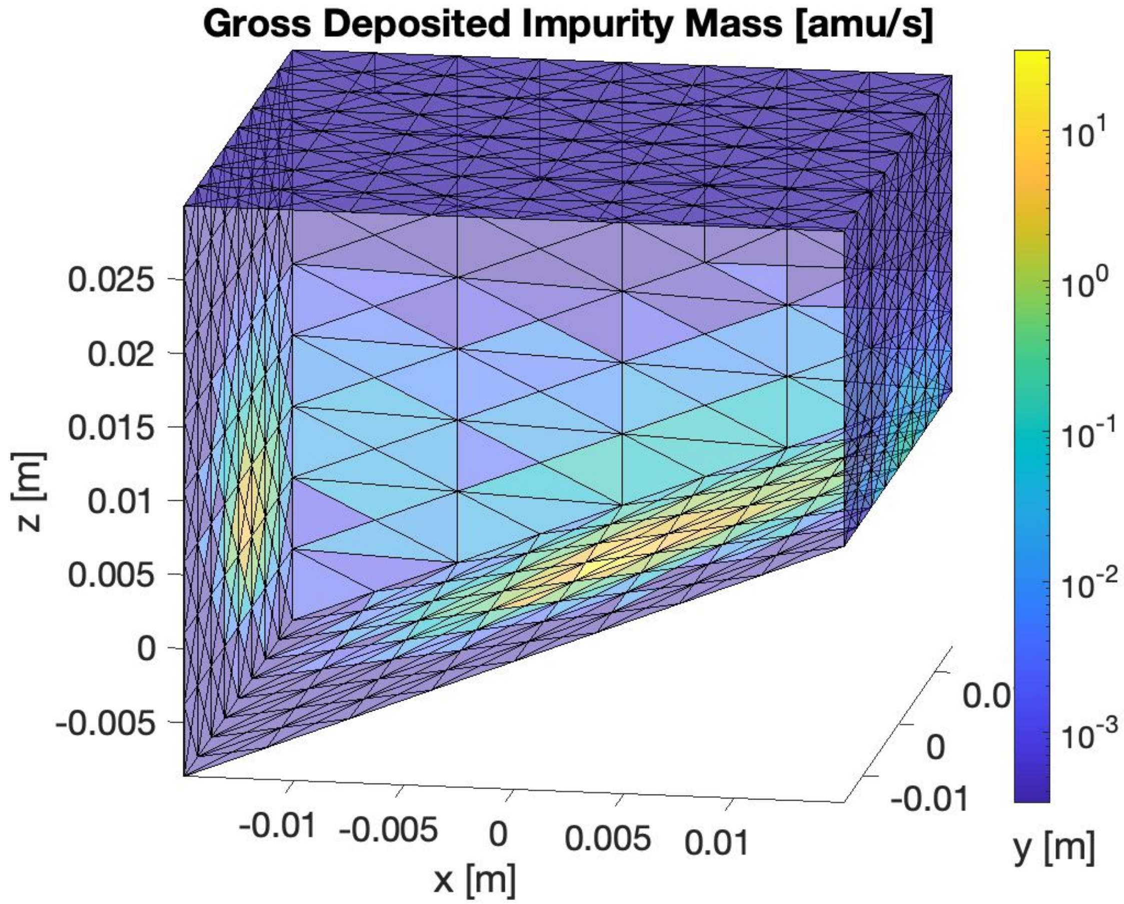
The outcome

- This example ignores the details of transport, but as long as the particles continue to hit the walls, there will be deposition, sputtering, and reflection.
- The weight of the particles will continue to approach zero.

$$grossDeposition = nP*(1-R)\sum_{i=1}^{\infty}(Y+R)^i$$
$$= nP * \frac{1-R}{1-(Y+R)} \quad (9)$$

The outcome

```
K>> sum(grossDep(:))

ans =

     1.249999839624124e+03

K>> sum(grossEro(:))

ans =

     1.249999839624136e+03

K>> sum(grossDep(:))-sum(grossEro(:))

ans =

    -1.227817847393453e-11

K>> sum(weight(:))

ans =

     1.217912297328868e-11
```

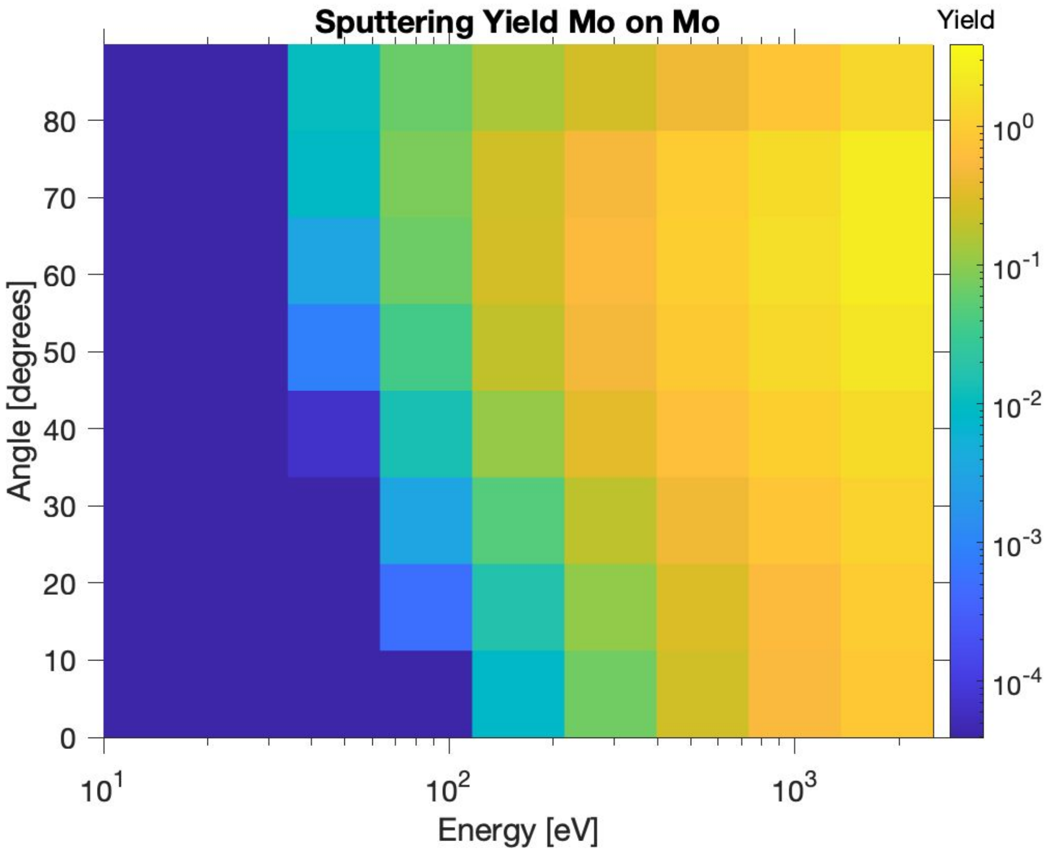


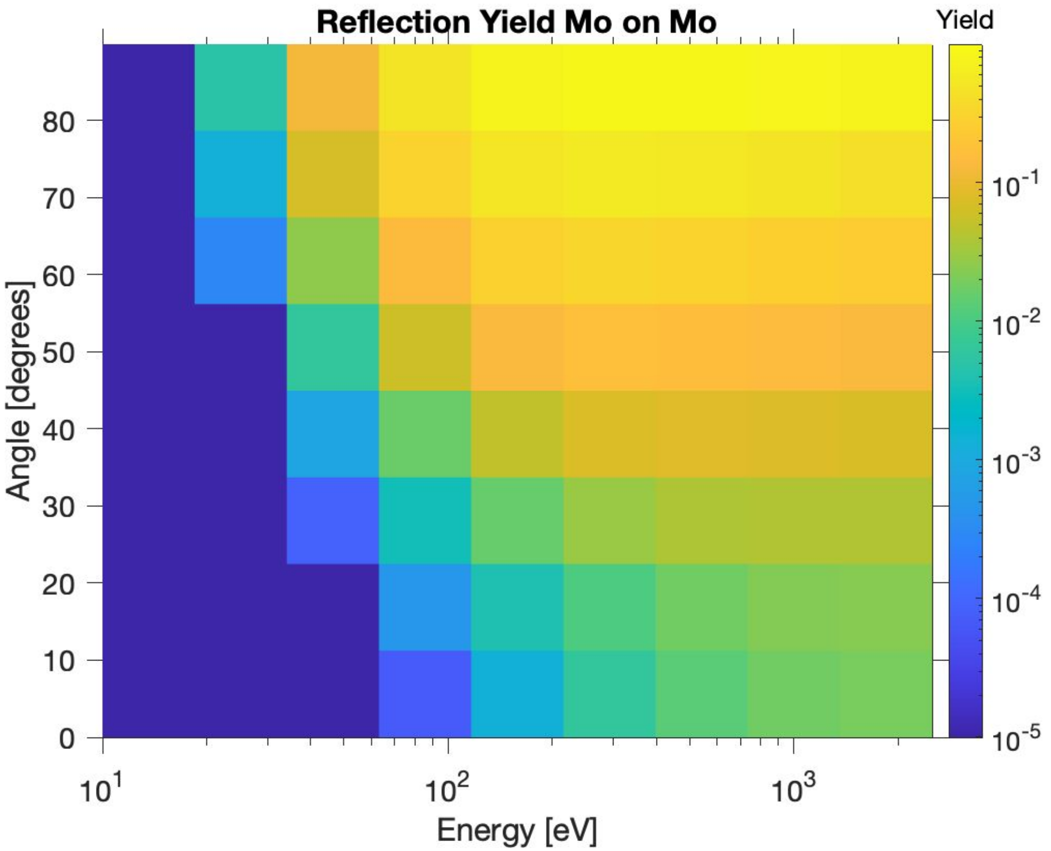
Good things about this approach

- The benefit of this approach is that we are using all of our simulated particles all the time (in this example where Y and R are always > 0).
- We know how many particles we have, so we can predict execution time (i.e., we’re not spawning new particles which could add to unpredictability in runtime).
- We are getting better statistics than we would if we were killing off 40% of our particles each generation of impact (We’re getting more lower weight impacts, as opposed to a single weight 1 impact for each sputtered/reflected particle).

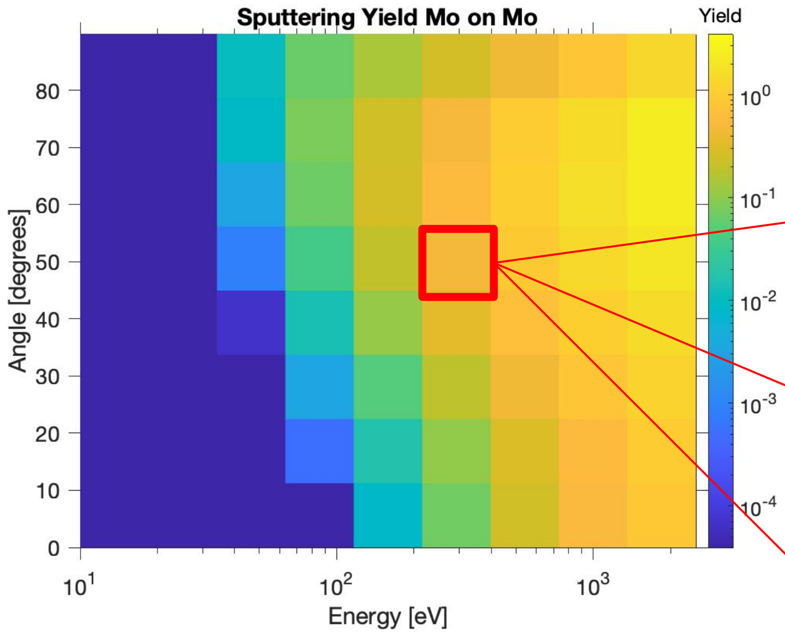
How do we use F-TRIDYN

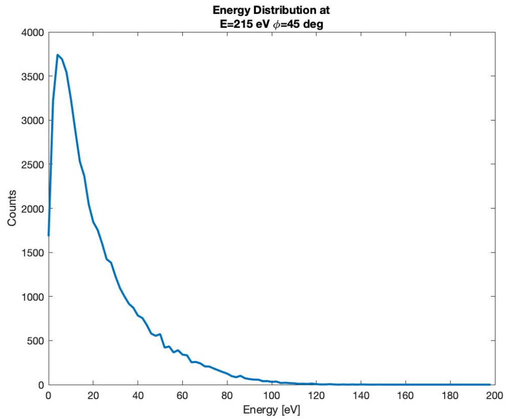
We run lots of FT simulations with fixed energy and angle of impact to create look-up tables for GITR.



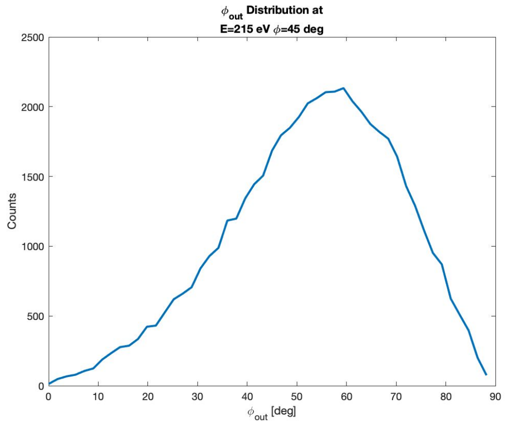


Each tile gives 3 distributions

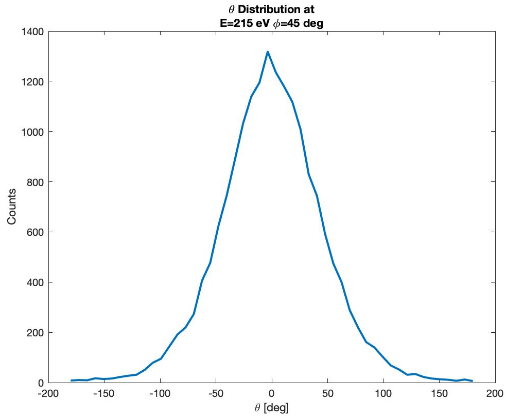




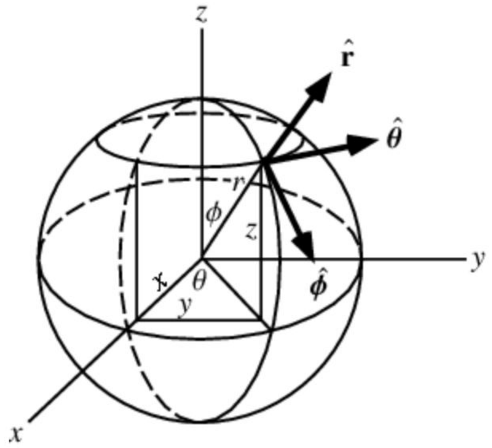
f(E)



f(phi)



f(theta)



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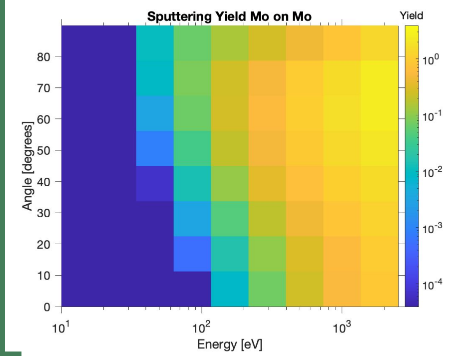
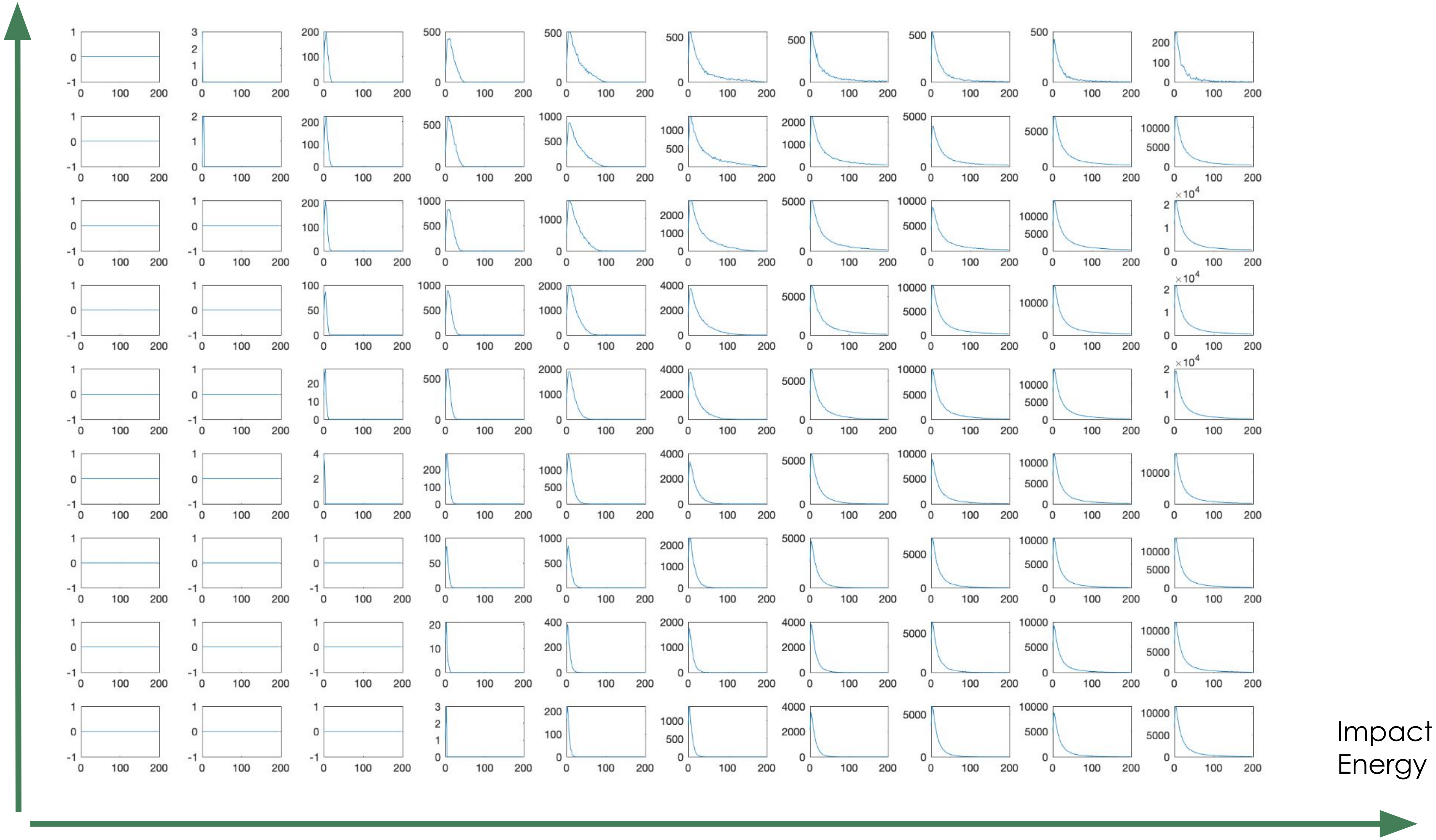
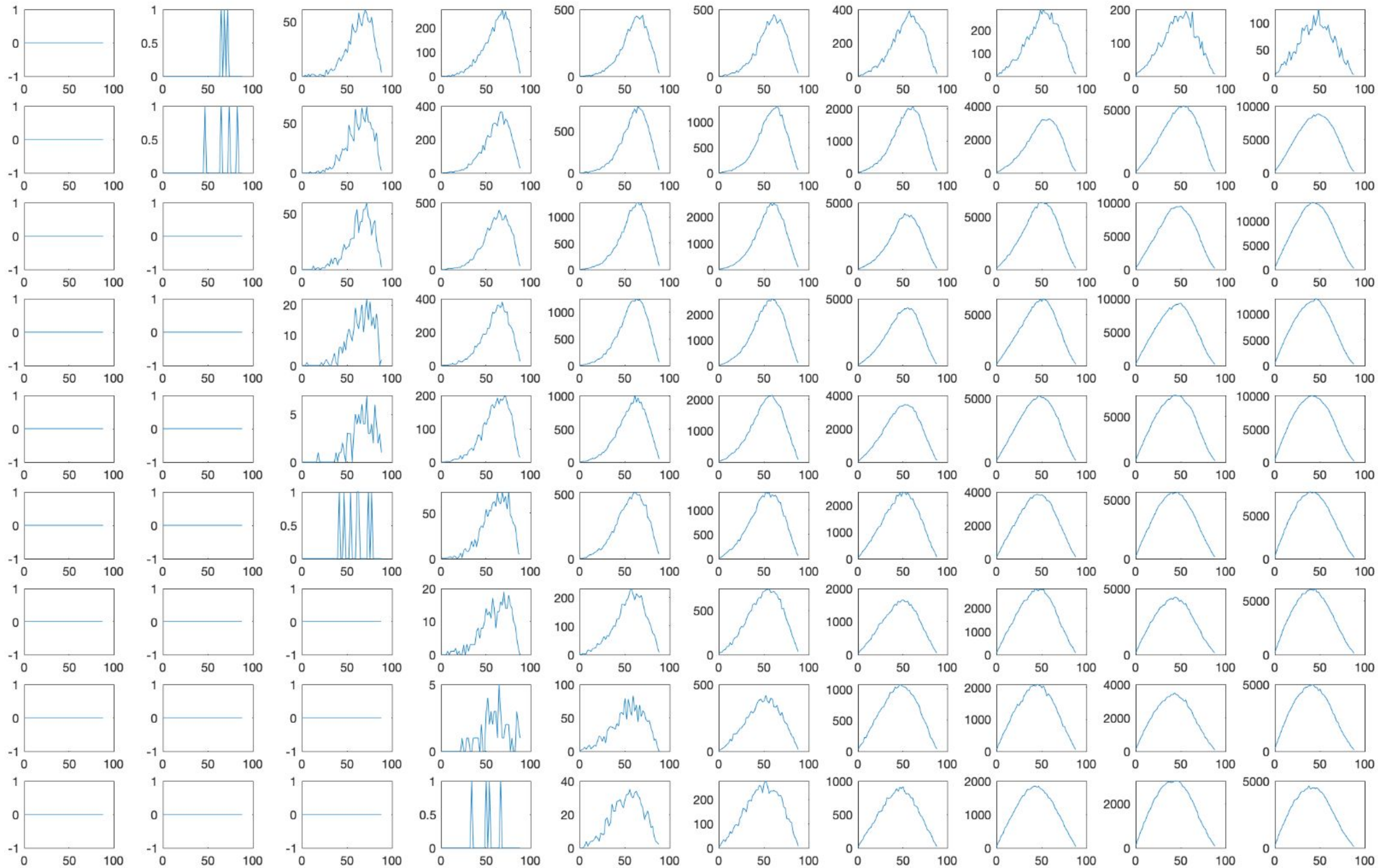
Sputtered Atom Energy Distribution

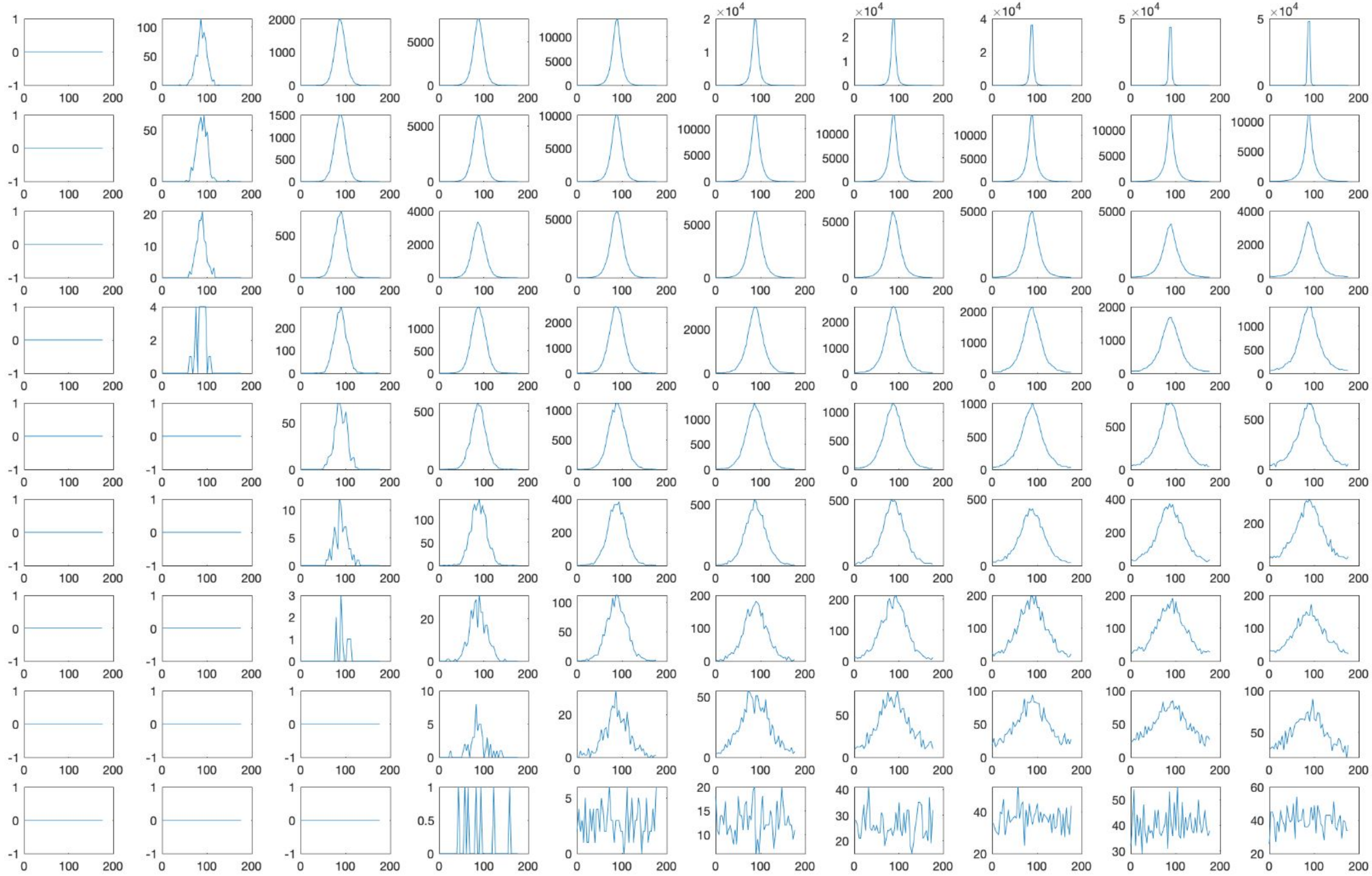
Impact Angle



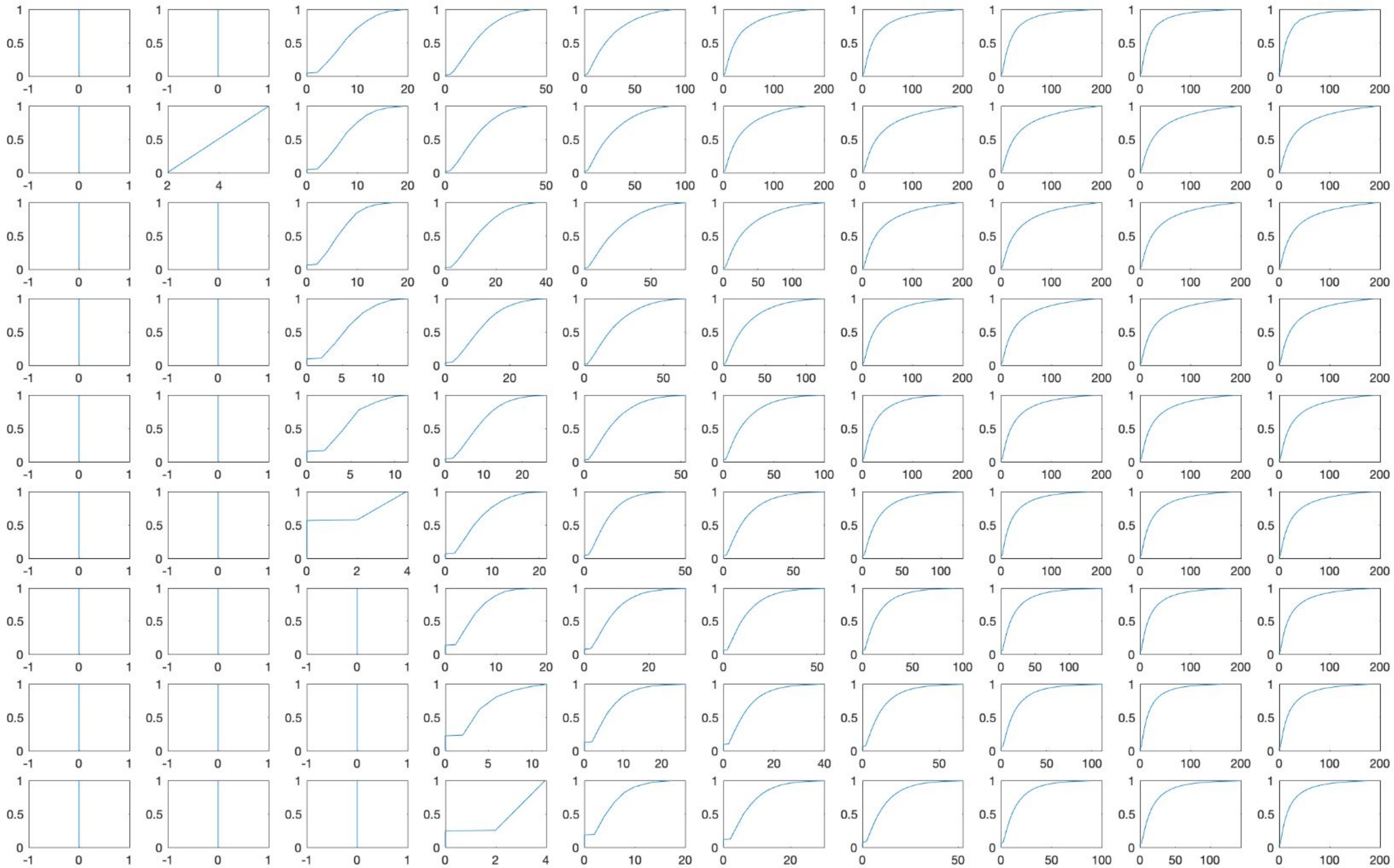


Impact Energy





Further processing within GITR makes these into regularly spaced CDFs



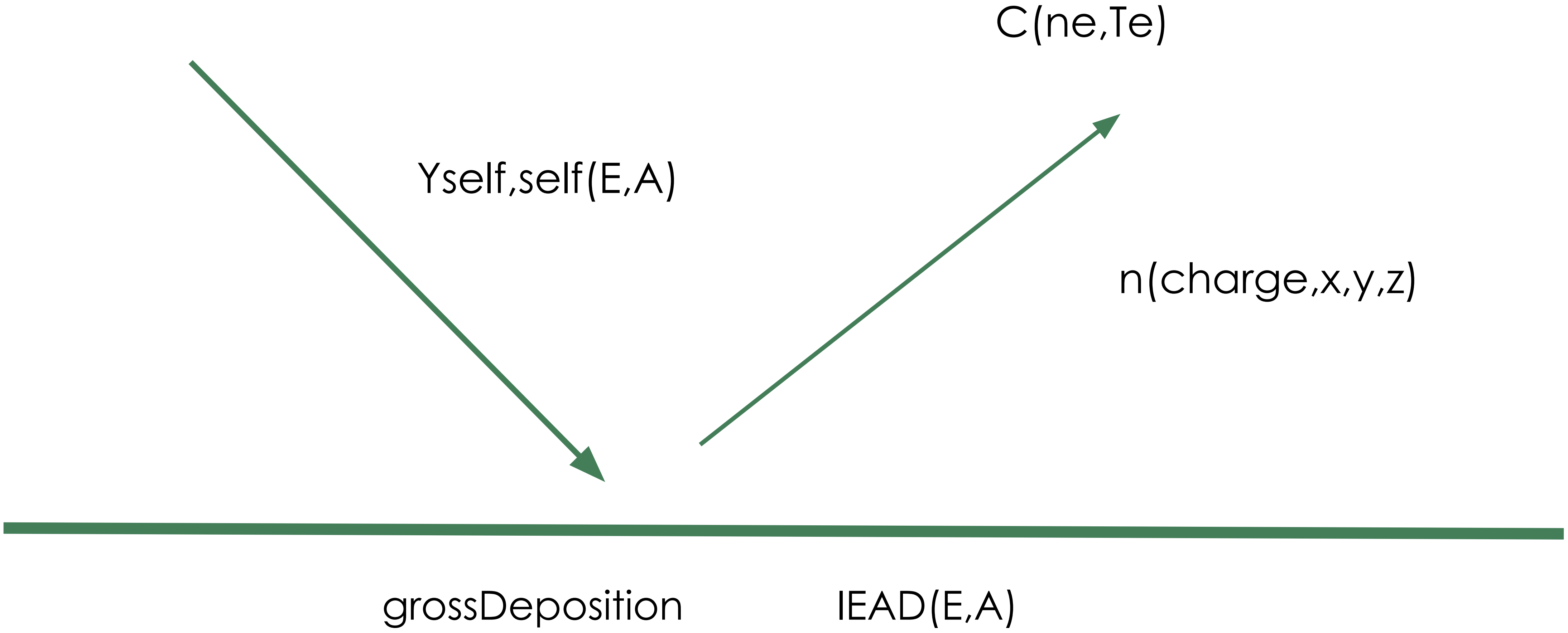
Drawbacks to current surface model

- No correlation between 1D distributions (energy, angles) - low energy sputtering may be high angle and vice versa, but GITR averages over them all.
- Low sputtering yield will inherently have bad distributions. Adding more particles will give lower yields which will also have poor distributions.
- Interpolation between energies/angle distributions doesn't really represent the physical processes

Going to Multi-species

- Currently, GITR simulations of different species can be run separately.
- This omits the effect of impurities reflecting off of and sputtering material of a different surface composition.

This requires added dimensions for storage arrays (inputs and outputs)



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