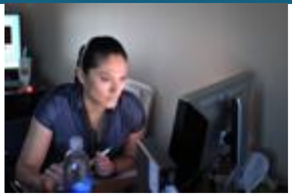
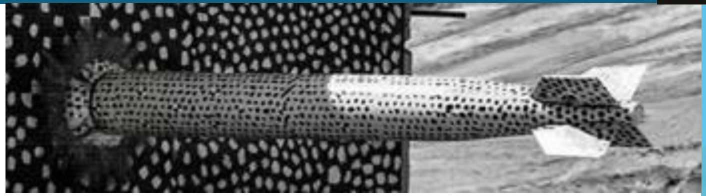
General Thermal-Field Emission and Space-Charge Limits for Particle-In-Cell and Nexus Theory





MeVArc Workshop 2024

Adam M. Darr

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Space-Charge Limited (SCL) and General-Thermal-Field (GTF)

Gauss's Law gives the fields (displacement, $\vec{D} = \epsilon_0 \vec{E}$ [electric field $\vec{E}$], sans polarization)

$$\nabla \cdot \vec{D} - \rho = 0$$

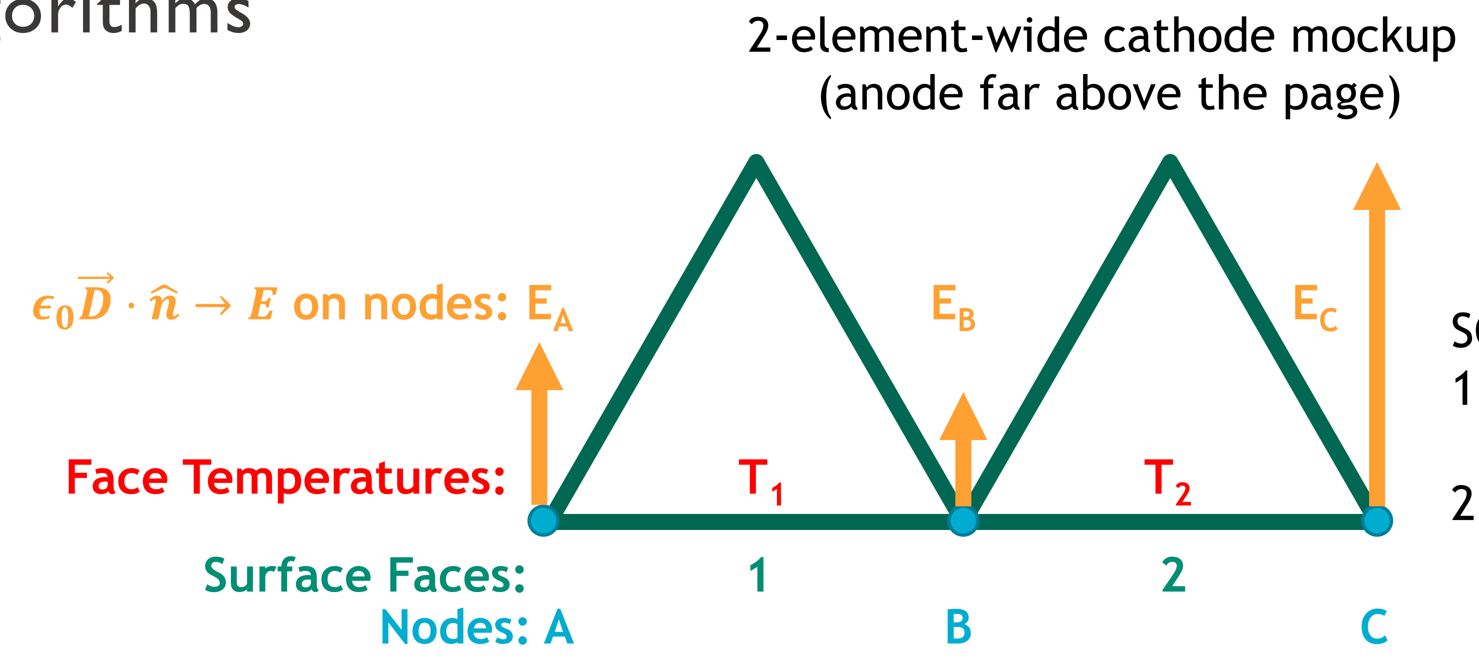
However, for classic Child's equation, $\vec{D} \cdot \hat{n} \rightarrow 0$ at the emitter. Weak form of Gauss's Law allows implied $\vec{D} \cdot \hat{n} = 0$ to be achieved each timestep by injection of additional charge.

Slight variation on the computation allows $\epsilon_0^{-1} \vec{D} \cdot \hat{n}$ to be exposed for GTF. Temperature T is handled by Empire (constant, scaled to time, or self-consistent over time). Then,

$$J_{GTF} = J_{GTF}\left(\vec{E} \cdot \hat{n}, T\right)$$

See Kevin Jensen, "A reformulated general thermal-field emission equation," *Journal of Applied Physics* **126**, 065302 (2019).

Algorithms



SCL:

1. Calculate charge creation on nodes.
2. Emit on surfaces the node is a member of.

GTF (present):

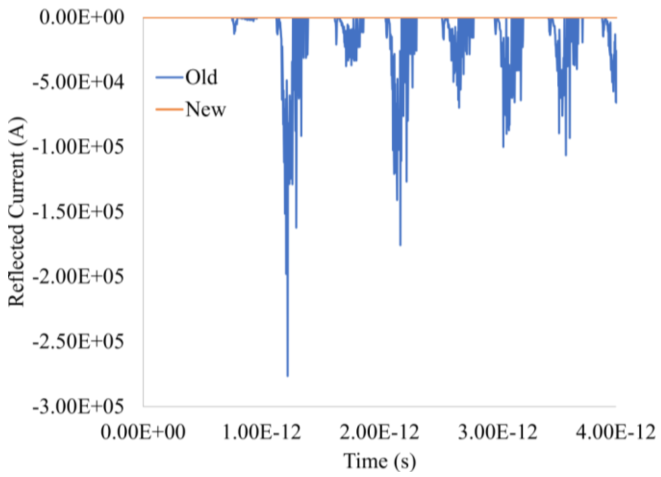
1. Calculate average current density on surfaces: $J_1 = [J(E_A, T_1) + J(E_B, T_1)]/2 \equiv (J_{1A} + J_{1B})/2$.
2. Calculate charge created: $Q_1 = J_1 A_1 \Delta t$.
3. Split Q among nodes the surface is a member of (??).
4. Emit on surface the node is a member of (????). $Q_1 = \Delta t(0.5 J_{1A} A_1 + 0.25 J_{1B} A_1 + 0.25 J_{2B} A_2)$.

GTF (future):

1. Calculate current density. Average on surfaces? Average on nodes? On nodes with average T?
2. Once surface current density is known, emit calculated charge on surface [eliminate legacy steps 3-4, $Q_1 = A_1 \Delta t (0.5 J_{1A} + 0.5 J_{1B}) = J_1 A_1 \Delta t$]. Better ways to do this?

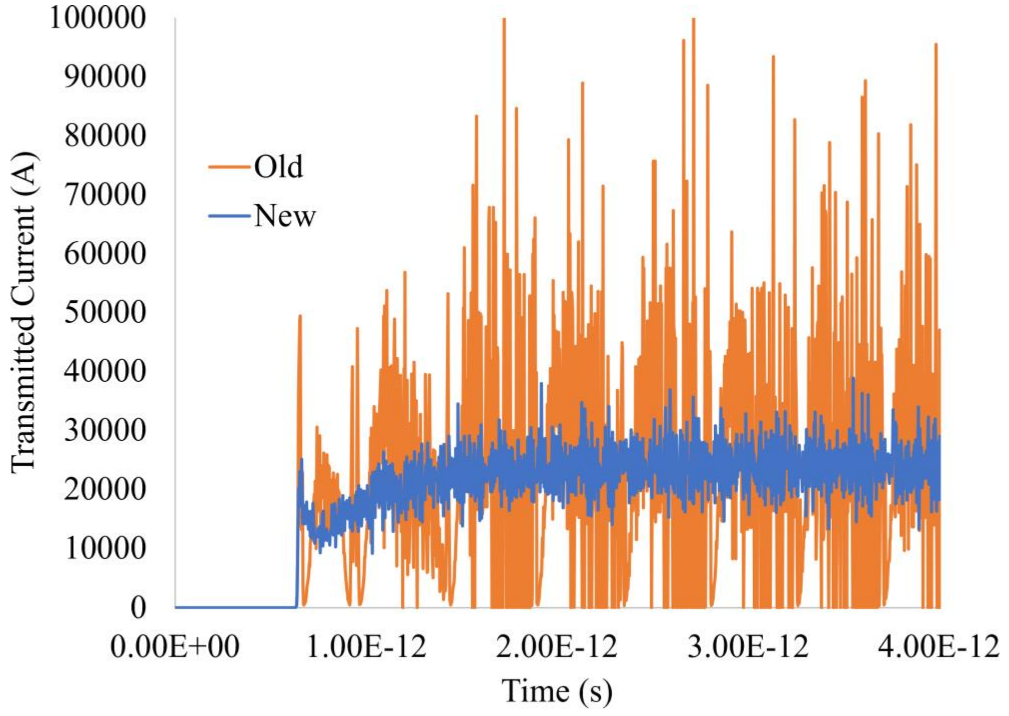
Algorithms

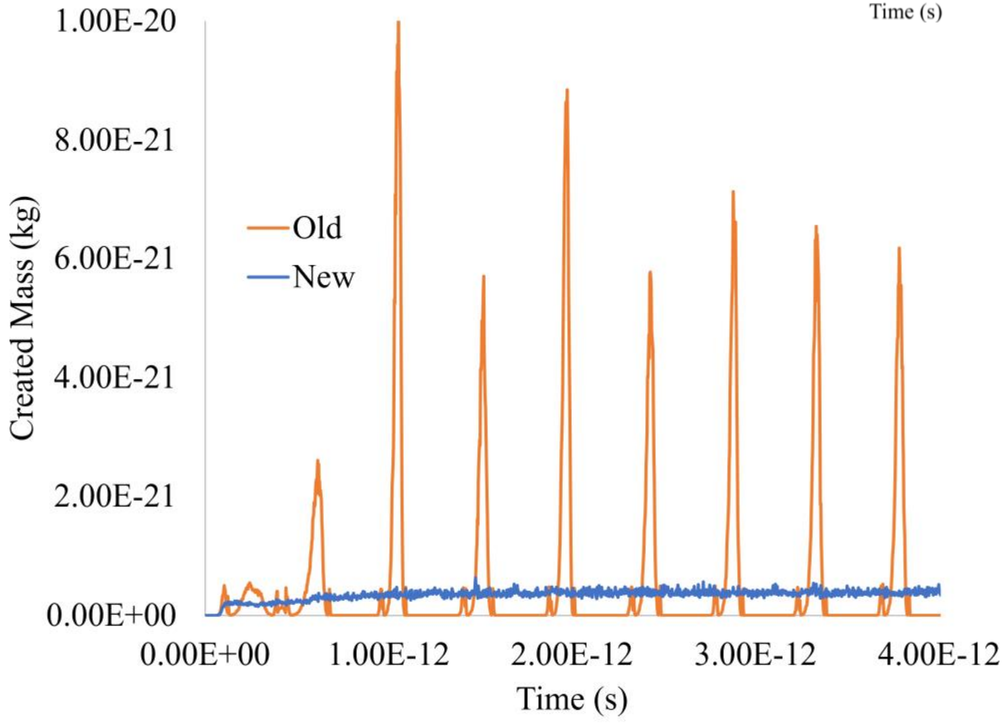
Old did not account for boundary-cell charge



On the importance of good Electric Field calculations.

Note: time-averaged answers both agree with theory (!!)





Nexus Theory

Single-physics is easy! With voltage V, gap distance D, temperature T, work function Φ…

Field emission (Fowler-Nordheim; approximate, since even one electron still modifies E):

$$J_{FN} = A_{FN} E^2 \exp\left(-\frac{B_{FN}}{E}\right) \approx A_{FN} \left(\frac{V}{D}\right)^2 \exp\left(-\frac{B_{FN} D}{V}\right)$$

Thermal emission (Richardson-Laue-Dushman; A_{RLD} is a bundle of fundamental constants):

$$J_{RLD} = A_{RLD} T^2 \exp\left(-\frac{\Phi}{k_B T}\right)$$

Space-charge limited emission (Child-Langmuir):

$$J_{CL} = \frac{4}{9}\epsilon_0 \sqrt{\frac{2e}{m}} \frac{V^{3/2}}{D^2}$$

Forbes-Deane gives lovely, fundamental forms and a few elliptic integrals for A_{FN}, B_{FN}

Standard references apply

Nexus Theory

Handwaving the non-dimensionalization (bars; cf. A. M. Darr et al. Phys. Rev. Res. **2**, 033137, 2020):

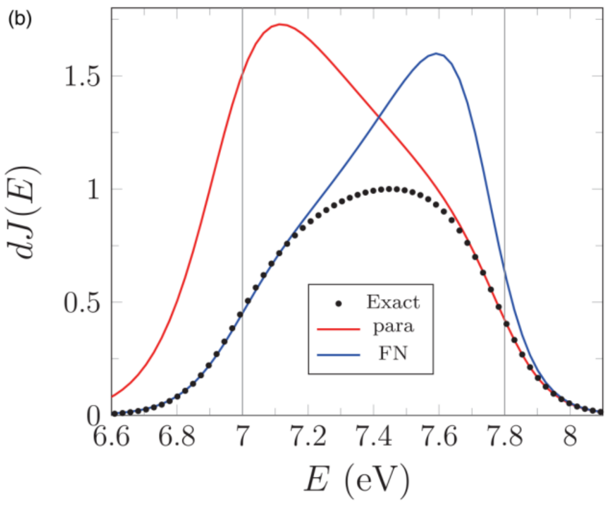
$$\bar{J}_{FN} = \bar{V}^2\bar{D}^{-2}\exp(-\bar{D}/\bar{V})\,;\bar{J}_{RLD} = \frac{9}{4}\bar{T}^2\exp(-1/\bar{T})\,;\bar{J}_{CL} = \frac{4\sqrt{2}}{9}\frac{\bar{V}^{3/2}}{\bar{D}^2}$$

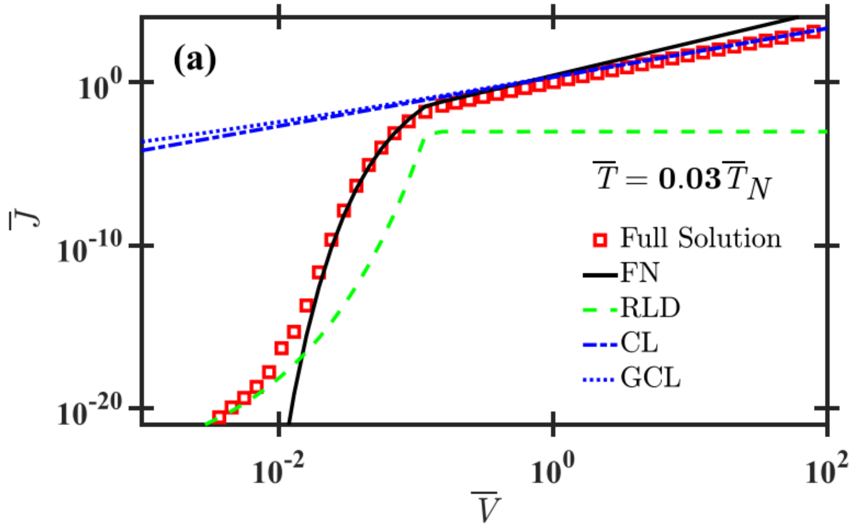
Trivially, we may compute $\bar{V}$, $\bar{D}$, and/or $\bar{T}$ tuples where

$$\bar{J}_{FN} = \bar{J}_{RLD} \textbf{ or } \bar{J}_{FN} = \bar{J}_{CL} \textbf{ or } \bar{J}_{RLD} = \bar{J}_{CL} \textbf{ or } \bar{J}_{FN} = \bar{J}_{RLD} = \bar{J}_{CL}$$

We know from Jensen that $\bar{J}_{GTF} > \bar{J}_{FN} + \bar{J}_{RLD}$, especially when $\bar{J}_{FN} \approx \bar{J}_{RLD}$. We also know that Child-Langmuir reflects over-emission, and drives $\bar{E} \to 0$ besides.

K. Jensen, *J. Appl. Phys.* **126**, 065302 (2019).

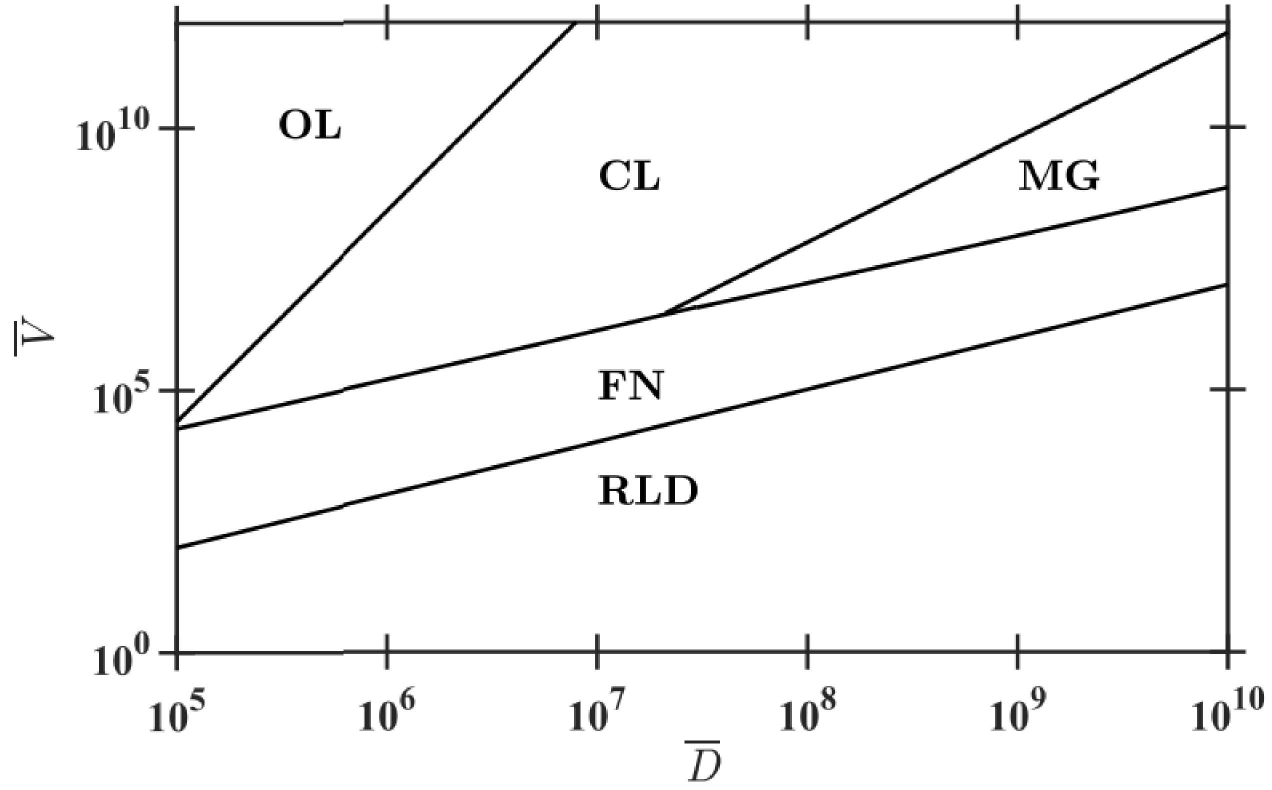




Nexus Theory

Can divide up parameter space into "physics-dominant" regions (nexus phase plot), separated by "two physics equate" curves (nexus curves). A. M. Darr et al. Phys. Rev. Res. **2**, 033137 (2020).

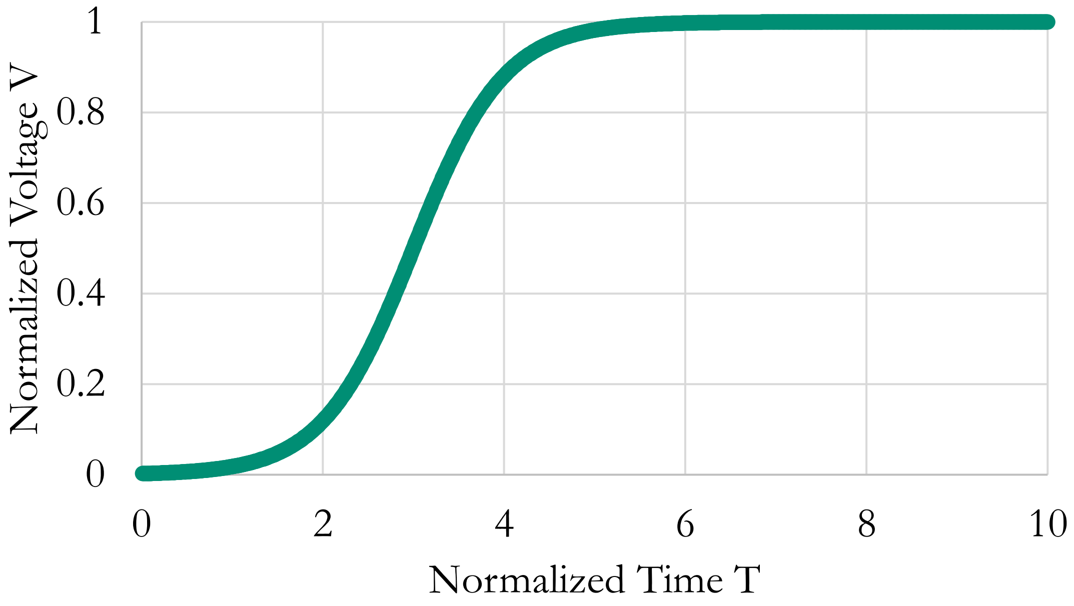
"Close" to nexus curves, though, still need multiphysics. Can we figure out how close?

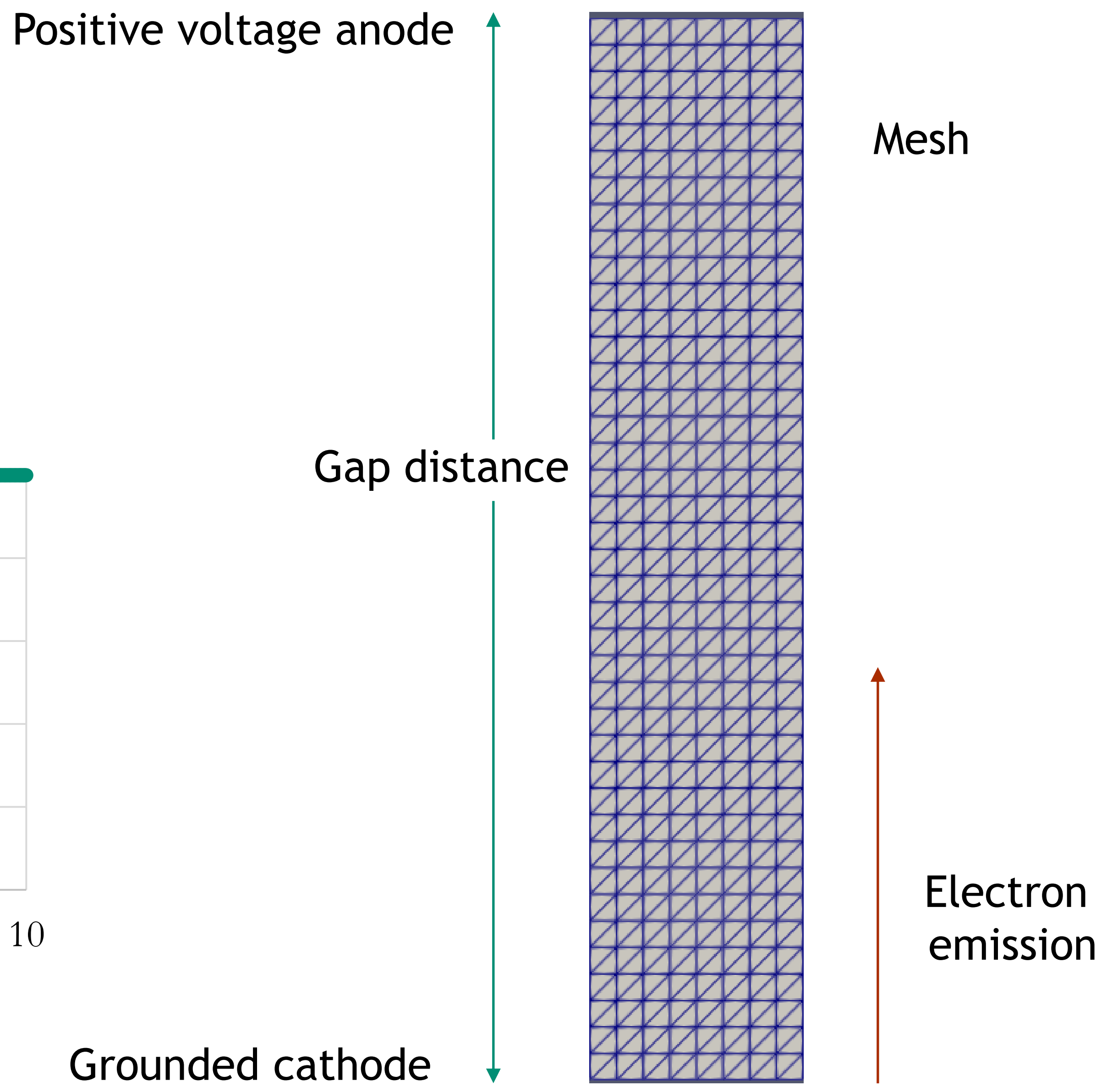


Simulation

Voltage Waveform (electrostatic)

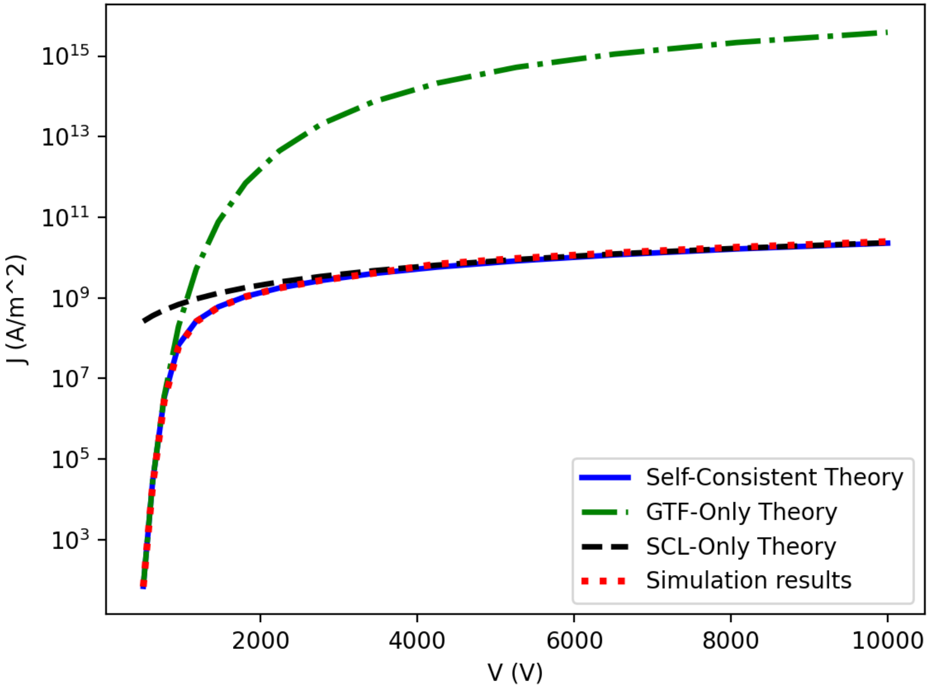
V{0.5 + 0.5 tanh[(t-3T)/T]}

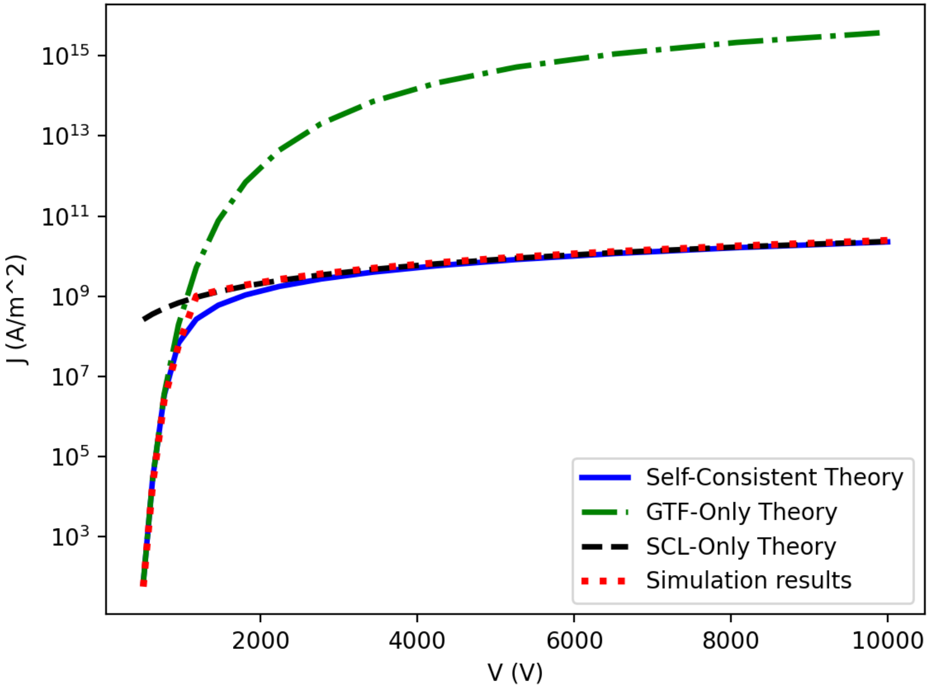




Simulation

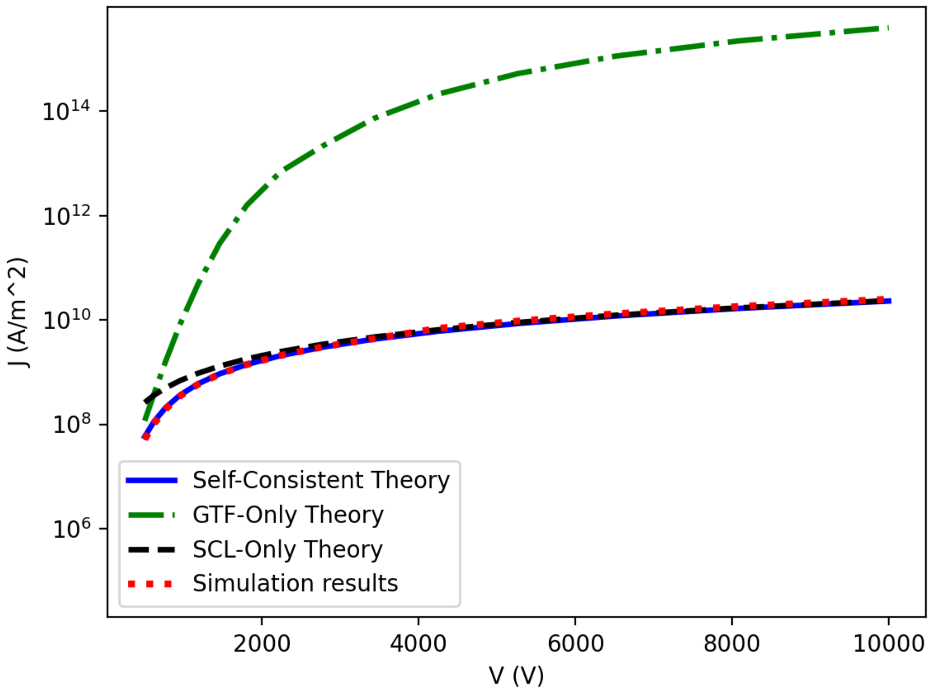
Full Physics vs. "Sharp" nexus (300 K)

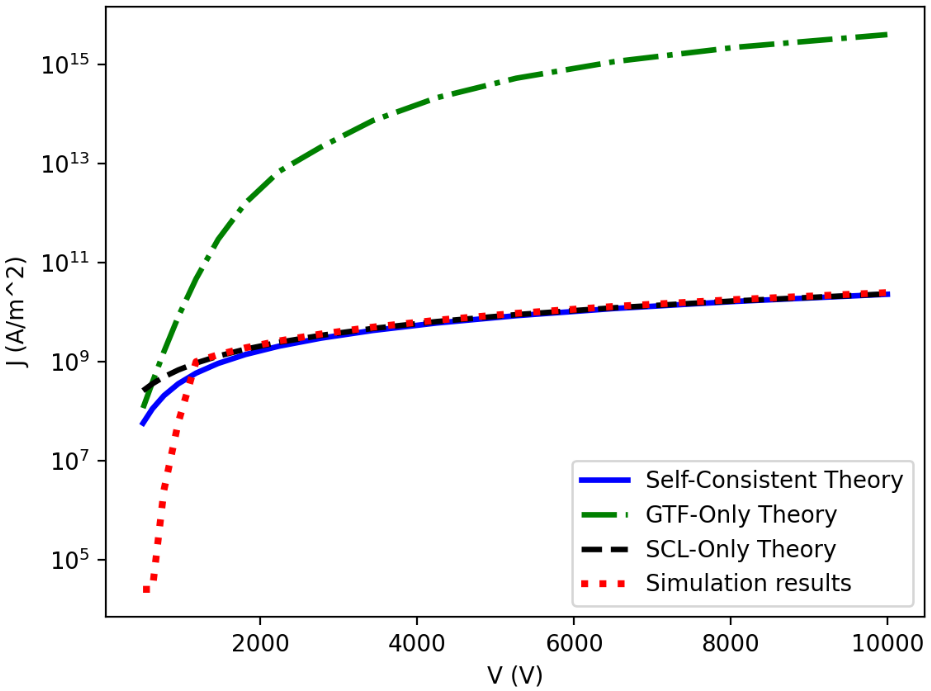




Simulation

Full Physics vs. “Sharp” nexus (3000 K)

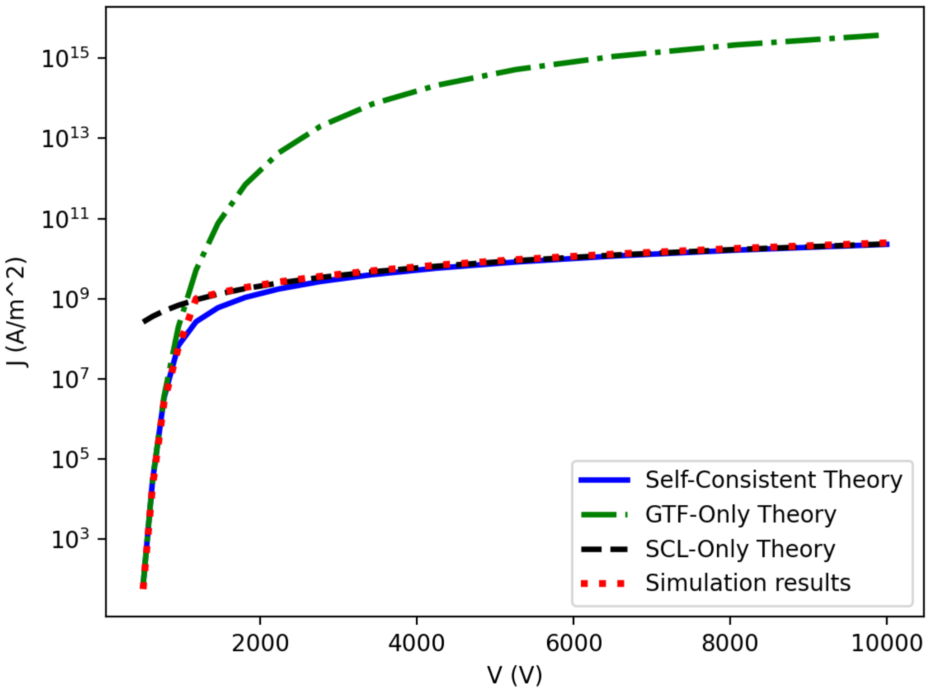




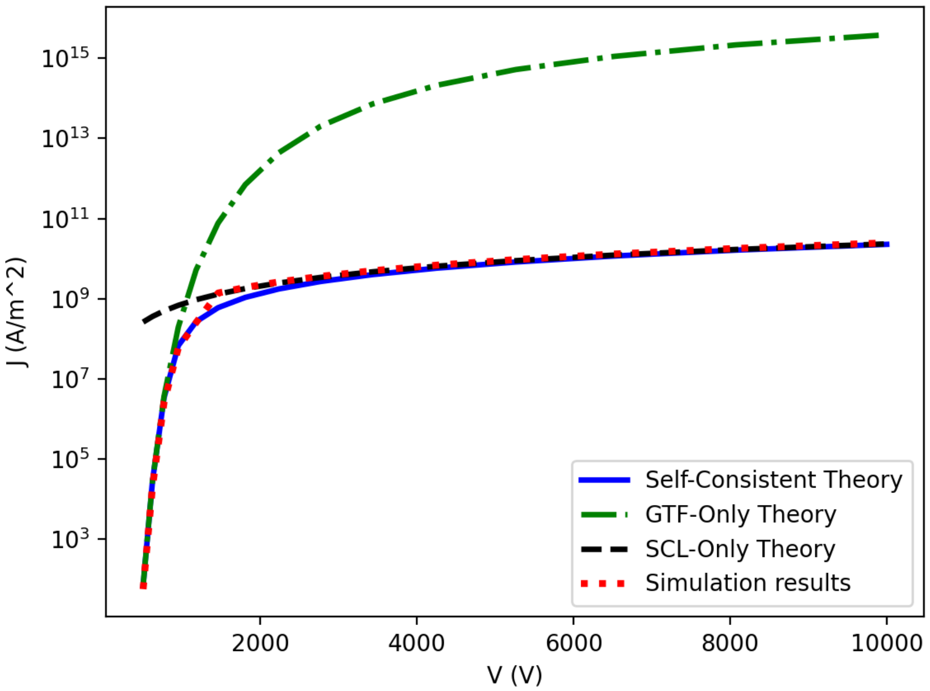
Simulation

Transition Nexus Theory (300 K)

0% ("Sharp")



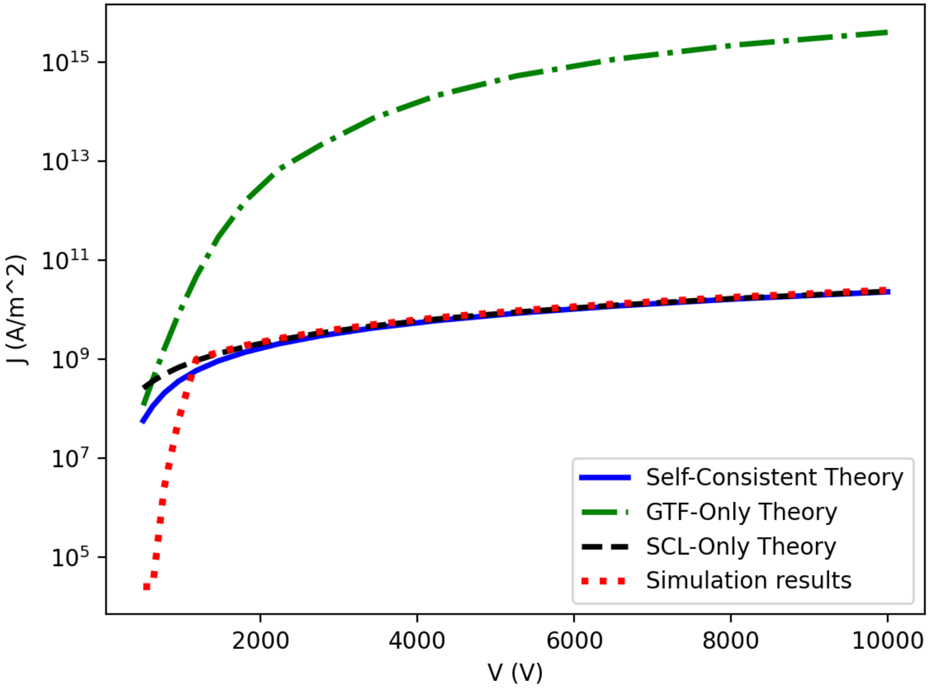
1000%



Simulation

Transition Nexus Theory (3000 K)

0% ("Sharp")



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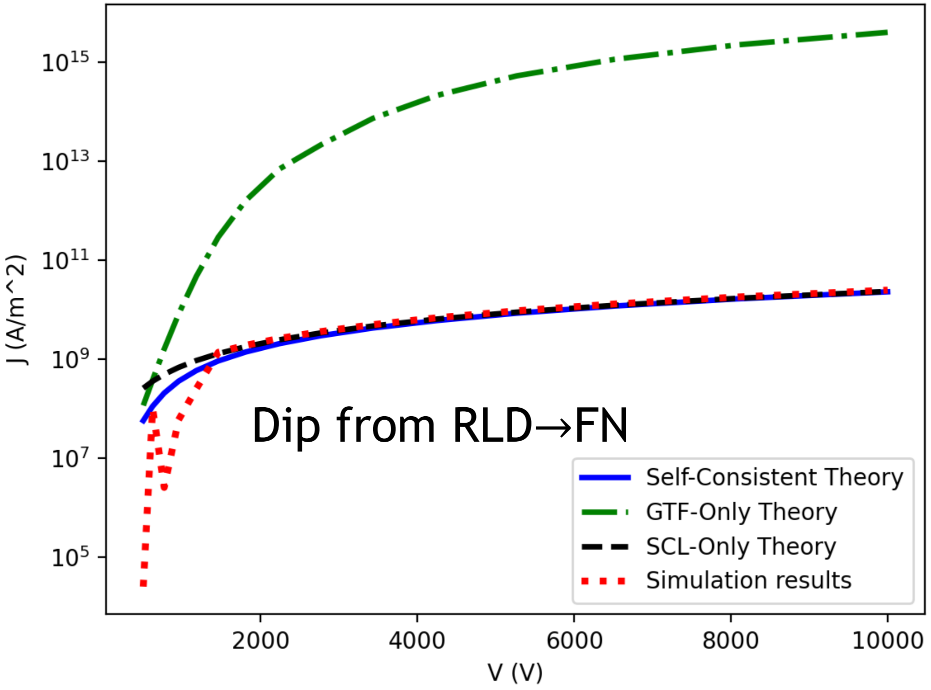


Nexus Theory

Order of magnitude analysis is insufficient for thermal → field emission. See Fig.

Fine for FN/RLD/GTF → SCL, at least it overestimates…

Physics vary too rapidly for order of magnitude analysis to be immediately useful.

Look instead at the effects?

Figure source: K. L. Jensen et al., *J. Appl. Phys*. **125**, 234303 (2019).

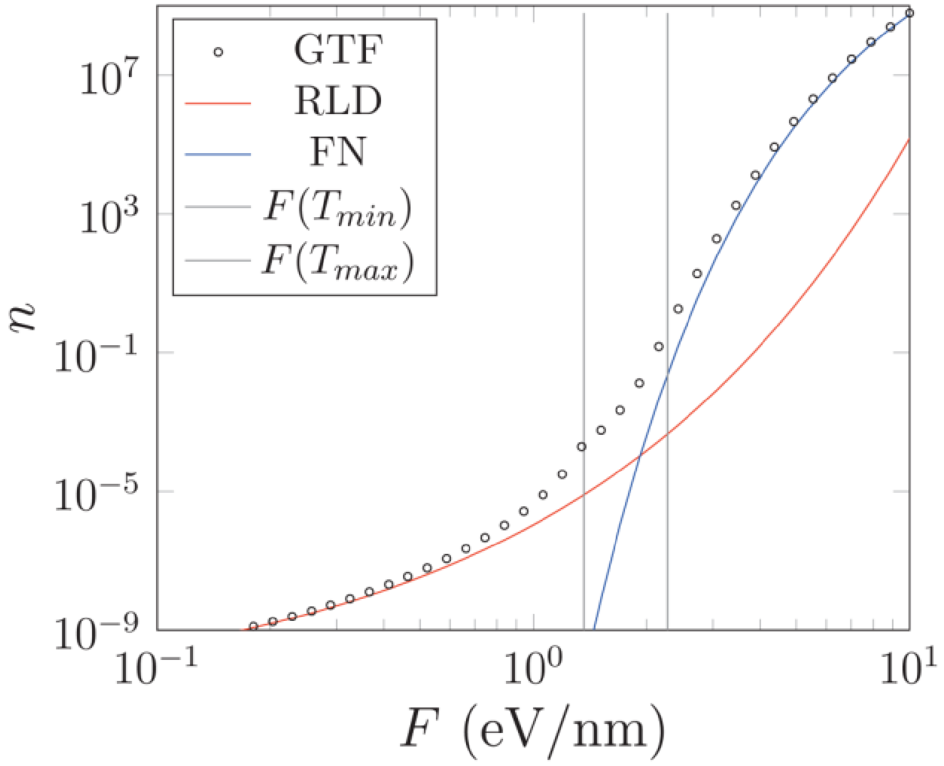


FIG. 28. $J_{GTF}(F, T)$ as a function of F for $T = 1173\,\text{K}$ and $\Phi = 4.5\,\text{eV}$. Also shown are Eq. (A20) (red) and Eq. (A21) (blue) and gray lines corresponding to $F(T_{min}) = 1.361\,\text{eV/nm}$ and $F(T_{max}) = 2.273\,\text{eV/nm}$ as per Eq. (A12).

Nexus Theory

Look at GTF emission and space-charge limited emission (CL).

What's the mutual assumption? GTF says $E_{cathode} \sim V/D$. SCL says $E_{cathode} \ll V/D$.

Transit time, based on average velocity, is on order

$$v_{ave} \approx \frac{1}{2}\sqrt{\frac{2eV}{m}};\ \tau \approx D\sqrt{\frac{2m}{eV}}$$

Given some J_{GTF}, per unit area the field perturbation (Gauss's law) is about

$$\Delta E_{cathode} = \frac{\sigma}{2\epsilon_0} \approx \frac{J_{GTF}\tau}{2\epsilon_0} \approx \frac{J_{GTF}}{\epsilon_0}\sqrt{\frac{mD^2}{2eV}}$$

$$\Delta E(V/D)^{-1} \approx \frac{J_{GTF}}{\epsilon_0}\sqrt{\frac{mV}{2e}}$$

Nexus Theory

However, this doesn't fix the problem since ΔE exponentially increases. Need at least rudimentary feedback with emission. Assume large J_{GTF} scales similarly to J_{FN} for expediency

$$\Delta E \approx \frac{J}{\epsilon_0}\sqrt{\frac{mD^2}{2eV}};\quad J \approx J_{GTF}E^2E_0^{-2}\exp\left(-\frac{B_{FN}}{\beta}\left(\frac{1}{E}-\frac{1}{E_0}\right)\right);\quad E_0 = \frac{V}{D}$$

Assuming constant B_{FN} (again, expediency), and knowing $E = E_0 - \Delta E$,

$$\Delta E \approx \frac{J_{GTF}}{\epsilon_0}\sqrt{\frac{mD^2}{2eV}}E^2E_0^{-2}\exp\left(-\frac{B_{FN}}{\beta}\left(\frac{1}{E}-\frac{1}{E_0}\right)\right)$$

$$\Delta E \approx \frac{J_{GTF}}{\epsilon_0}\sqrt{\frac{mD^2}{2eV}}\left(1-\frac{\Delta E}{E_0}\right)^2\exp\left(-\frac{B_{FN}}{\beta}\left(\frac{1}{E_0-\Delta E}-\frac{1}{E_0}\right)\right)$$

Large when SCL-like

$$\Delta E \approx \frac{J_{GTF}}{\epsilon_0}\sqrt{\frac{mD^2}{2eV}}\left(1-\frac{\Delta E}{E_0}\right)^2\left(1-\frac{B_{FN}}{\beta E_0}\left(\frac{\Delta E/E_0}{1-\Delta E/E_0}\right)\right)$$

Nexus Theory

Solving quadratically after taking the first two polynomial terms of the exponential,

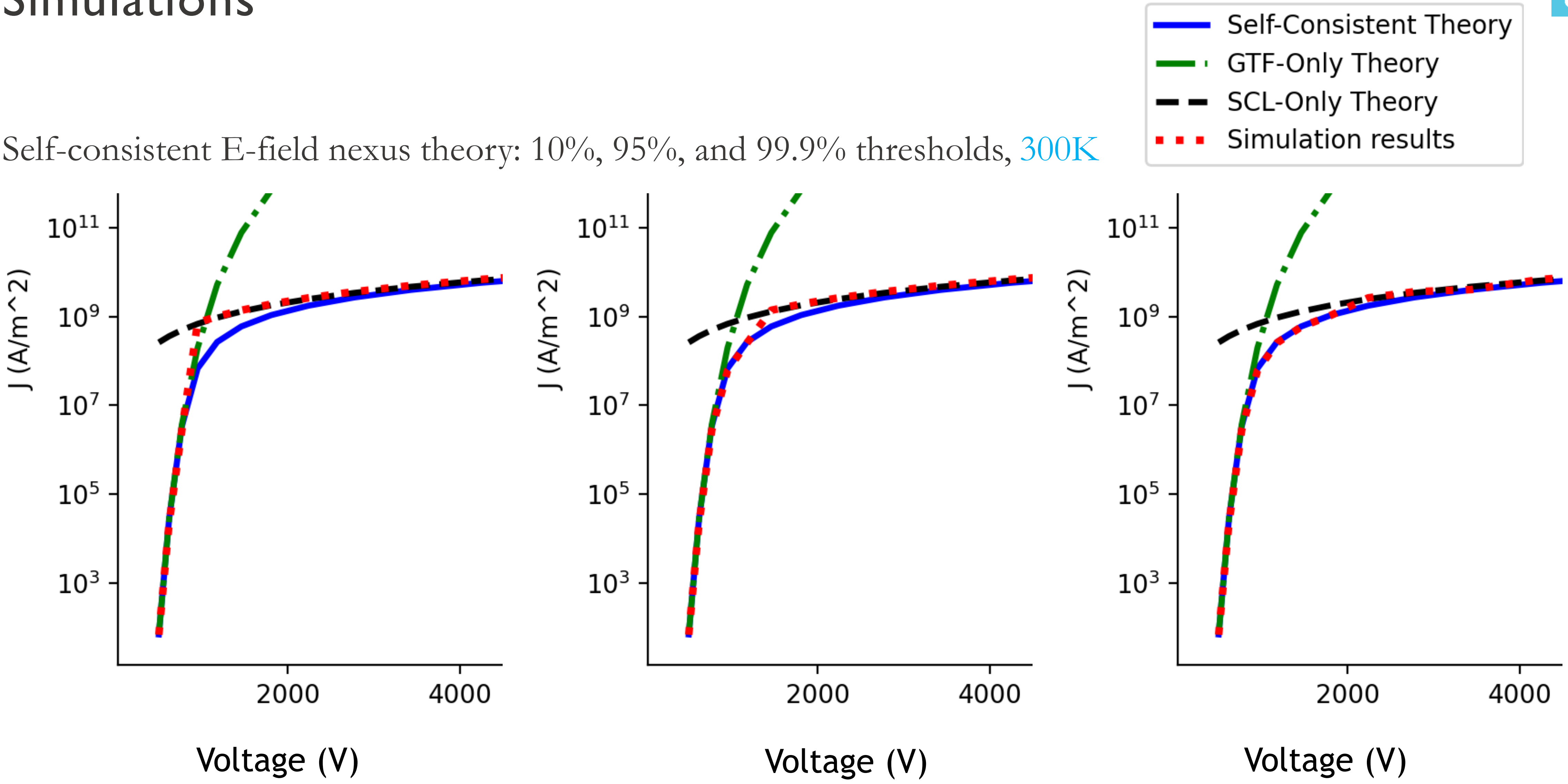
$$\Delta E \approx \frac{E_0^2 + 2E_0 j + bE_0 j + E_0\sqrt{E_0^2 + 4E_0 j + 2bE_0 j + b^2 j^2}}{2(j + bj)}$$

$$j = \frac{J_{GTF}}{\epsilon_0}\sqrt{\frac{mD^2}{2eV}}; \quad b = \frac{B_{FN}}{\beta E_0}$$

When this estimate of self-consistent ΔE reaches X% of V/D, go to SCL

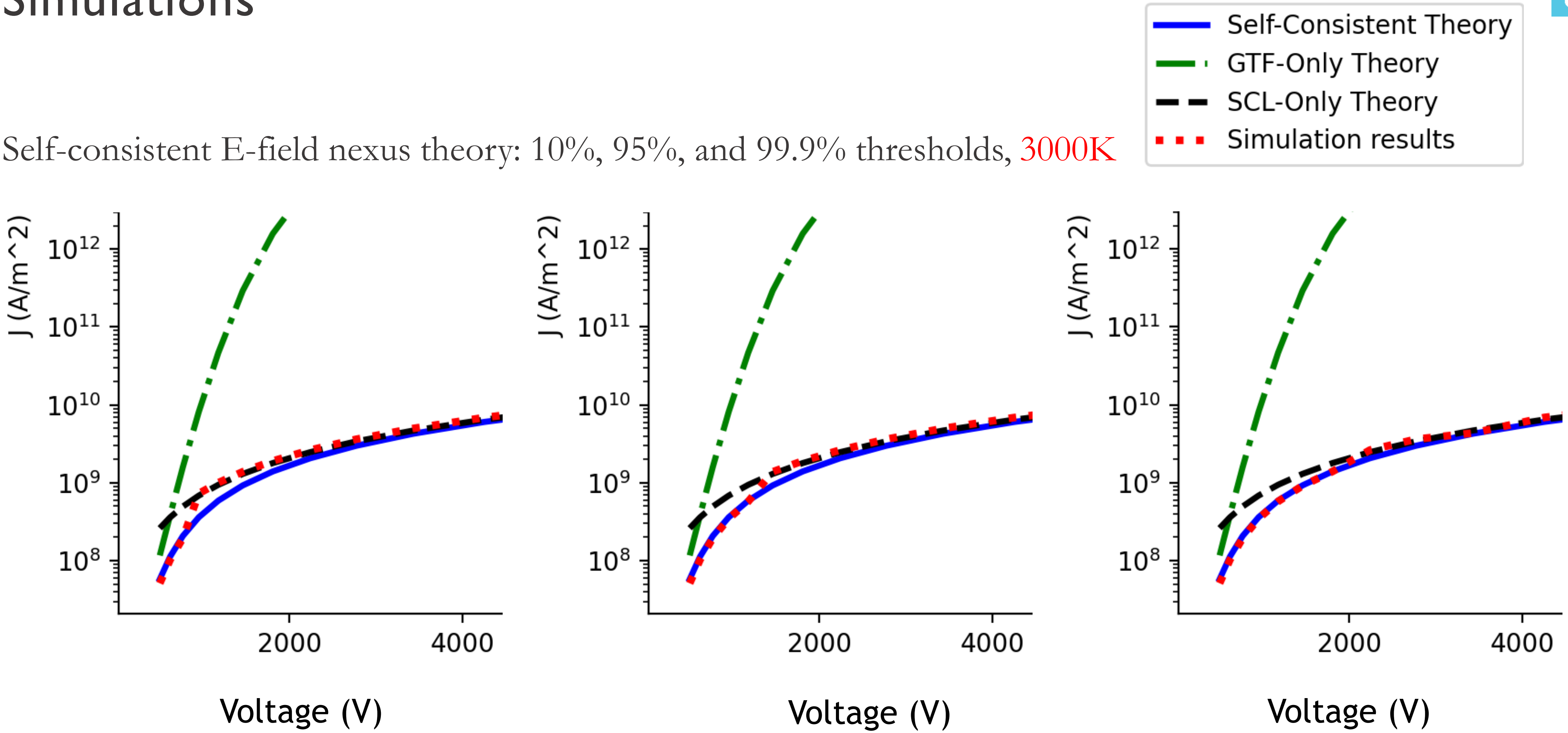
Simulations

Self-consistent E-field nexus theory: 10%, 95%, and 99.9% thresholds, 300K



Simulations

Self-consistent E-field nexus theory: 10%, 95%, and 99.9% thresholds, 3000K



Conclusions

General Thermal Field does a good job recovering space-charge limits.

Nexus theory trivially computes "dominant mechanisms," but struggles to identify multiphysics.

Lots of additional work to derive a reasonable GTF→CL transition region.

- The expression is easy to compute, though.

Questions?

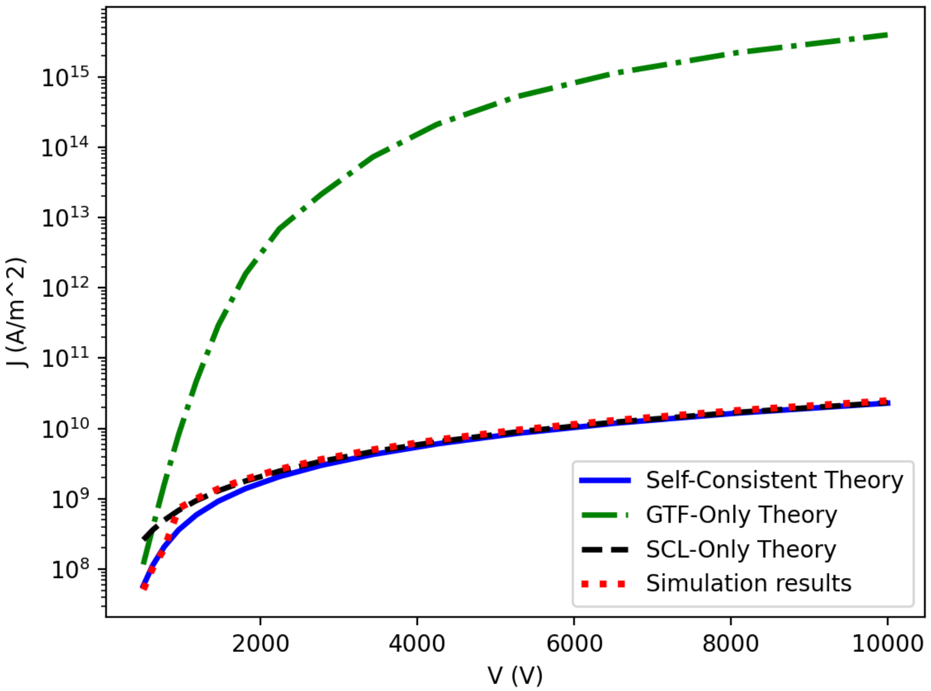
Simulation (Backup)

Self-consistent electric field (SCL for $\Delta E > 0.1E_0$)

300 K

3000 K

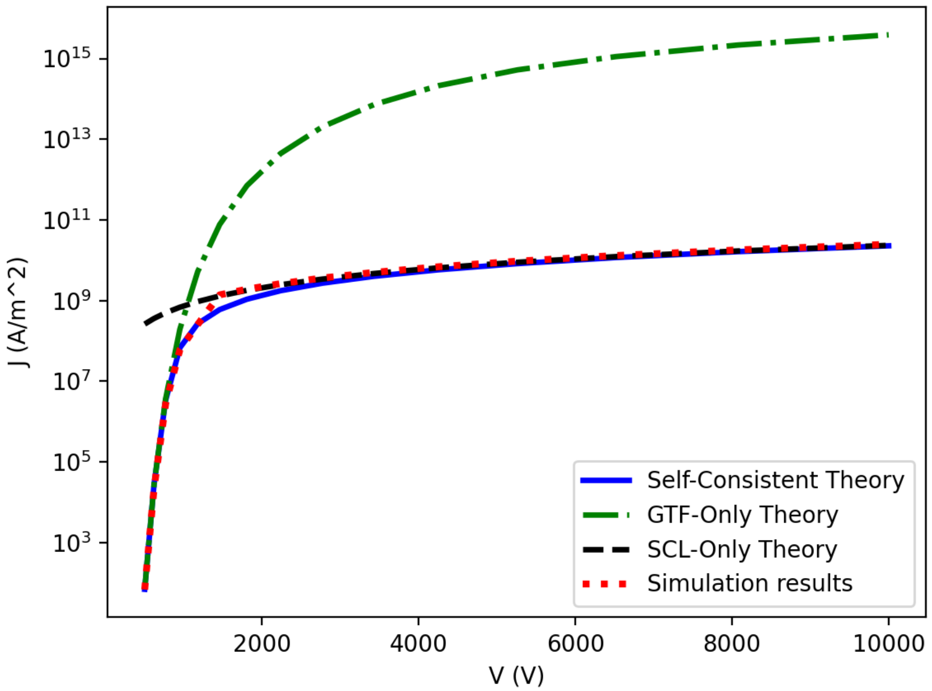
Self-consistent electric field (SCL for $\Delta E > 0.1E_0$)



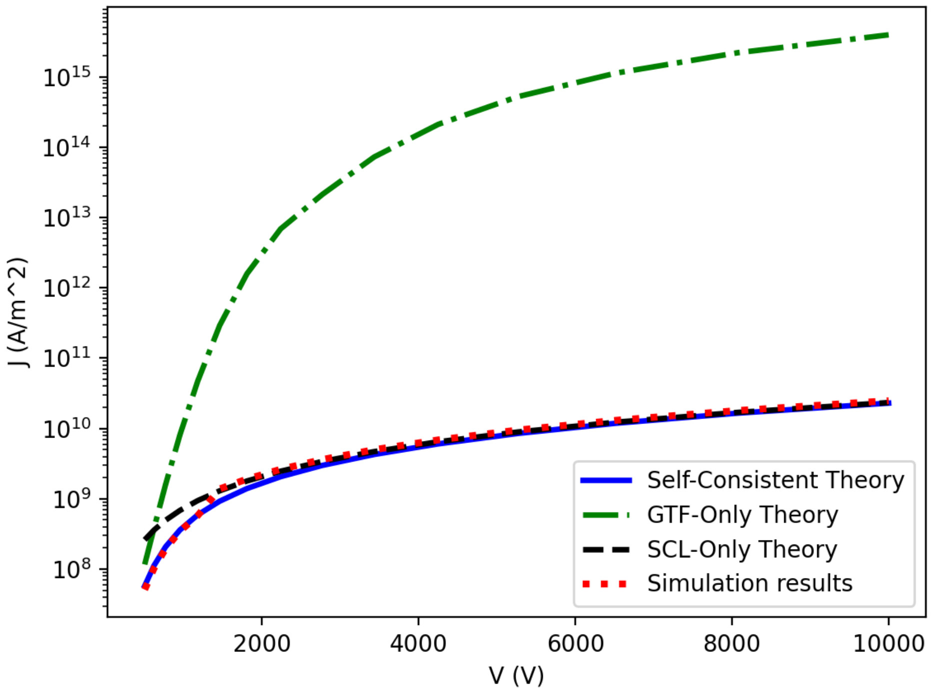
Simulation (Backup)

Self-consistent electric field (SCL for $\Delta E > 0.95 E_0$)

300 K



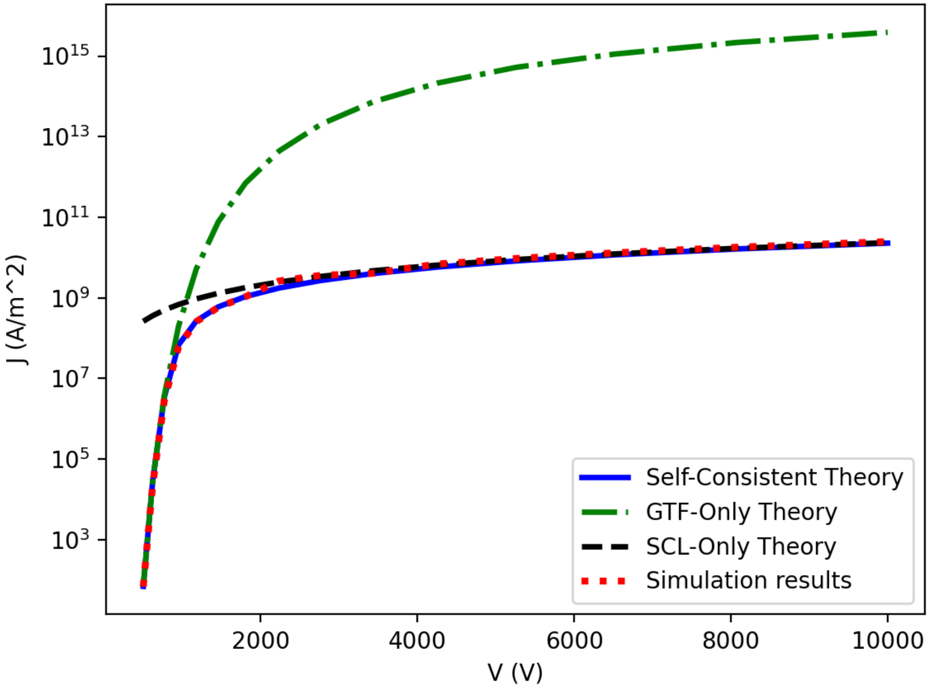
3000 K



Simulation (Backup)

Self-consistent electric field (SCL for $\Delta E > 0.999E_0$)

300 K



3000 K