High-fidelity three-dimensional simulations of thermionic energy converters

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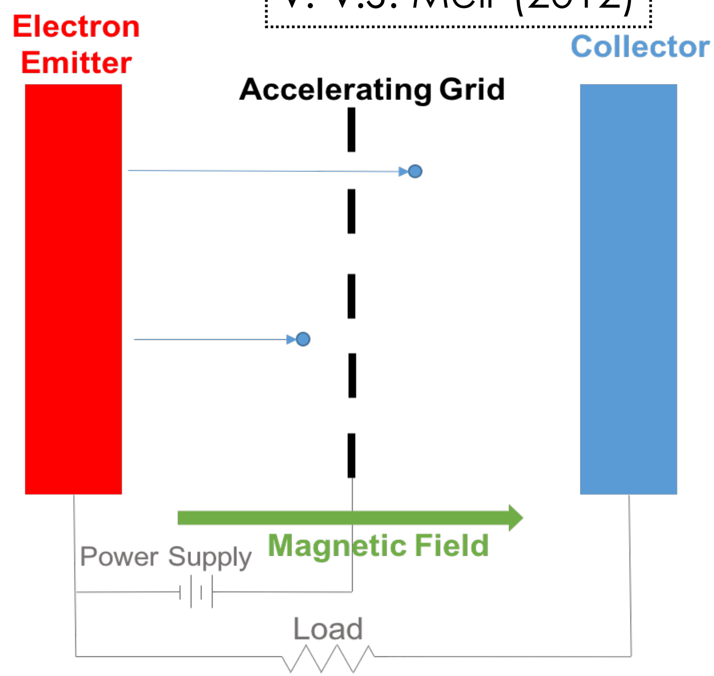
Thermionic Energy Converters as Alternative Electrical Generators

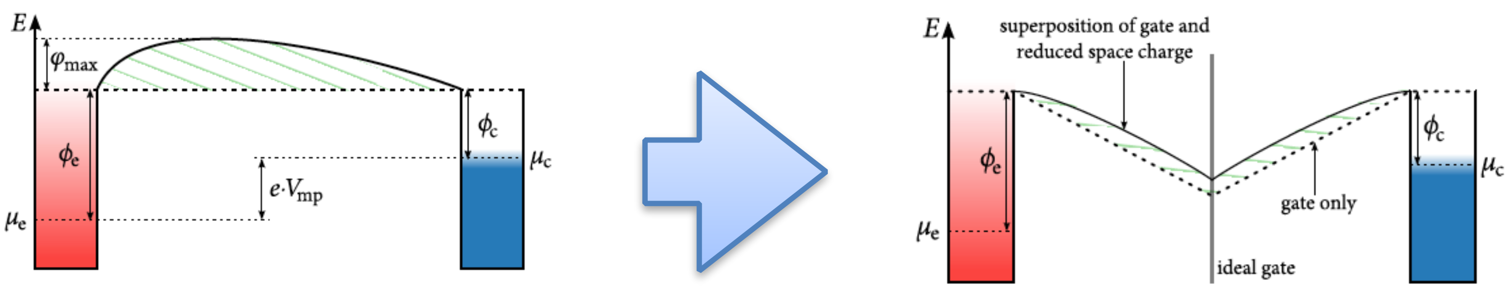
- Electricity generation in the United States (and elsewhere) is largely a product of old technologies
  - Large Scale (>MW): fuel drives turbines to generate current
    - High fixed costs for development and deployment - efficiency at large scale
    - Stagnant industrial progress
  - Small scale (<~KW): lithium-ion batteries
    - High materials cost limits price/stored-energy - not scalable
    - Battery technologies reaching limits on efficiency and size
- Thermionic Energy Converters (TECs)
  - Boil off electrons at hot emitter and absorb at cold collector to generate current.
  - Power is generated by difference in electrochemical potential
- Compelling features of TECs
  - High efficiencies approaching Carnot limit
  - Scalable, robust, no moving parts
  - Challenging to model! Complex dynamics!

V. V.S. Meir (2012)



TEC constraints and design strategies

- Thermionic emission scales strongly with temperature $$j_{\mathrm{T}} = AT^2 e^{-(\phi_w - \Delta\phi)/k_b T}$$
- Child-Langmuir limits peak current for simple diode $$j_{\mathrm{CL}} = \epsilon_0 \sqrt{\frac{2e}{m}} \frac{V^{3/2}}{d^2}$$
  - Lower temperature leads to reduced current
  - Biasing anode leads to lower efficiency
  - Reducing gap leads to cooling difficulties
- Solution: Inter-gap grid applies voltage



  - Increase effective space-charge limit without biasing anode
  - Grid is lossy. Its design and placement must be optimized

Realistic TEC efficiency includes loss channels

- Goal: Maximize current at collector, minimize losses

$$\eta = \frac{P_{\mathrm{load}} - P_{\mathrm{grid}}}{P_{\mathrm{ec}} + P_{\mathrm{R}} + P_{\mathrm{ew}}}$$

- Many possible energy loss channels during operation

1. Kinetic losses - excess electron kinetic energy heats surface

$$P_{\mathrm{ec}} = J_{\mathrm{e}}\left(\phi_{\mathrm{e}} + 2k_{\mathrm{B}}T_{\mathrm{e}}\right) - \mathrm{t}J_{\mathrm{c}}\left(\phi_{\mathrm{e}} + 2k_{\mathrm{B}}T_{\mathrm{c}}\right)$$

2. Grid losses - electron intercepted by accelerating gate

$$P_{\mathrm{grid}} = V_{\mathrm{grid}}\left(J_{\mathrm{grid}} + \mathrm{t}J_{c}\right)$$

3. Radiative losses - heat lost through emissivity

$$P_{\mathrm{R}} = \epsilon\sigma_{\mathrm{sb}}\left(T_{\mathrm{e}}^{4} - T_{\mathrm{c}}^{4}\right)$$

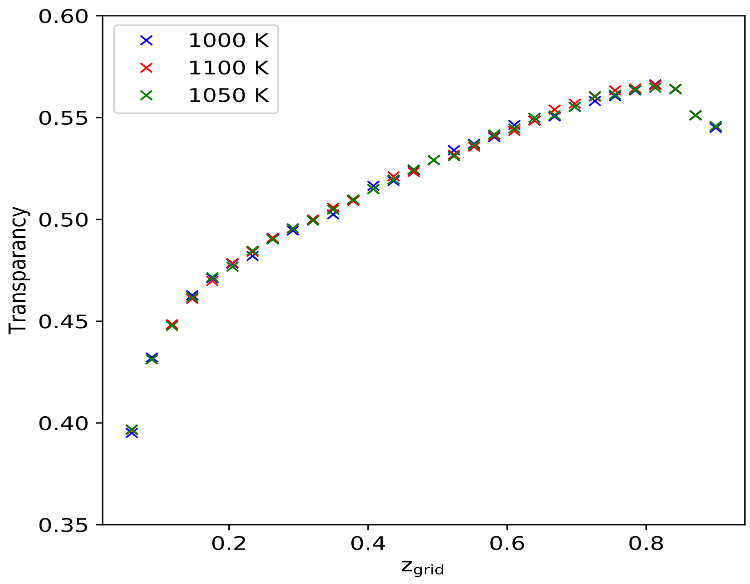
4. Resistive losses - losses in external circuit

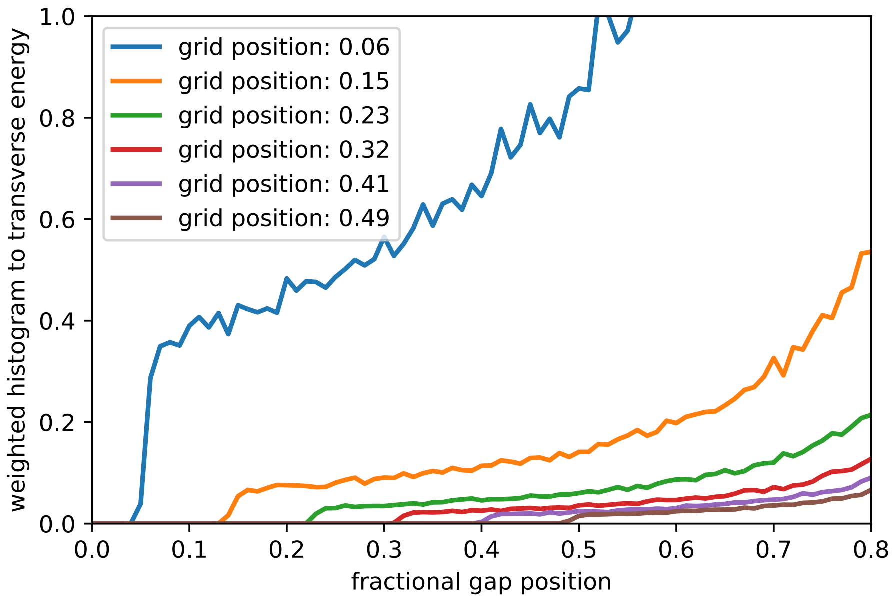
$$P_{\mathrm{ew}} = 0.5\left(\frac{L}{\rho_{\mathrm{ew}}}(T_{\mathrm{em}} - T_{\mathrm{env}})^{2} - \rho_{\mathrm{ew}}(J_{\mathrm{ec}} - \mathrm{t}J_{\mathrm{c}})^{2}\right)$$

For more on these models, see Voesch et al. *Energy Technology*, **5**(12):2234-2243, (2017).

Case Study: Grid transparency in relation to transverse dynamics

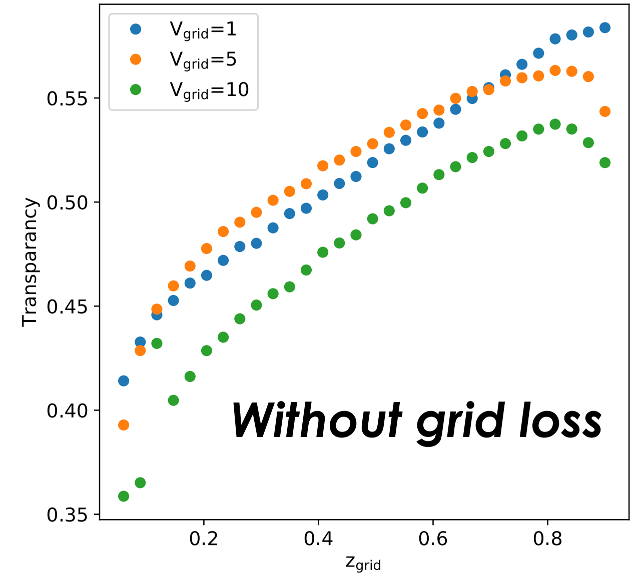
- For simple device, transparency peaks as grid approaches collector, even for different T_e and V_{grid}
  - Transverse kick from grid drives large oscillations
  - Effects of transverse motion mitigated closer to grid
  - This effect is dimensional in nature, coupling motion in both planes
    - Further reason why 3D dynamics are critical to optimizing
- **Conclusion:** Minimize transverse dynamics for maximum efficiency

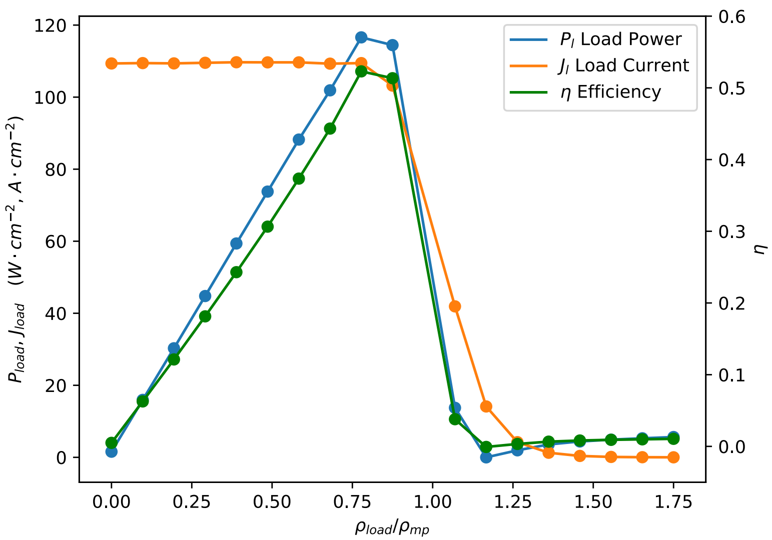


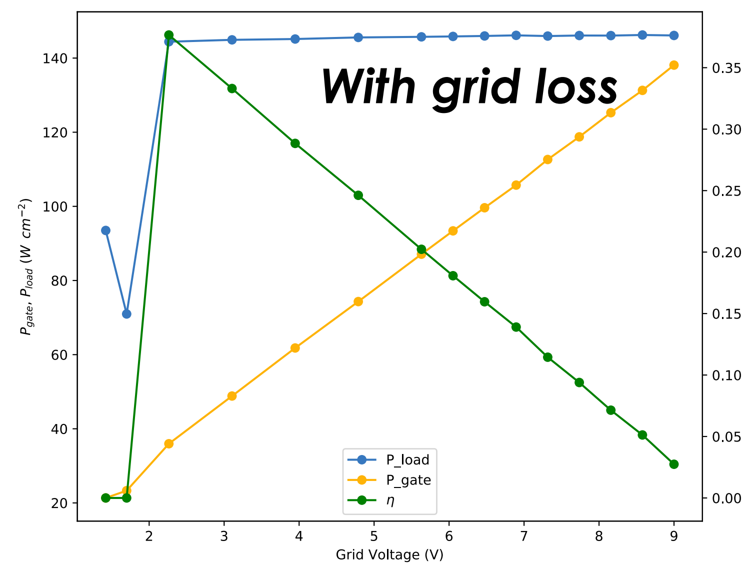


Case Study: Grid losses shift ideal operating point

- Ignoring grid losses, efficiency scales consistent across different voltages
- Introducing grid/anode losses significantly changes optimum
  - Losses scale strongly with voltage
  - But, grid voltage is important for extracting ideal current
- **Conclusion:** Voltage must optimize total current while minimizing energy-per-particle
  - Similar to an I-V characteristic







Improvements in modeling TECs using the Warp Code

- An open-source* plasma and accelerator simulation framework, developed by Lawrence Berkeley National Laboratory, now a part of the Berkeley Lab Accelerator Simulation Toolkit[&]
  - 2D, R-Z, and 3D geometries featuring electrostatic and electromagnetic particle-in-cell
  - Macro-particle, Multi-species, beam-envelope, transverse slice, emission models
  - Internal conductors, dielectrics, adaptive mesh refinement
  - RadiaSoft efforts to support vacuum devices[#]:
    - Enhance dielectric capabilities and extend solver to 3D and parallel use
    - Improve and validate emission models for novel cathodes
    - New geometry capabilities (mesh-refinement/"cut-cells" with internal boundaries)
    - CAD input-output with support for standard files

* https://bitbucket.org/berkeleylab/warp/src/master/

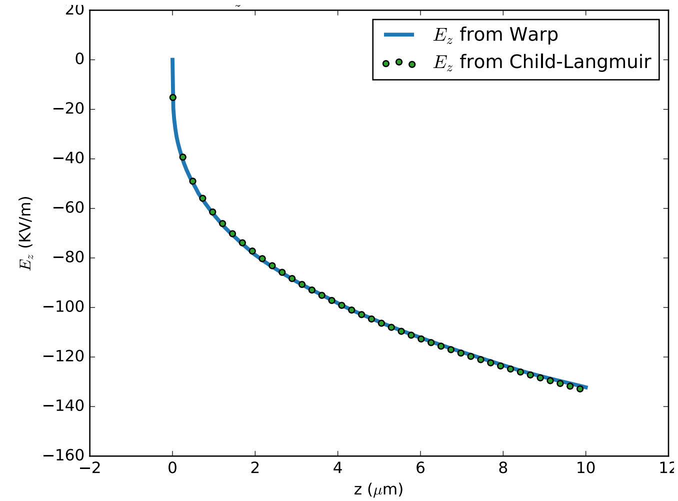
& http://blast.lbl.gov/blast-codes-warp/

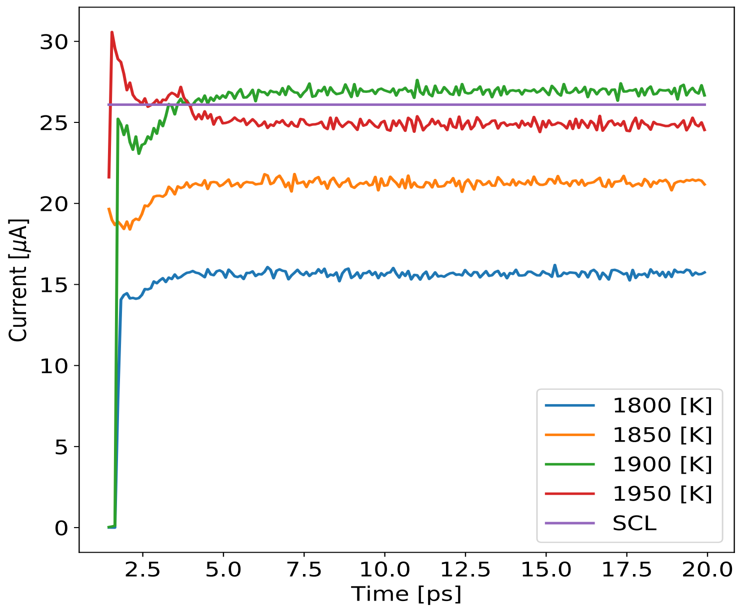
\# https://bitbucket.org/radiasoft/warp/src/master/

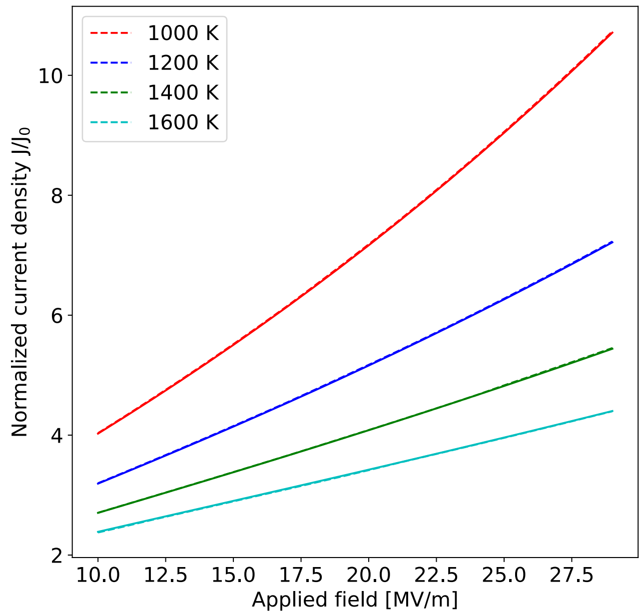
Additional developments for plasma dynamics at Exascale - R. Ryne 10/21

Requirements: Emission in the space-charge limited regime

- TECs are most efficient when space-charge limited
  - Child-Langmuir is a cold limit
  - Approaching C-L at high temperature introduces some transient effects which quickly dampen
- Proper modeling of field enhancement, "Schottky emission" is required due to applied field
  - Field enhancement is critical for advanced emitters
  - Warp implementation shows good agreement



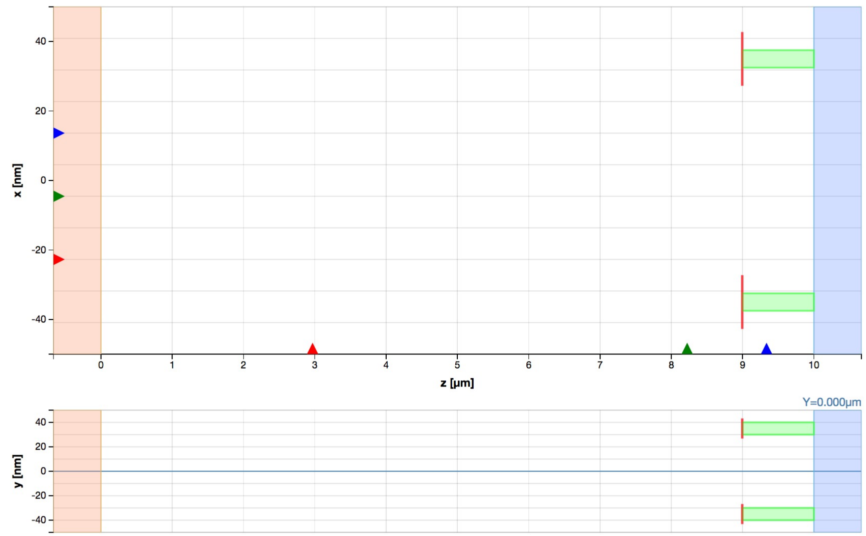


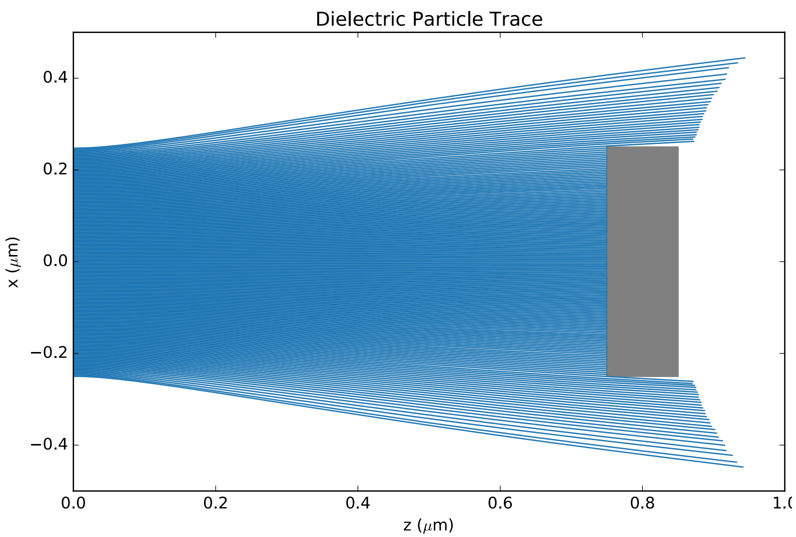


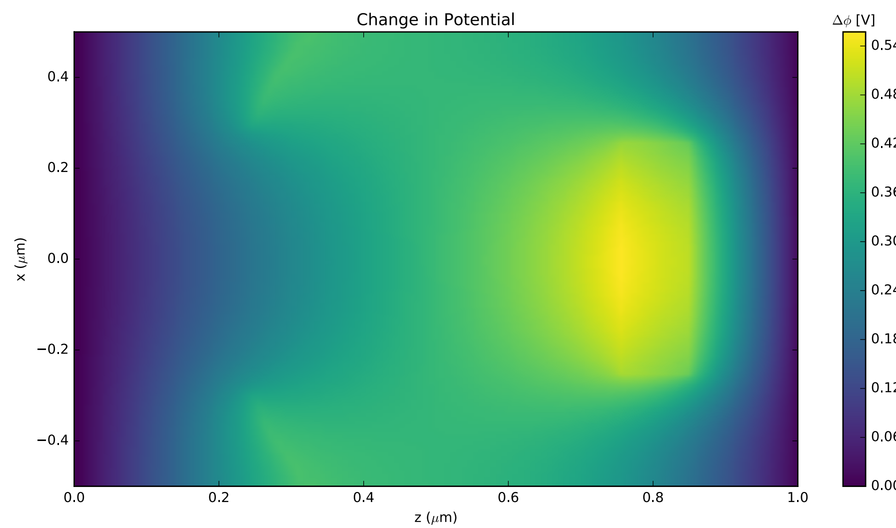
radiasoft

Requirements: Self-consistent dielectric interactions

- TEC grids may require dielectric supports or anchors for mechanical stability
  - Isolated from an external circuit, these supports may charge and deflect particles
- Improvements to Warp's capabilities
  - Extended MultiGridDielectric solver from 2D to 3D, parallelization
  - Installing dielectrics is now consistent with installing conductors
  - New "Dielectric Particles" permit charging of dielectric surfaces

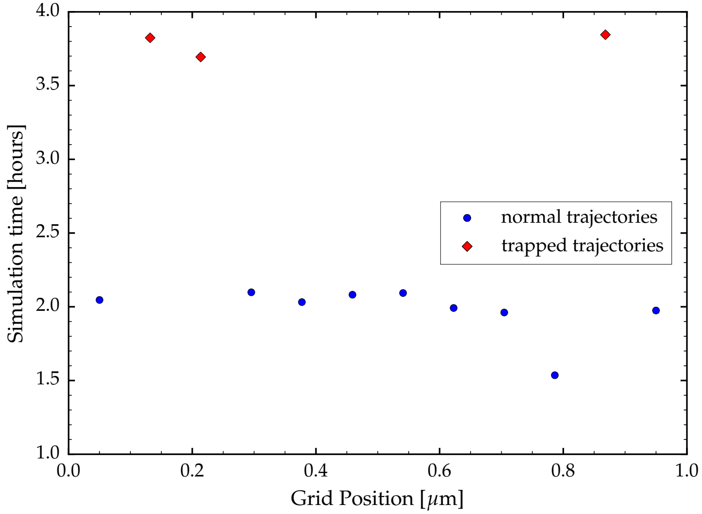


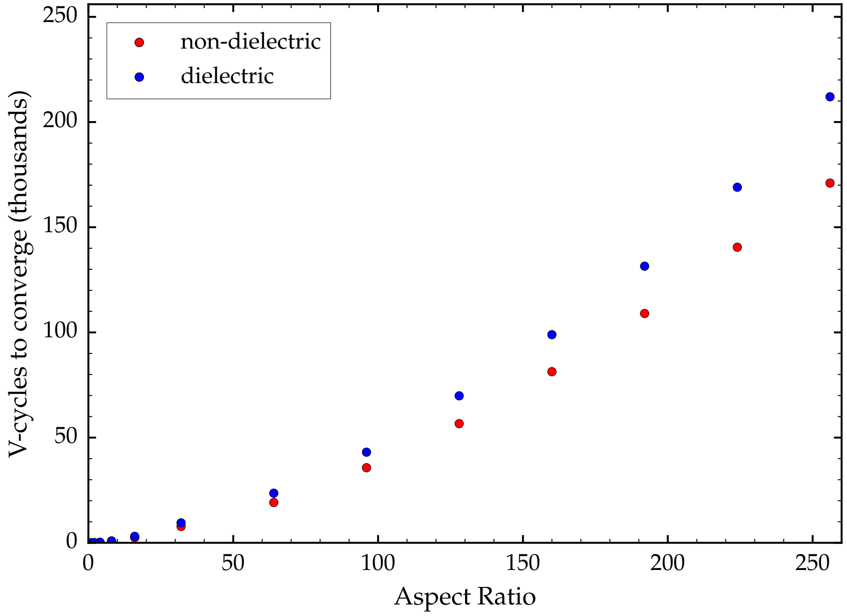


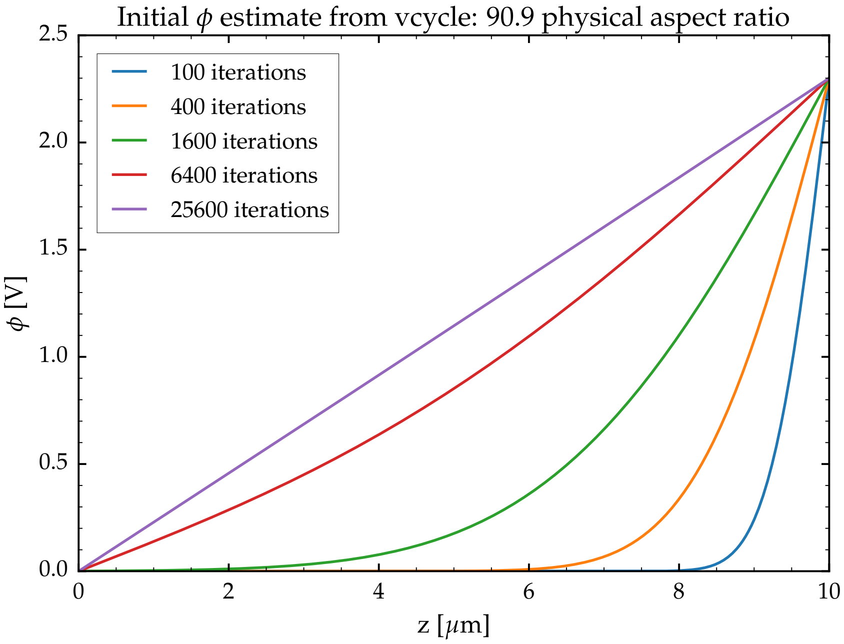


Challenges: Reducing computational expense

- Most of a TEC is empty space
  - Areas of interest are separated by vacuum region
  - Transit time between theses areas of interest is significant fraction of simulation
  - Reflection and oscillatory dynamics introduce transient behavior extends simulation duration
- High aspect ratio limits solver speed
  - Cell-centered dielectric solver is slower as coarseness of V-cycle is limited by extra cells

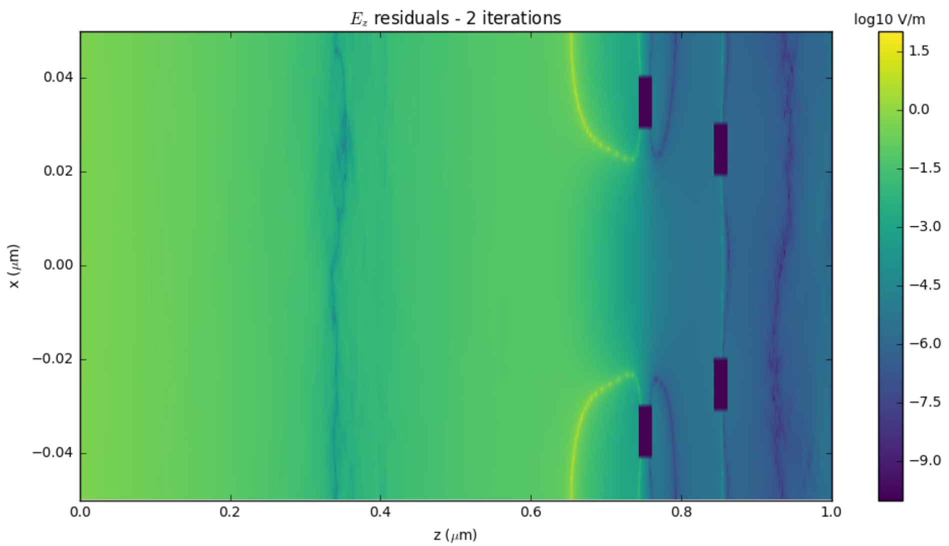


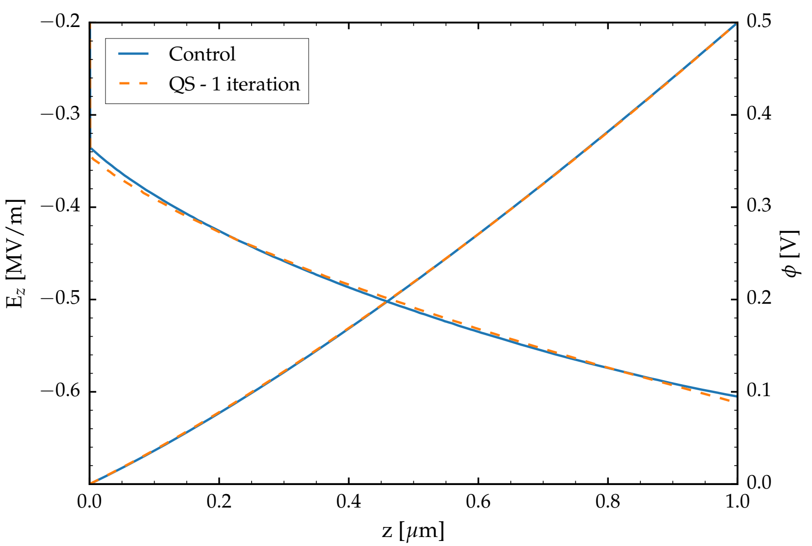




A hybrid quasi-static approach to reduce computational demands

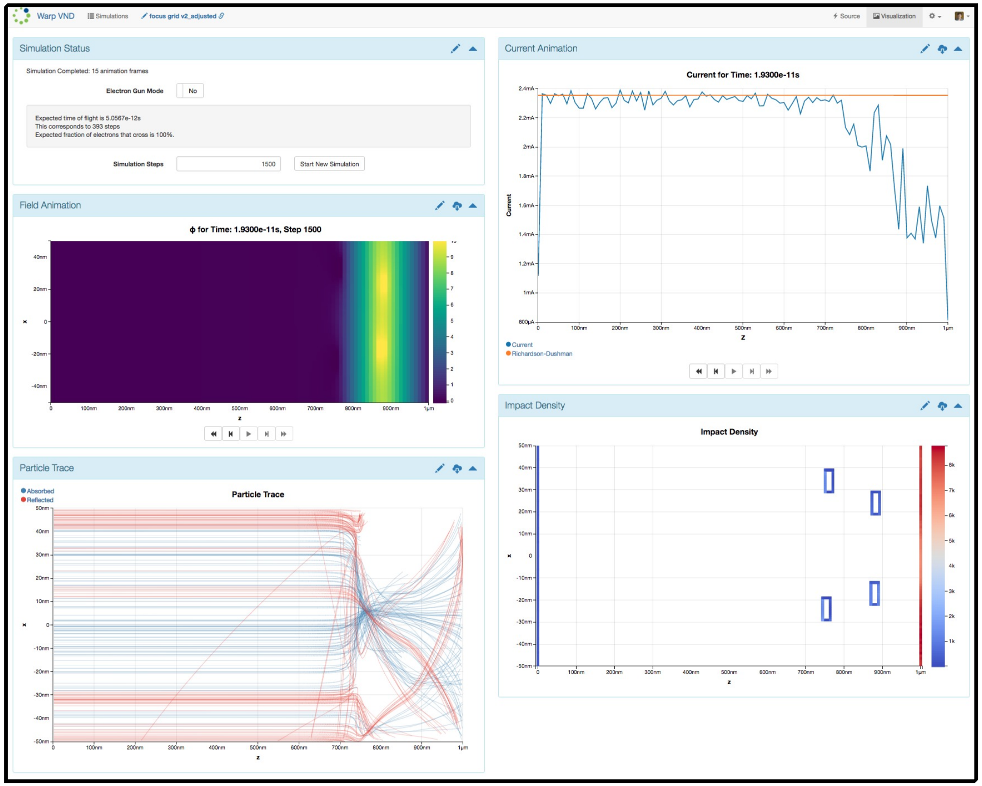
- Achieving steady-state drains significant resources (25-30% of total)
  - Especially significant for 3D simulations with small grid features and small time-step
- Use quasi-static solver: iterative emission converges to steady-state solution much faster!
  - Successful strategy for gun/source studies with clearly defined geometries
  - Efficient when current is evenly distributed, less efficient for sharp bottlenecks in current
  - Still suffers from captured trajectory problem
- Planned improvements:
  - Parallelization for future efforts with 3D optimization
  - Resolve captured trajectories through smart "time-out"

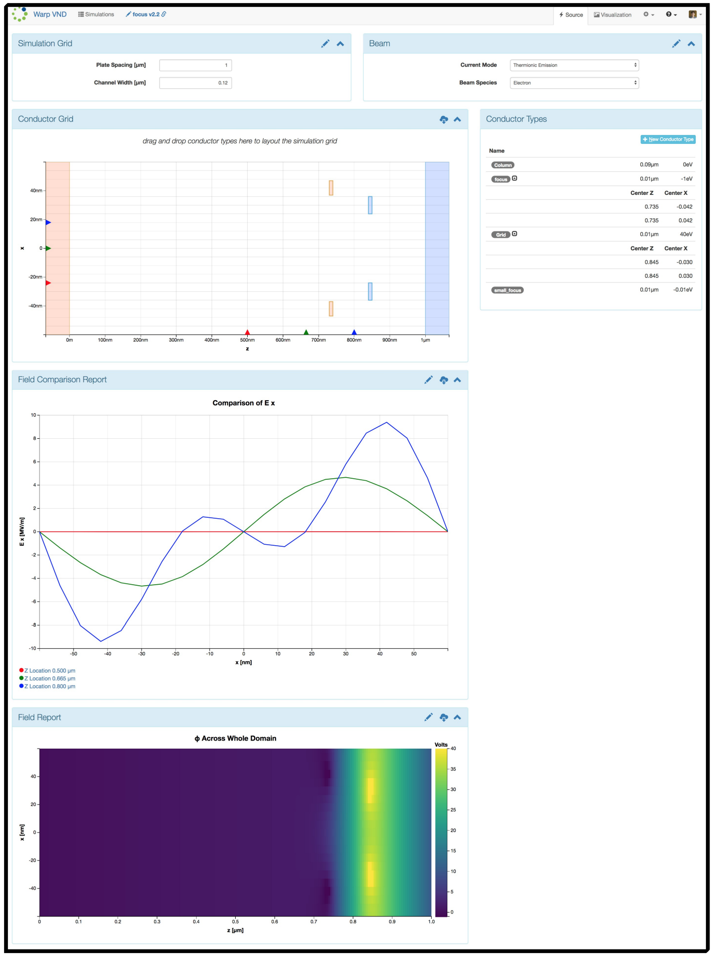




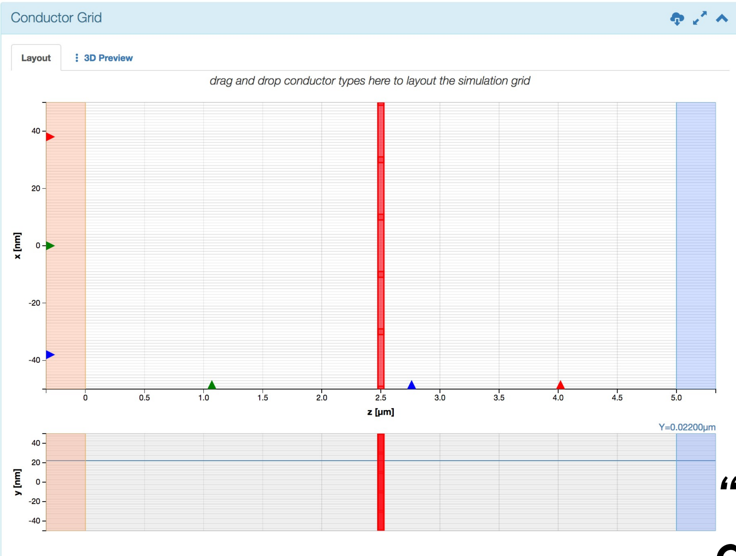
A cloud-based platform for VNDs via Sirepo

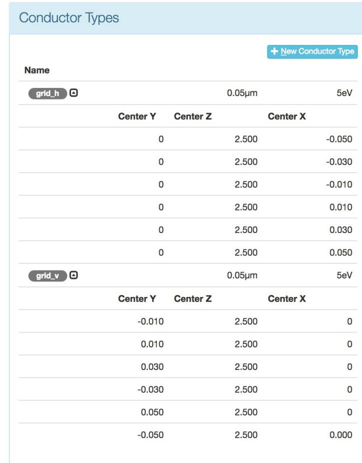
- Complex simulation tools require expertise and dedicated support for training and troubleshooting
- We are developing a 3D interface on RadiaSoft's Sirepo platform - https://alpha.sirepo.com/#/warpvnd
- Automated Diagnostics - fields, particles, loss diagrams
- Choice of Solvers - multigrid, dielectric, quasi-static
- Automated Visualizations - 2D/3D rendering with VTK.js





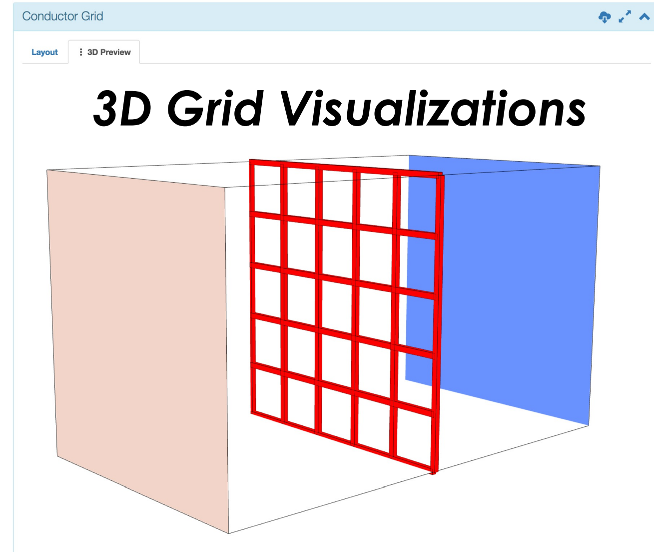
Streamlining TEC designs in Sirepo



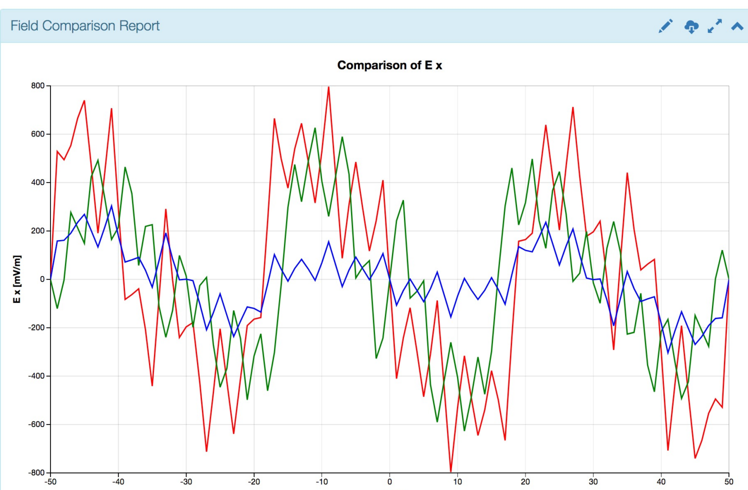


Center Y	Center Z	Center X
0	2.500	-0.050
0	2.500	-0.030
0	2.500	-0.010
0	2.500	0.010
0	2.500	0.030
0	2.500	0.050

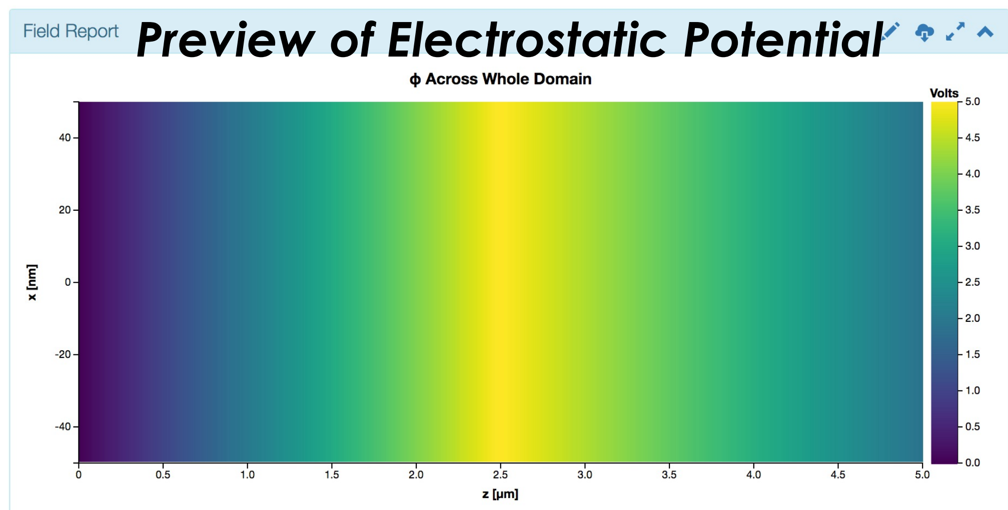
Center Y	Center Z	Center X
-0.010	2.500	0
0.010	2.500	0
0.030	2.500	0
-0.030	2.500	0
0.050	2.500	0
-0.050	2.500	0.000



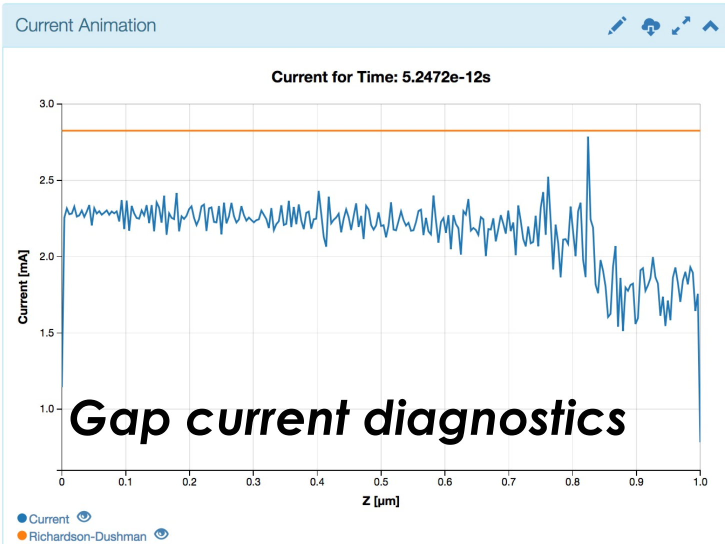
"Drag and drop" grid design

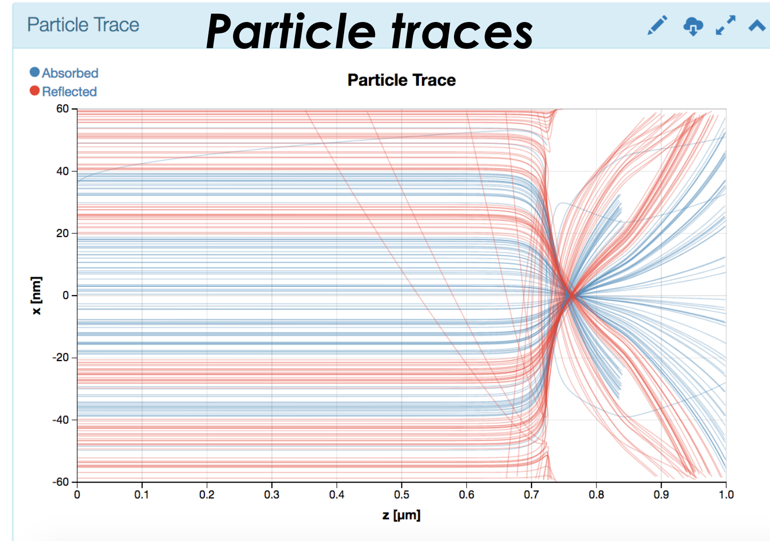


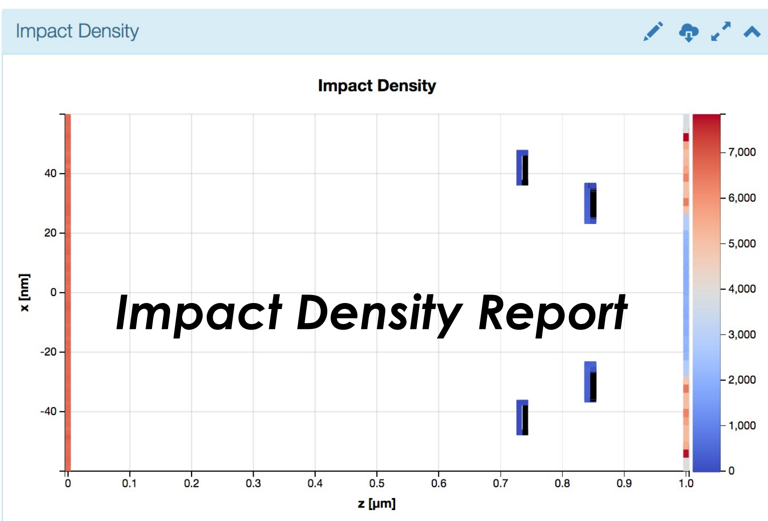
Preview Electric Fields

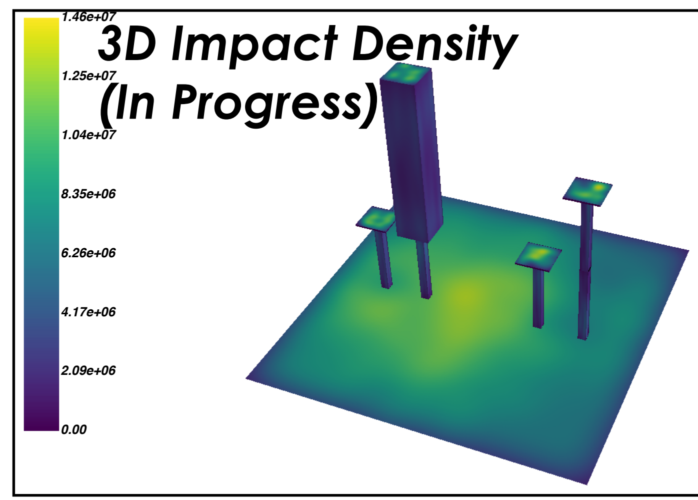


Rapid design evaluation in Sirepo



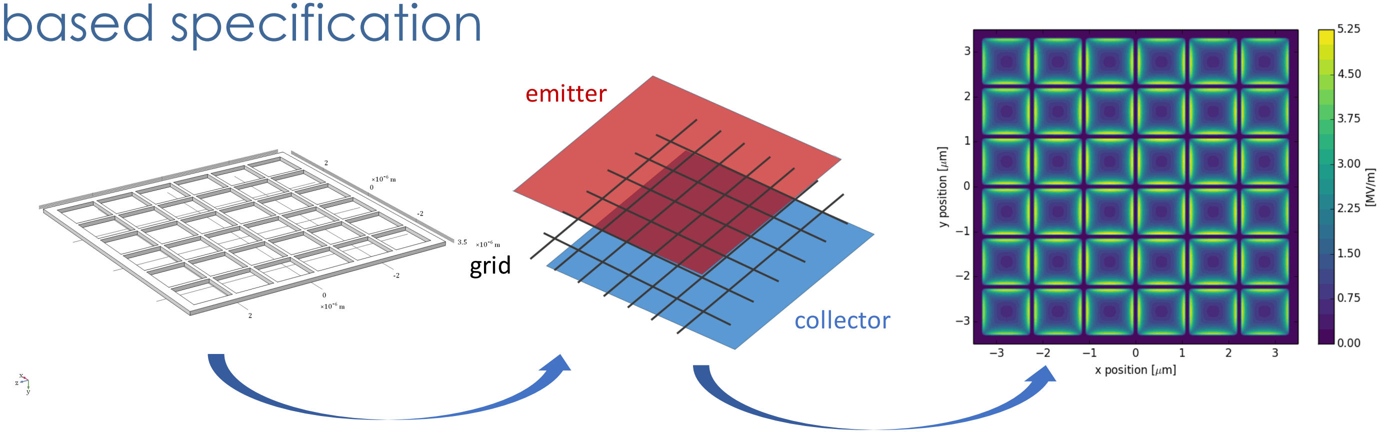




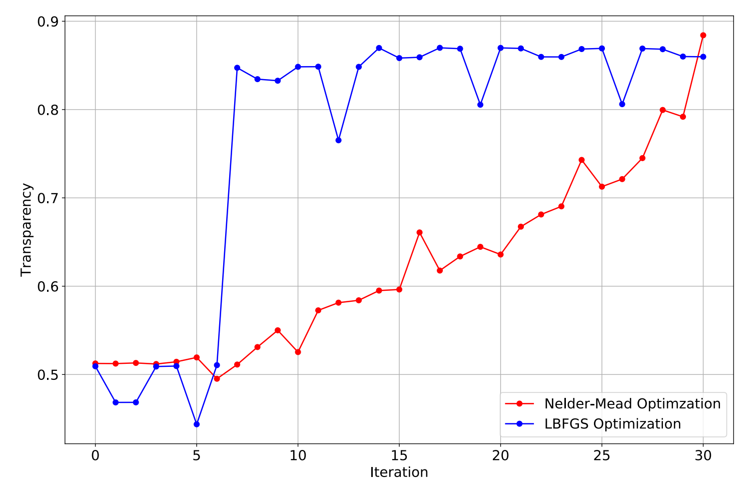


Future Interface Plans

- Generalized CAD support
  - Leverage cut-cells/mesh refinement
  - Vertex-based specification
  - STL I/O



- Launching of jobs at NERSC
  - NEWT (NERSC Web Toolkit) for queue management and authentication
  - Shifter for container management
- Integrate and improve optimization
  - Native Warp with Python hooks
    - Standard Scikit + genetic algorithms



Conclusions

- Thermionic energy converters present attractive solutions for efficiency energy production
  - Scalable from personal (KW) to community (MW) sources
  - Novel emitter technologies promise higher efficiency
  - Novel production techniques promise portability
- Optimization of these devices requires careful simulation studies
  - Proper measurement of steady-state system
  - Rigorous efficiency model to capture discrete loss channels
- Using Warp, we are improving the capabilities to model and optimize TECs and similar nano-electronics
  - Enhanced dielectric solver for realistic structures
  - Improved geometry-handling for complex emitters/grids
  - New optimization tools for deploying Warp simulations
- These tools are being made available via a browser-based platform for scientific computing, https://www.sirepo.com

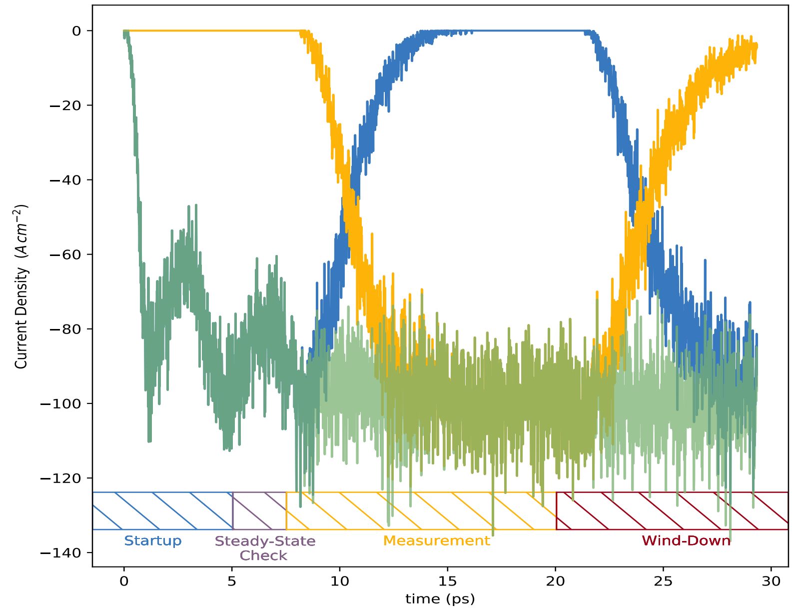
Additional material

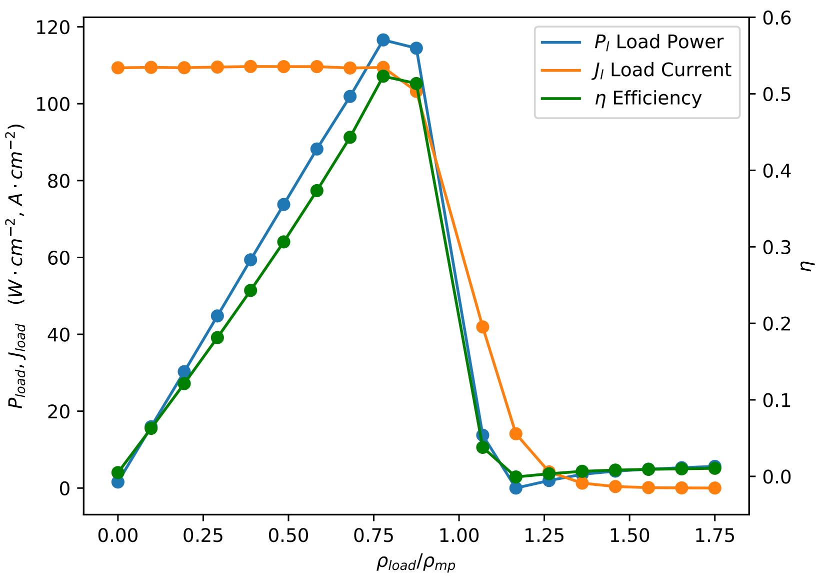
Anatomy of a TEC Simulation

Four Stages of Simulation

- Startup: Begin emission
- Steady-state check: Validate current
- Measurement: Begin collection
- Wind-Down: End collection

Required statistics are device specific!





External circuit model required to maintain feedback

- V_{load} must bridge gap in work functions
- The load resistance must be chosen based on the operating conditions
- If σ is too small, low voltage
- If σ is too large, low current