TECH-X

SIMULATIONS EMPOWERING YOUR INNOVATIONS

NIBS 2018

FLUID MODELING OF NEGATIVE HYDROGEN ION SOURCES

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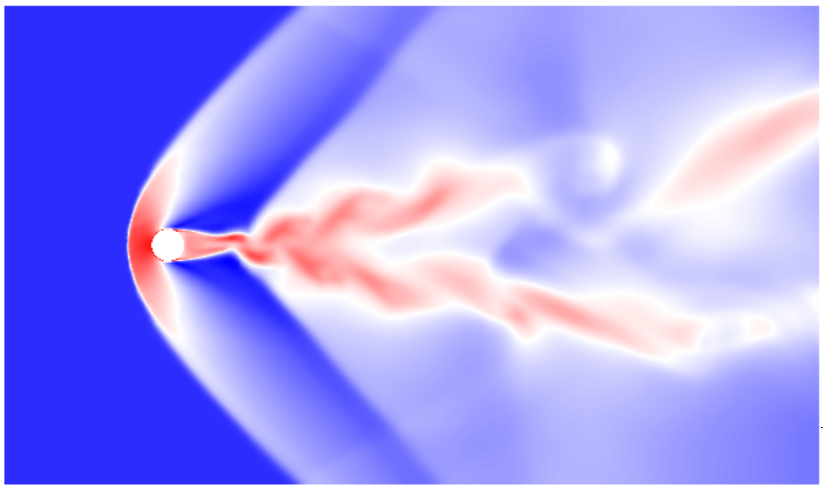
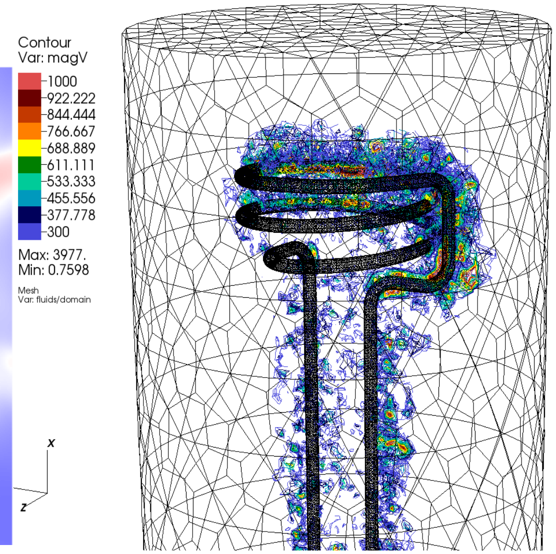
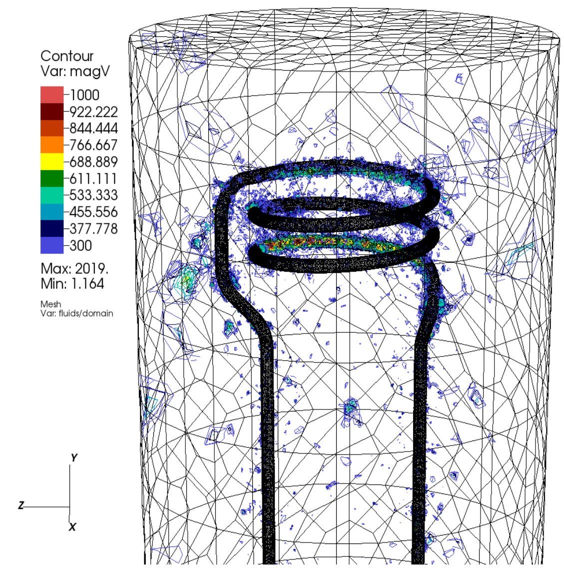
We are using a plasma fluid modeling tool to simulate the performance of ion sources

USim





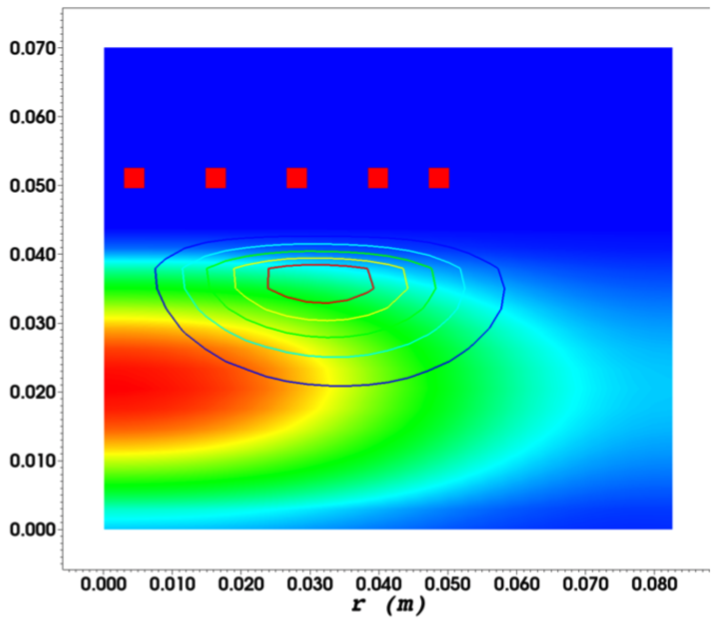


A computational fluid dynamics (CFD) code, unstructured meshes, charged or neutral fluids

We have used USim to model plasma interaction with antenna surfaces in SNS H^- ion source; Help improve internal antenna design for improved reliability at SNS

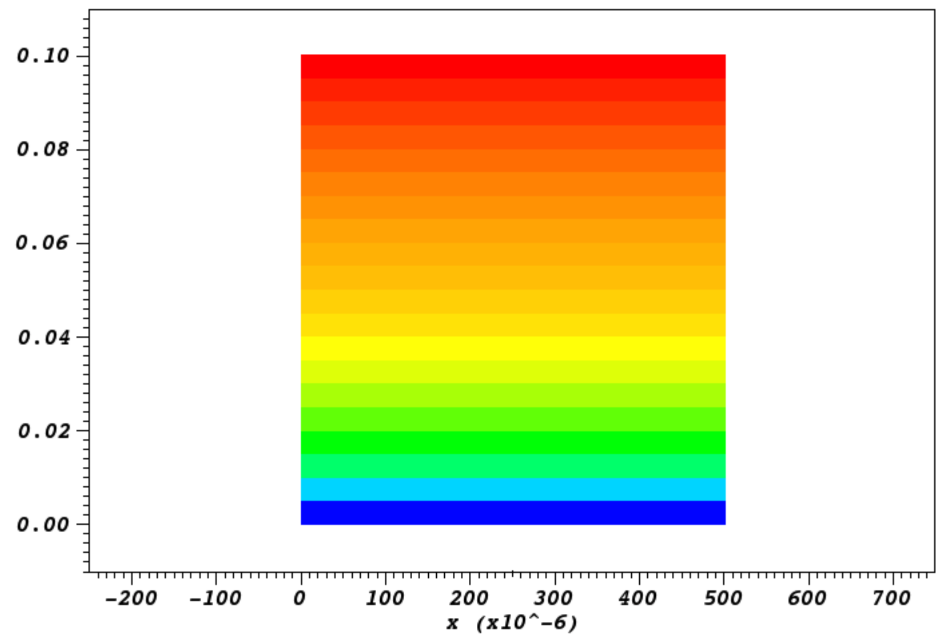
We have developed two models for ion sources in

Multi-fluid electromagnetic



Multi fluid, spectral EM
Appropriate to higher density, ICP
Computationally intensive
Discussed at NIBS 2016

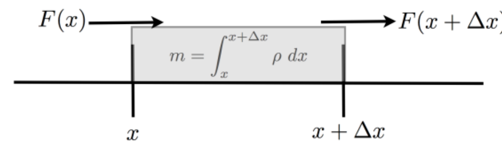
Multi-fluid drift-diffusion

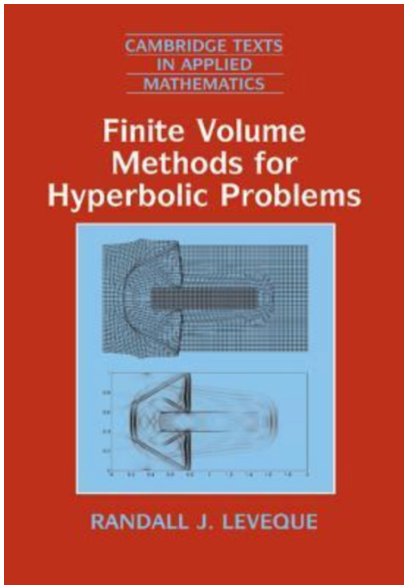


Multi-fluid, electrostatic
Appropriate to lower density
Computationally simple
Today's presentation

USim solves flux-conservative equation sets using finite volume algorithms

$$\frac{\partial q}{\partial t} + \nabla \cdot F(q) = S$$





Many of the USim algorithms are described in detail in this book

One example is convective drift equations*:

$$\frac{\partial n_e}{\partial t} + \nabla \cdot n_e \mu_e E = S_n$$

$$\frac{\partial u_e}{\partial t} + \nabla \cdot u_e \gamma \mu_e E = S_u$$

*USim includes non-hyperbolic terms, like diffusion, separately with algorithms like STS

Drift-diffusion models are most applicable when electron-neutral collisions dominate

The drift-diffusion model works best with:

- *High pressure* (collision frequency larger than plasma frequency implies v ~ E)
- *Low voltage* (drift velocity smaller than thermal velocity implies v ~ E)
- *Low plasma density* (Debye length long implies field penetrates into plasma)

For example, assuming: T_e ~ 4 eV, $v_{th}=10^6$ m/s, E ~ 1 kV/m, $\sigma_{elastic} = 10^{-19}$ m^{-2}

Neutral pressure (torr)	Collision frequency (s^{-1})	Mean Free Path (m)	Electron Drift Velocity (m/s)	Plasma density (m^{-3})	Plasma frequency (s^{-1})	Debye length (m)	Drift diffusion applicable?
10	3×10^{10}	30×10^{-6}	10^4	**10^{12}**	10^7	0.01	**Y**
0.1	3×10^8	3×10^{-3}	10^6	**10^{14}**	10^8	0.001	**Maybe**
0.01	3×10^7	0.03	10^7	**10^{15}**	3×10^8	3×10^{-4}	**N**

The USim model solves the full drift diffusion equation with sources

$$\frac{\partial n_e}{\partial t} + \nabla \cdot n_e \mu_e E - \nabla \cdot D_n \nabla n_e = S_n$$

$$\frac{\partial u_e}{\partial t} + \nabla \cdot u_e \gamma \mu_e E - \nabla \cdot D_u \nabla n_u = S_u$$

$$\mu_e = \frac{q}{m N_0 \sigma_0 v_{th}} \approx \frac{4x10^{24}}{N_0}$$

- USim includes an RK-like super-time-stepping scheme for stepping over diffusion time scales
- USim can also include any number of ion species in the same way

Drift-diffusion model includes joule heating, ionization and excitation through source terms

$$S_n = n_e N_0 k$$

ionization density source

$$S_u = n_e \mu E^2 - D_n E \nabla n_e - n_e N_0 k \epsilon$$

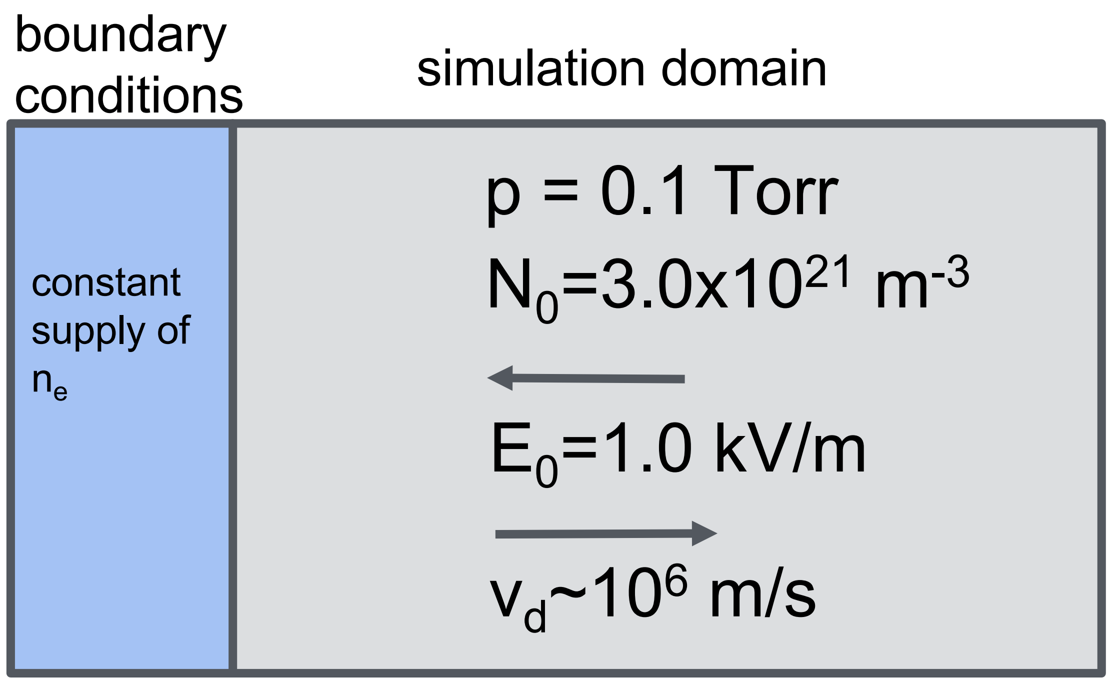
convective joule heating

diffusive joule heating

ionization energy losses

- We can track an arbitrary number of these reactions
- k can be temperature dependent

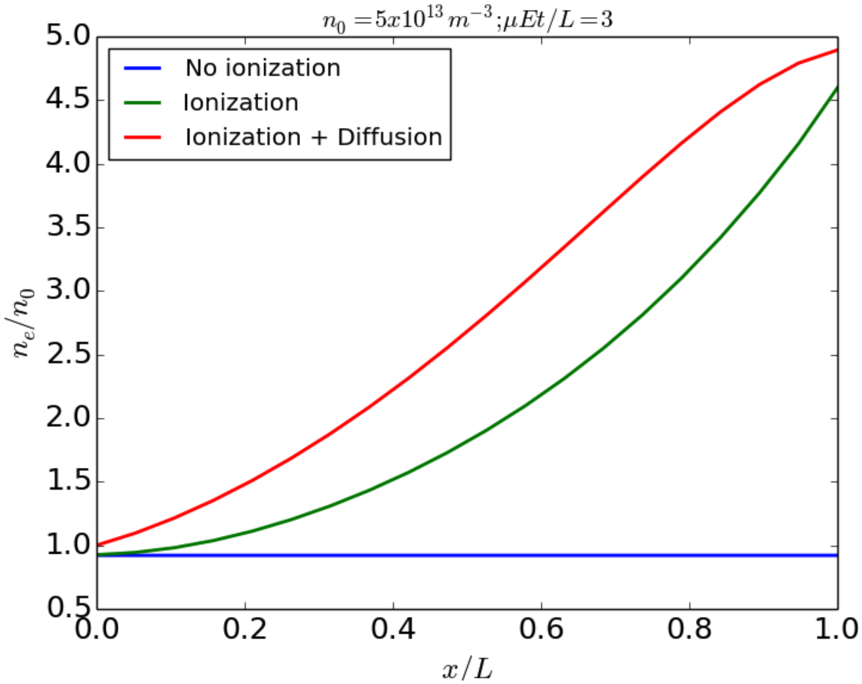
As a test-bed for this model, we use a rectangular region of constant gas density and electric field



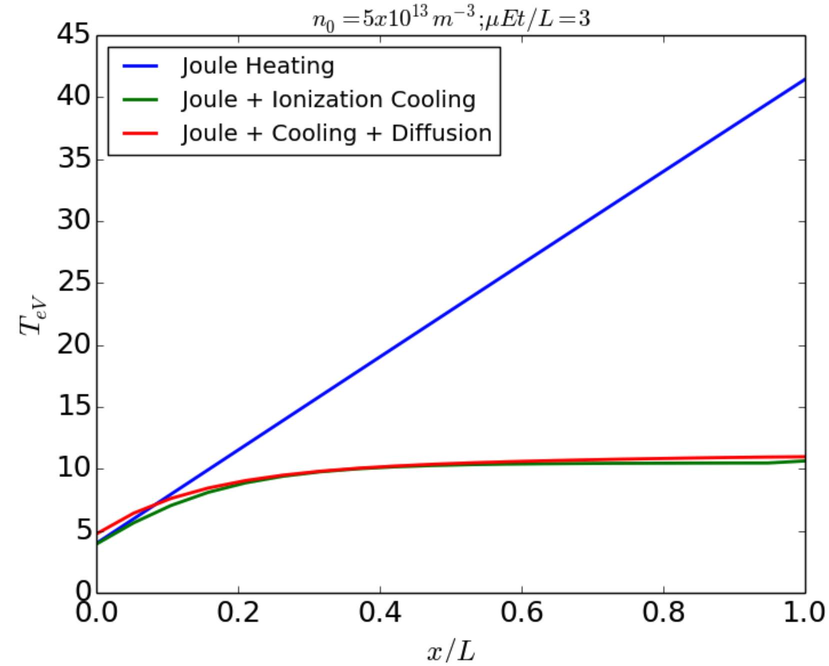
- We assume a reservoir of electrons with n_e ~ 5.0x10^{12} m^{-3} and Te = 2 eV on the left boundary

First test case includes H_2 ground state impact ionization

Electron Density

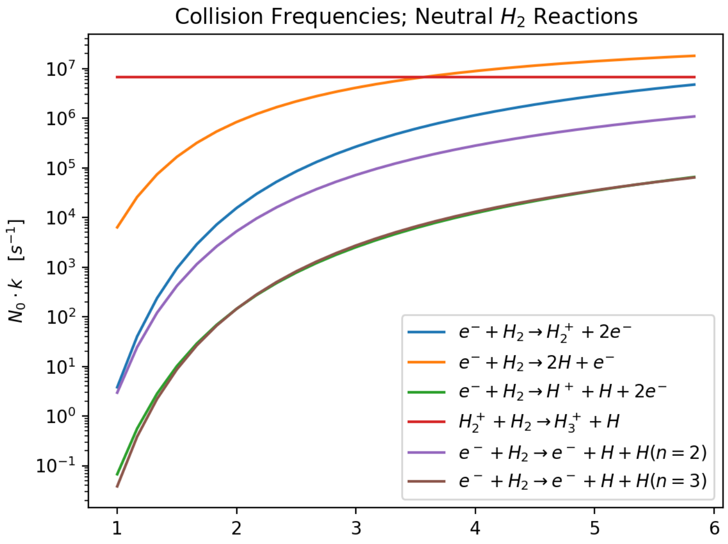


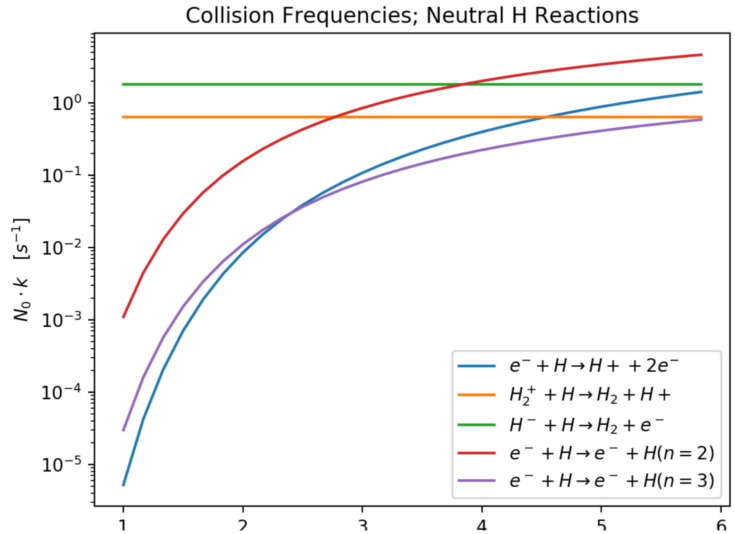
Electron Temperature

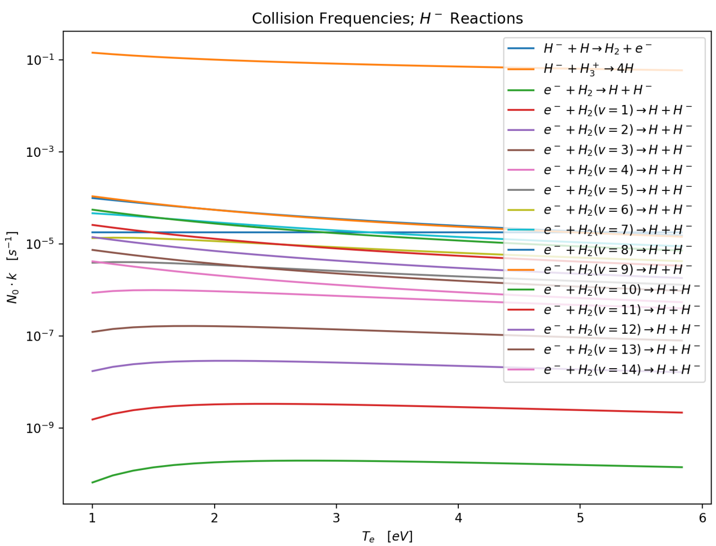


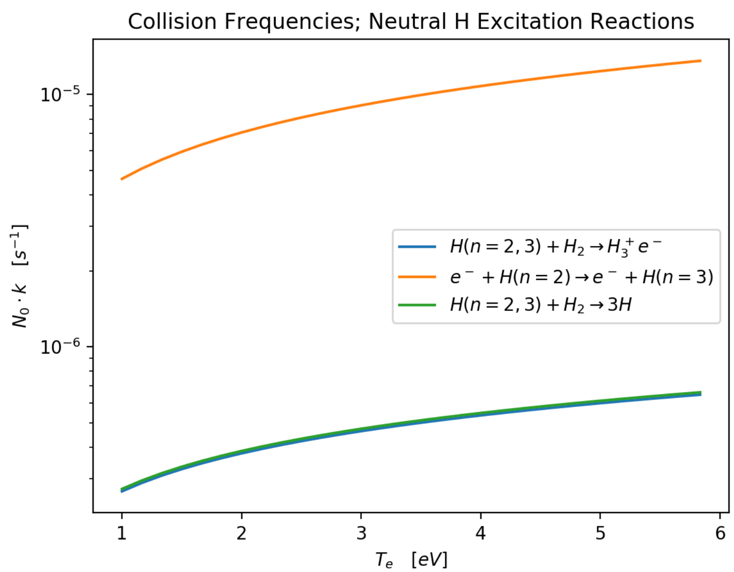
- We evolve system to steady steady (a few electron crossing times)
- Ionization adds density, diffusion acts to smooth
- Ionization energy loss acts to cool the plasma

Reaction Sources

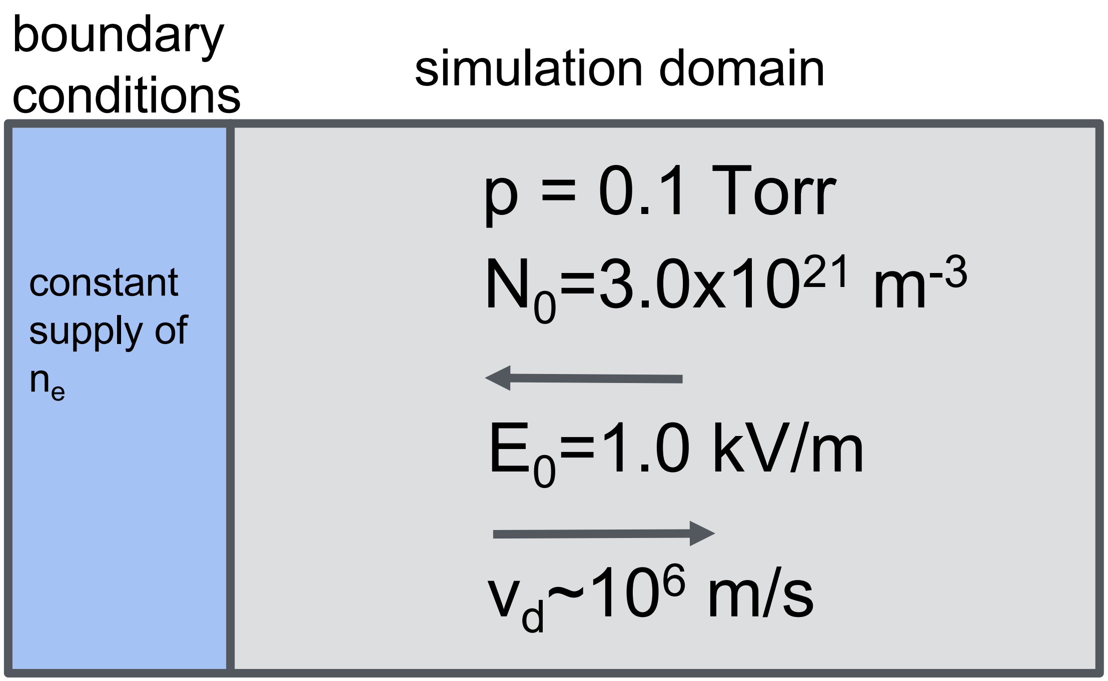






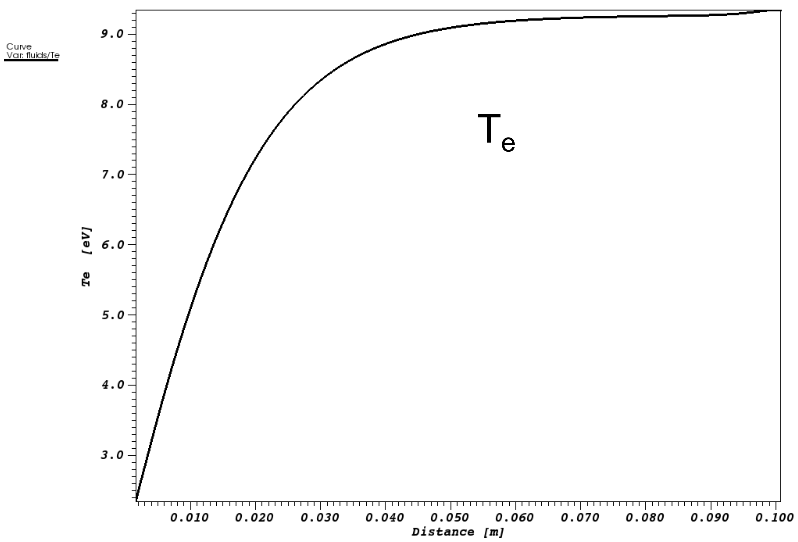


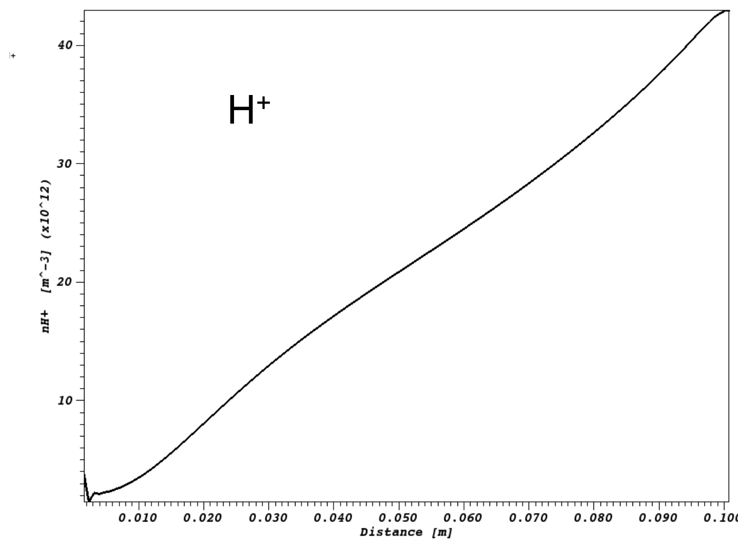
We perform simulations with reaction sources in a system similar to our previous simulations



- We assume a reservoir of electrons with n_e ~ 5.0x10^{12} m^{-3} and Te = 2 eV on the left
- Add reactions
- Increase physical dimensions

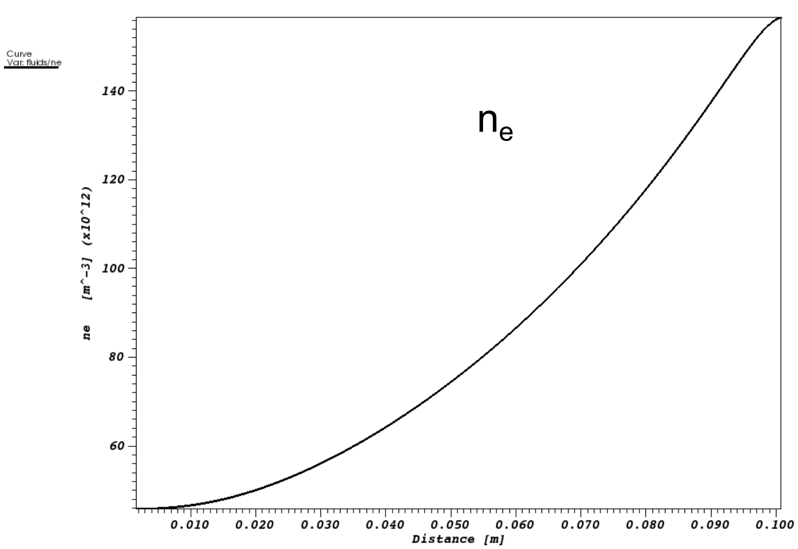
Results with Ionization and Dissociation

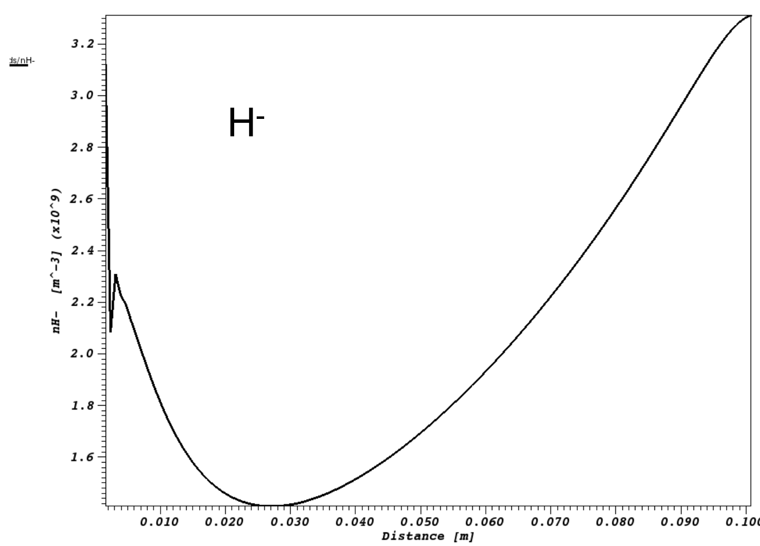




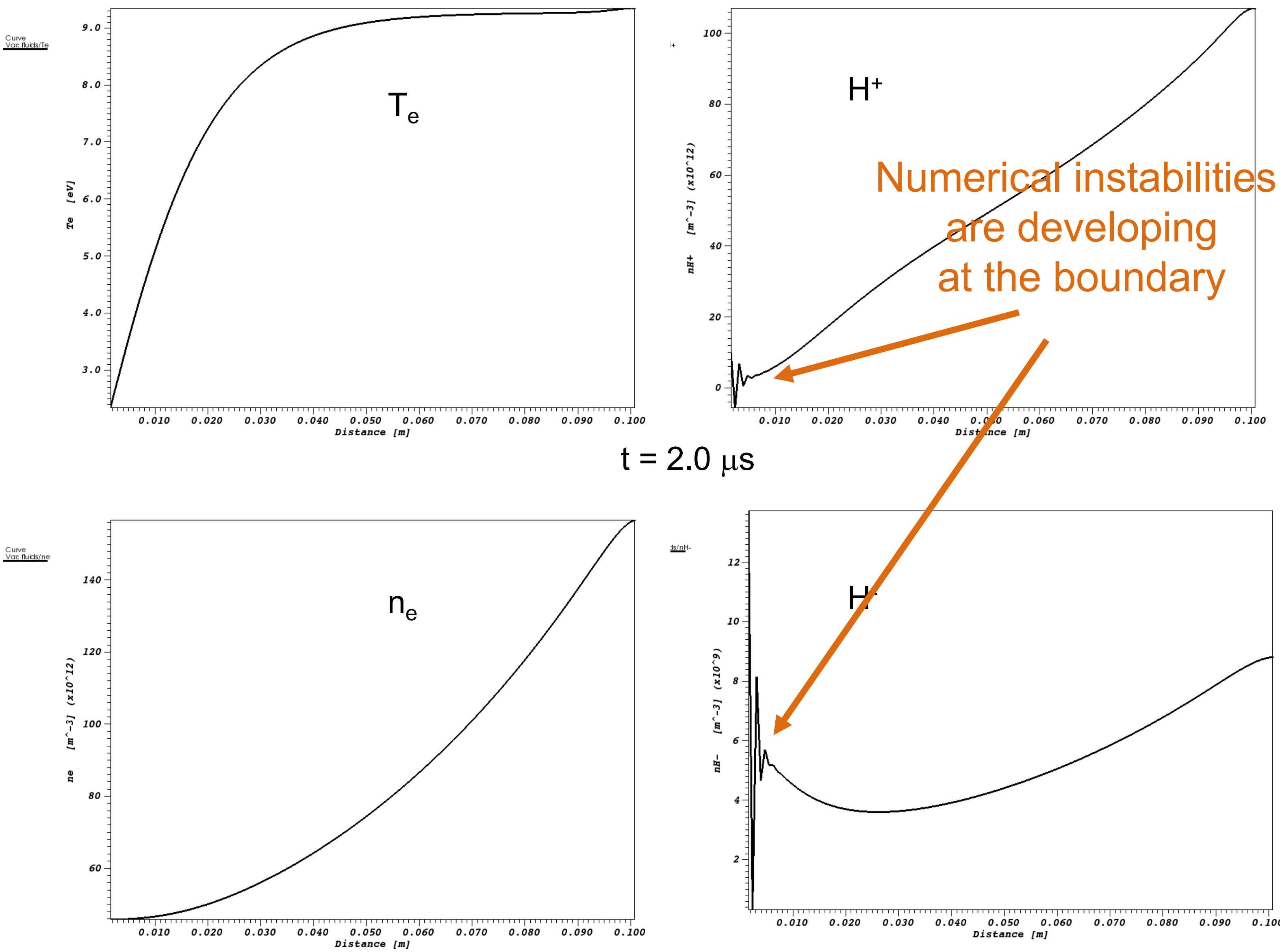
$$e^- + H_2 \rightarrow H_2^+ + 2e^-$$
$$e^- + H_2 \rightarrow 2H + e^-$$
$$e^- + H_2 \rightarrow H + H^-$$
$$e^- + H_2 \rightarrow H^+ + H + 2e^-$$
$$e^- + H \rightarrow H^+ + 2e^-$$
$$e^- + H^- \rightarrow H + 2e^-$$
$$e^- + H_2^+ \rightarrow 2H$$
$$e^- + H_2^+ \rightarrow H + H^+ + e^-$$

t = 0.7 μs





Results with Ionization and Dissociation and Vibrational Creation of H^-



$e^- + H_2 \rightarrow H_2^+ + 2e^-$
$e^- + H_2 \rightarrow 2H + e^-$
$e^- + H_2 \rightarrow H + H^-$
$e^- + H_2 \rightarrow H^+ + H + 2e^-$
$e^- + H \rightarrow H^+ + 2e^-$
$e^- + H^- \rightarrow H + 2e^-$
$e^- + H_2^+ \rightarrow 2H$
$e^- + H_2^+ \rightarrow H + H^+ + e^-$
$e^- + H_2(v=1) \rightarrow H + H^-$
$e^- + H_2(v=2) \rightarrow H + H^-$
$e^- + H_2(v=3) \rightarrow H + H^-$
$e^- + H_2(v=4) \rightarrow H + H^-$
$e^- + H_2(v=5) \rightarrow H + H^-$
$e^- + H_2(v=6) \rightarrow H + H^-$
$e^- + H_2(v=7) \rightarrow H + H^-$
$e^- + H_2(v=8) \rightarrow H + H^-$
$e^- + H_2(v=9) \rightarrow H + H^-$
$e^- + H_2(v=10) \rightarrow H + H^-$
$e^- + H_2(v=11) \rightarrow H + H^-$
$e^- + H_2(v=12) \rightarrow H + H^-$
$e^- + H_2(v=13) \rightarrow H + H^-$
$e^- + H_2(v=14) \rightarrow H + H^-$

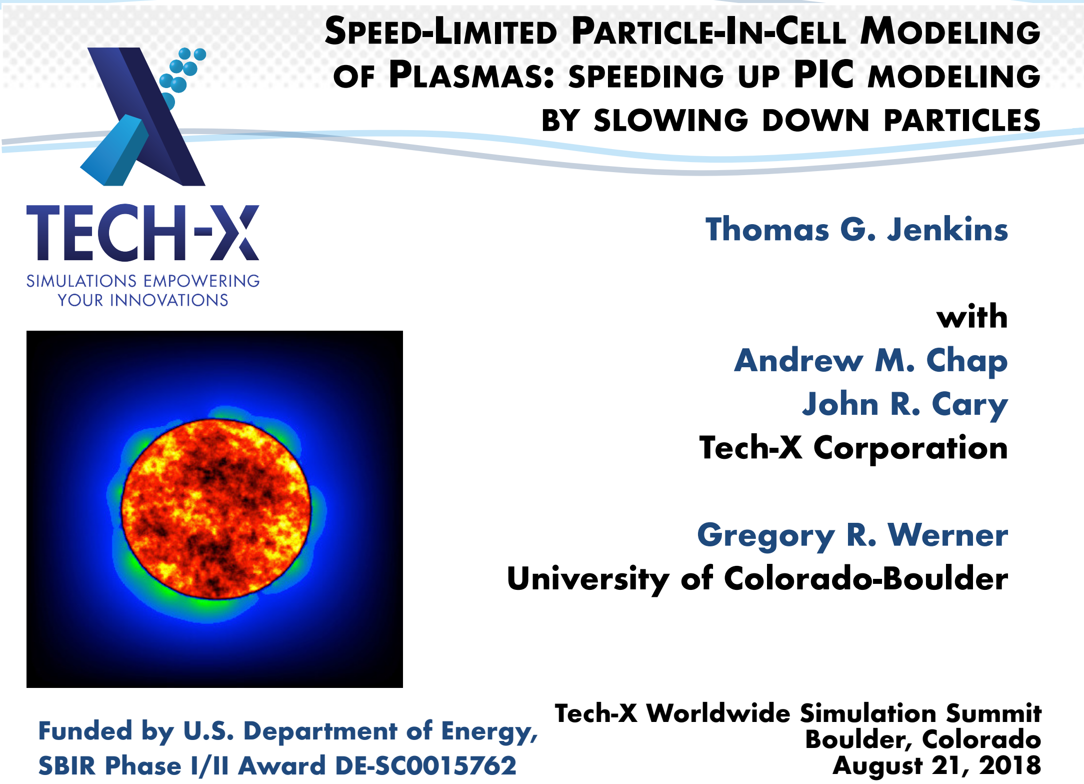
Conclusions and Next Steps

- We can use fluid models to simulate negative hydrogen ion sources with realistic plasma chemistry (an ongoing effort!)
- In some cases, a drift diffusion model is appropriate for this modeling

- 2-Dimensional cylindrical modeling with Hydrogenic chemistry
  -- Include RF power deposition
- -- Include wall production of H^-

- Deuterium plasma chemistry?
- Alternative Methods for speeding up ion source simulations, for instance, ECRs
- -- Speed Limited Particle-In-Cell Algorithms

Next Steps



- Fastest electrons set the timestep in PIC, even if their kinetics are not of interest
- SLPIC formalizes how to transform PIC equations of motion so that fast particles are accurately simulated without excessive time step restrictions

THANK YOU FOR YOU ATTENTION

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