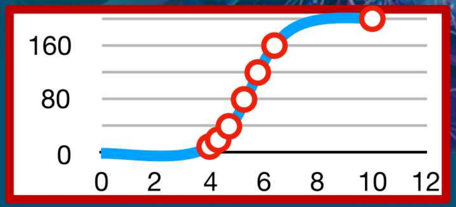
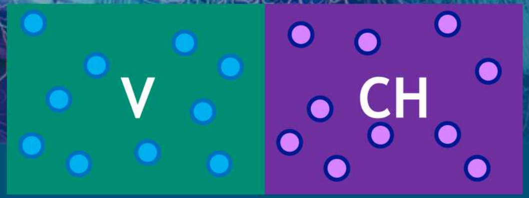
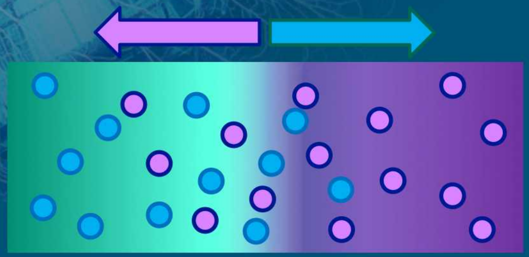
Sandia National Laboratories

SAND2018-12610C

Modelling Species Transport across a V/CH Interface







PRESENTED BY

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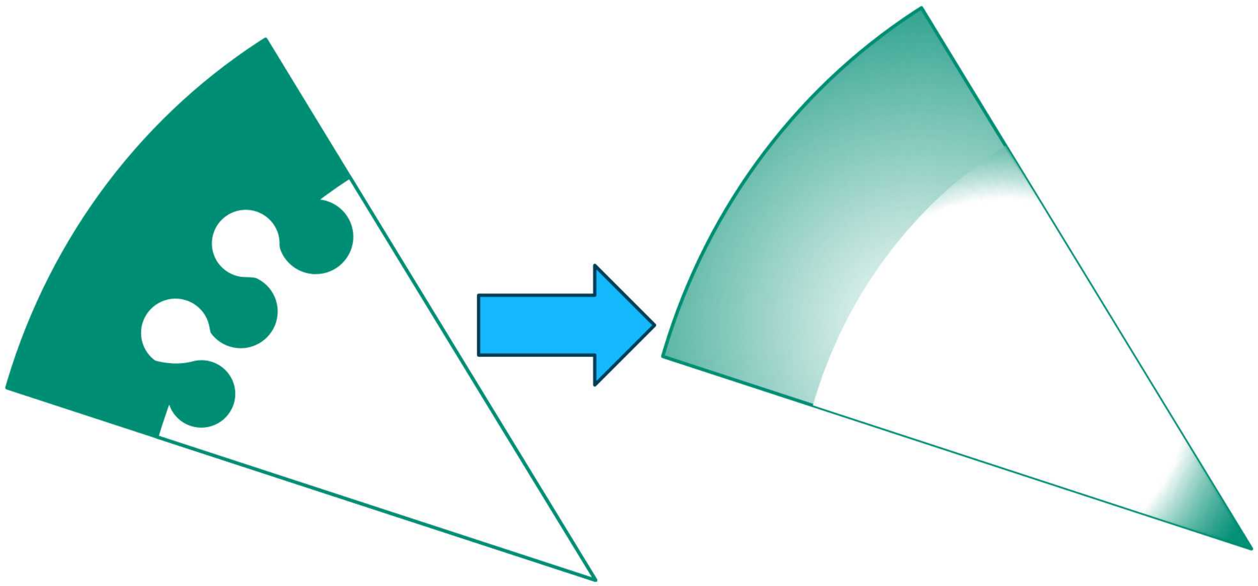
This project has been a large interdisciplinary effort

- Diagnostic Development
  - E.C. Harding, M. Schollmeier, G.P. Loisel, S.B. Hansen
- Sample Development
  - S.B. Hansen, P.J. Christenson, P.F. Knapp, T. Mattsson
- Target Fabrication
  - Haibo Huang, Reny Paguio, Brian Stahl
  - *General Atomics, La Jolla, CA*
- Modeling and Source Development
  - Roger Vesey, P. J. Christenson, T. Mattsson, K. Beckwith
- Multi-species BGK theory and code development
  - M. Murillo (MSU), J. Haack (LANL), L. Stanton (LLNL) and C. Hauck (ORNL)

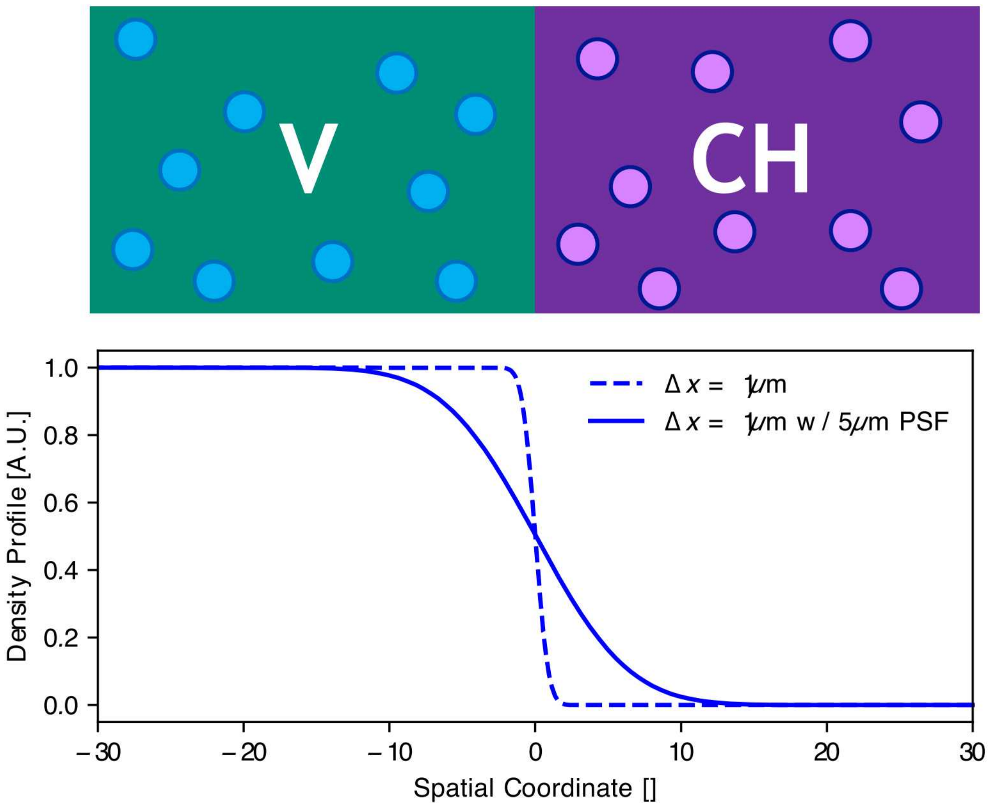
Understanding material transport across an interface is fundamentally tied to our understanding of mix

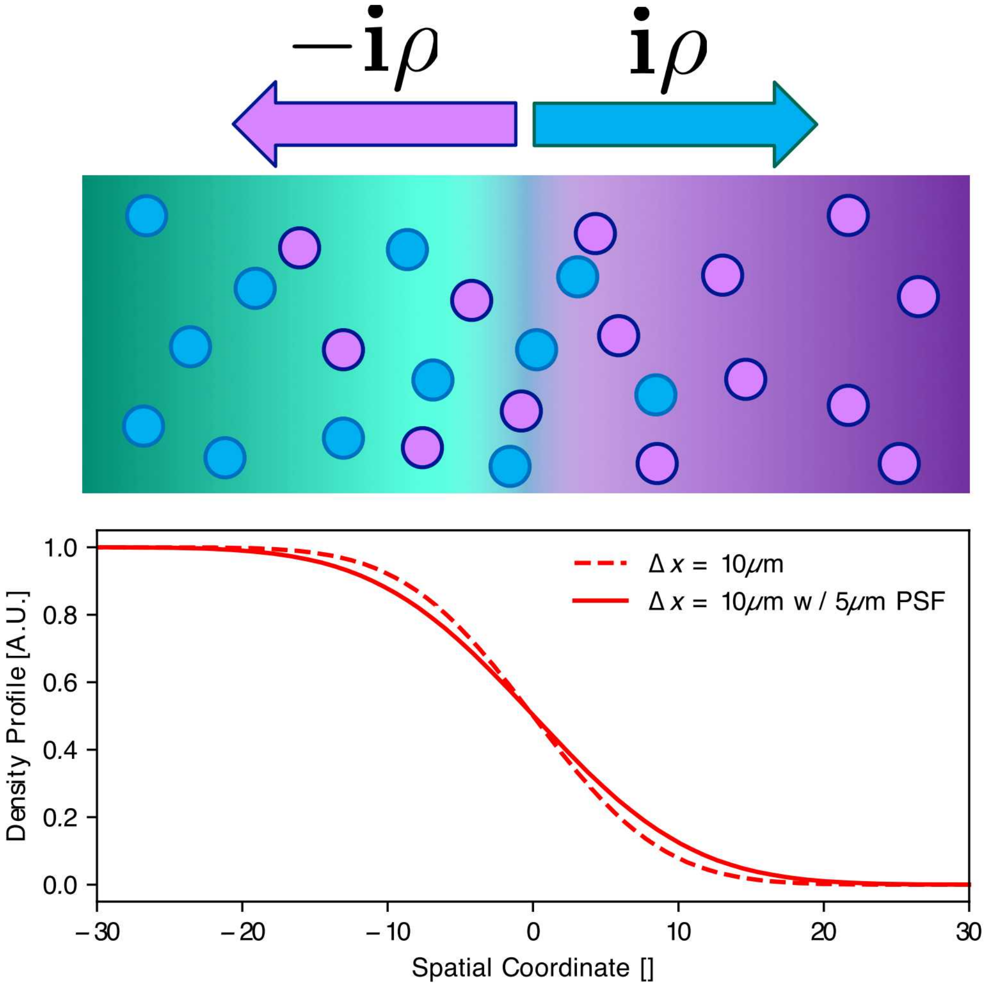


- In addition to distorting the hotspot shape and introducing vorticity, perturbations will
  - increase the surface area available for transport processes
  - decrease the scale length over which transport needs to operate to mix a volume
- Unfortunately fluid models don't account for transport processes well, particularly in strongly coupled plasmas

- How does an interface go from perturbed to mixed
- Is it just hydrodynamic stirring/turbulence?
- What role does diffusion play?

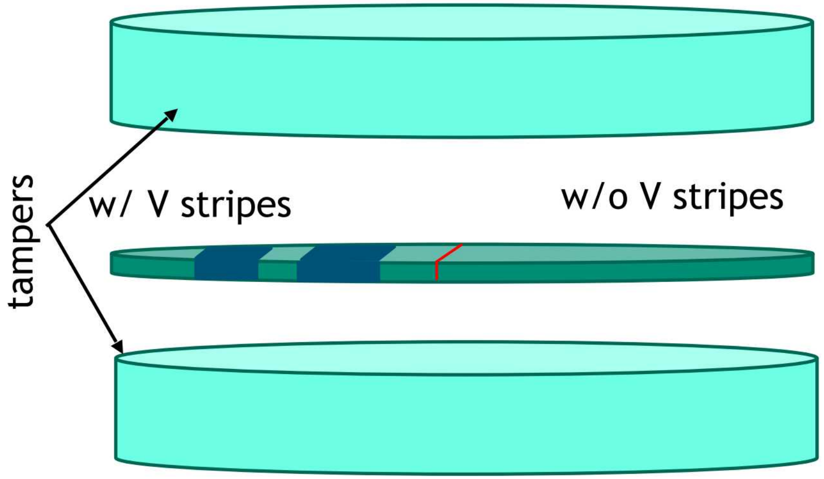
We want to measure the "blurring" of an interface between a strongly coupled mid-Z element and a low Z material





Plasma Transport Sample and Diagnostic Concept

Conceptual Sample



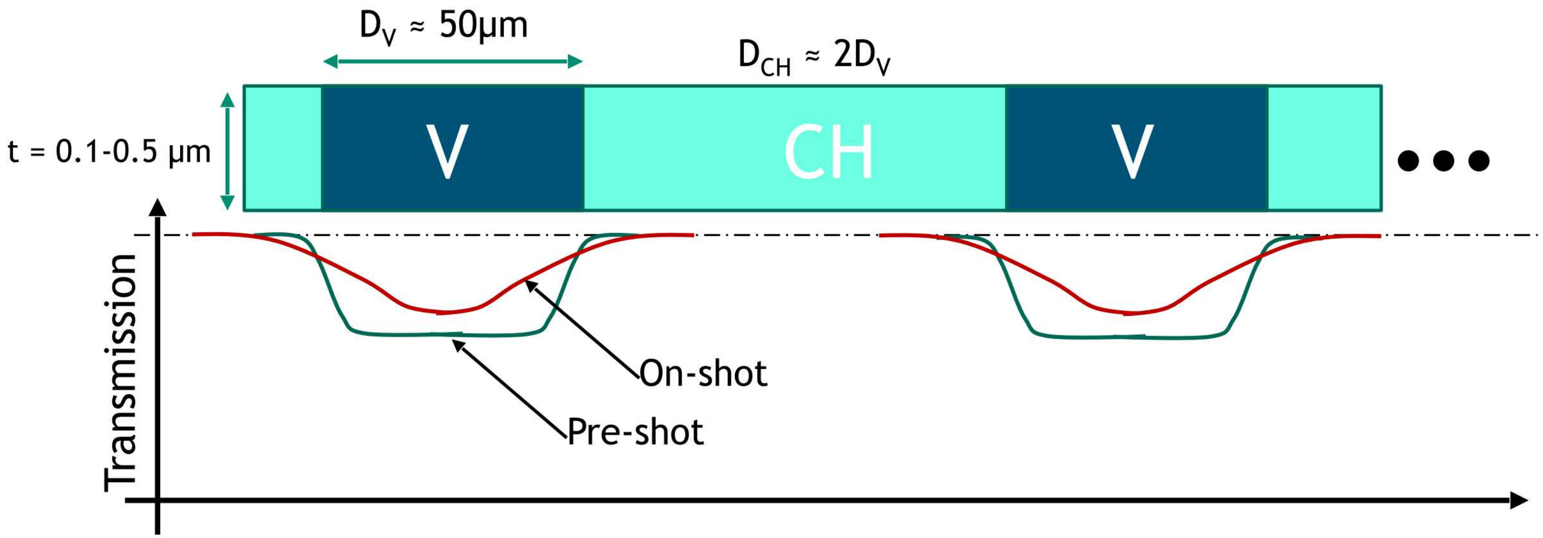
Half moon sample allows transmission to be obtained from the attenuation

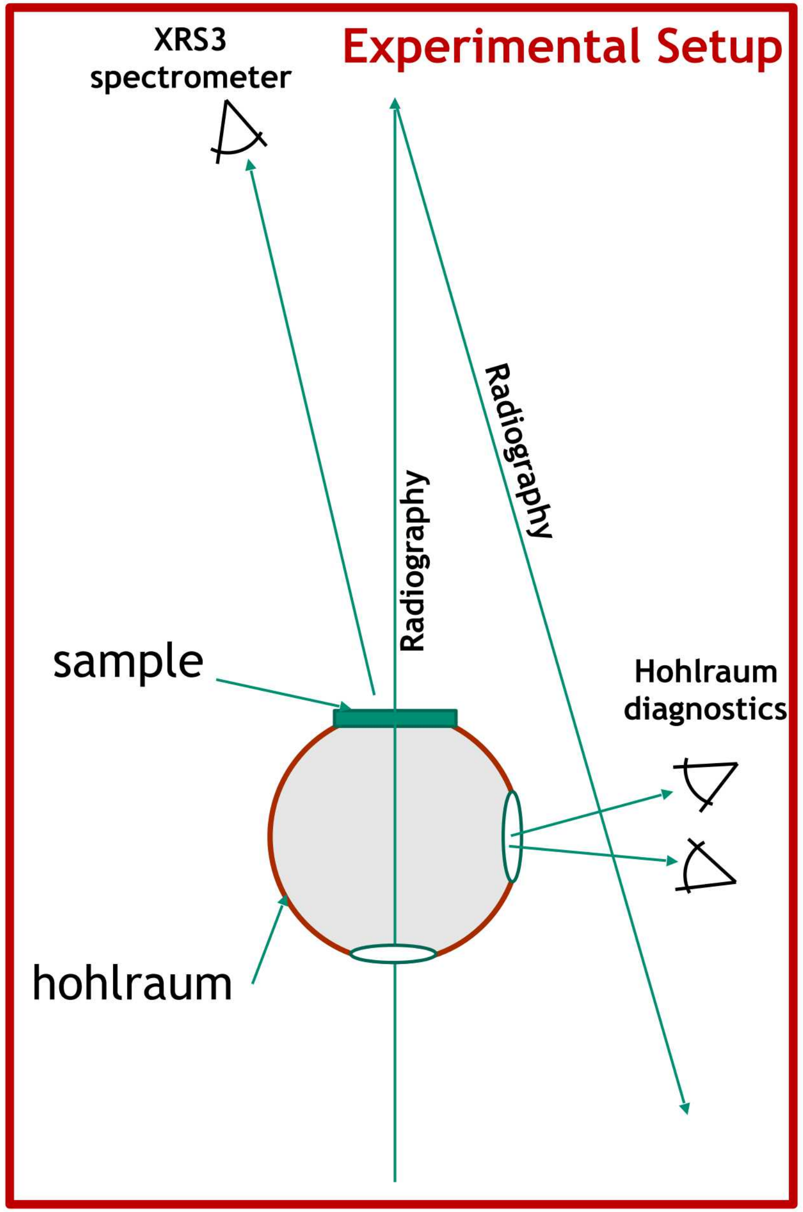
Linear array of High-Z material allows integration of data along one dimension

Sample heated using Hohlraum from one side

ZBL radiography used to image evolution of high Z strips

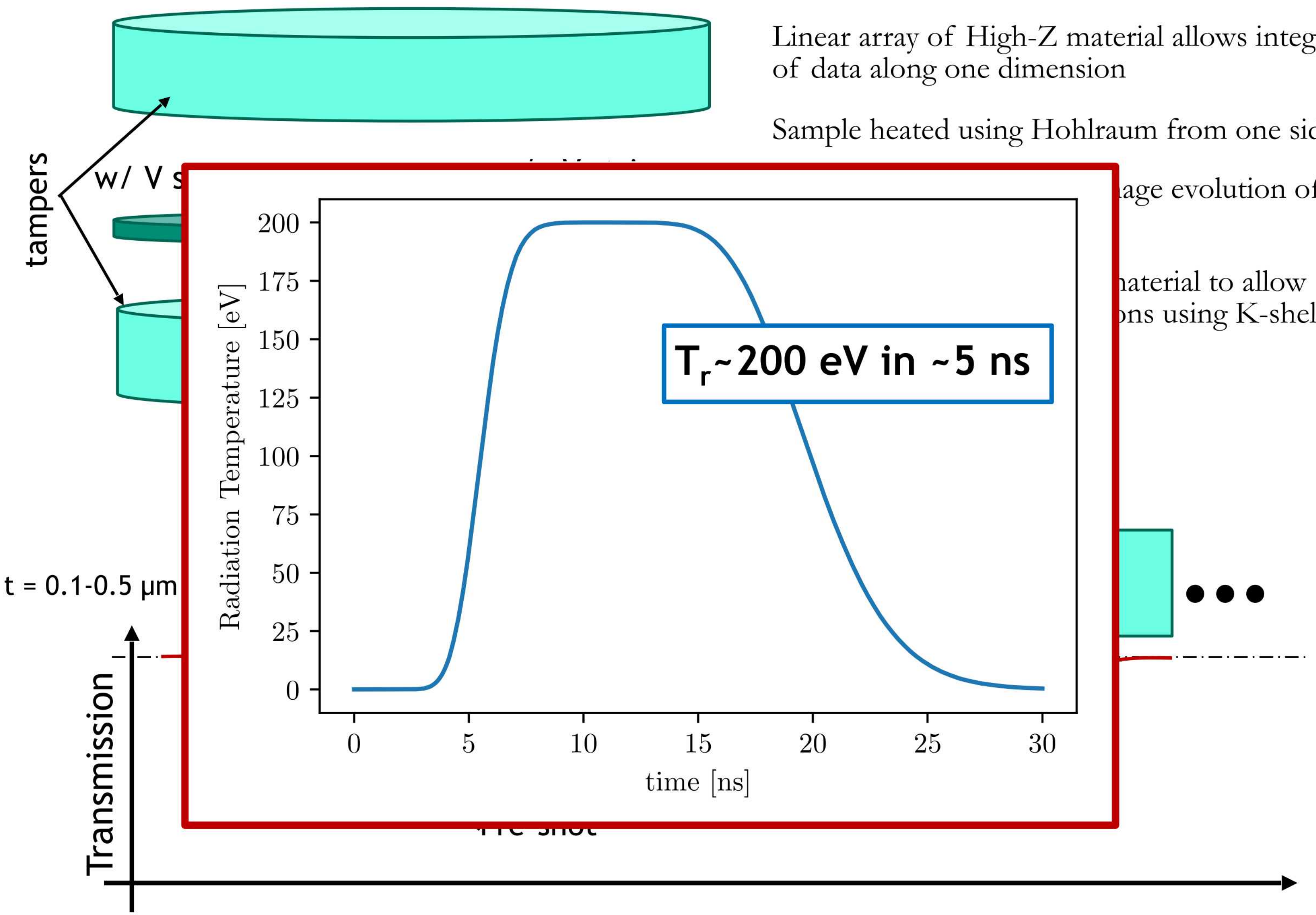
Sample doped with mid-Z material to allow diagnosis of sample conditions using K-shell emission spectroscopy





Plasma Transport Sample and Diagnostic Concept

Conceptual Sample



Half moon sample allows transmission to be obtained from the attenuation

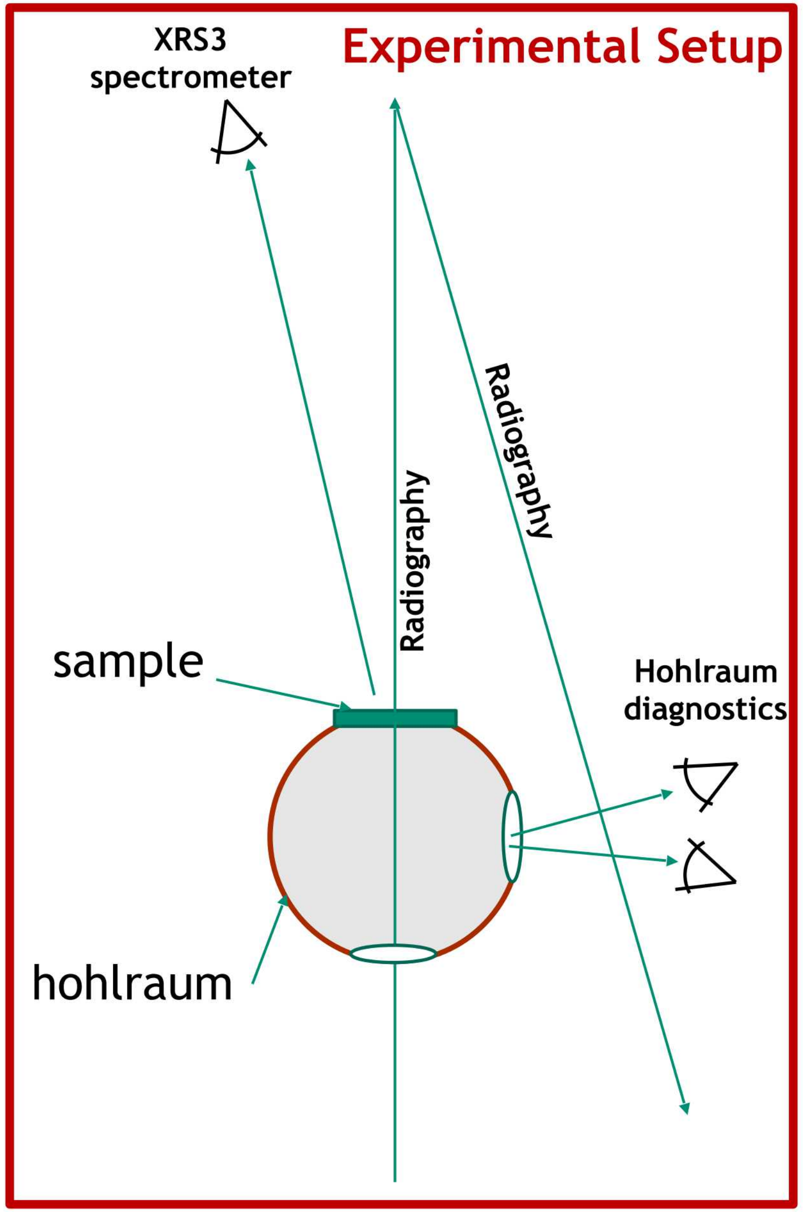
Linear array of High-Z material allows integration of data along one dimension

Sample heated using Hohlraum from one side

age evolution of high

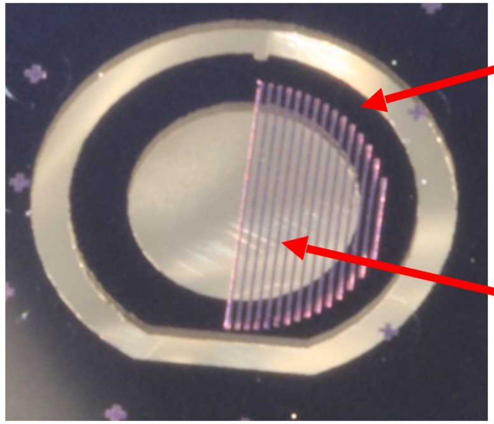
aterial to allow
ons using K-shell

Experimental Setup



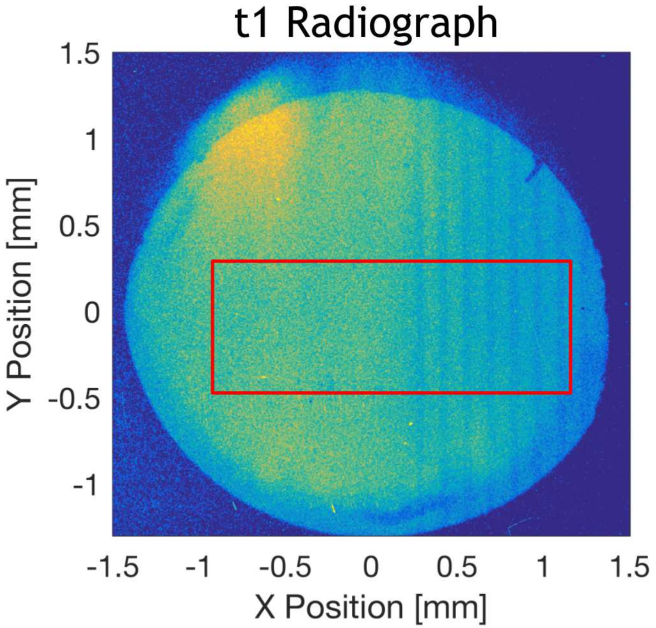
First plasma transport experiments have been executed on Z demonstrating the feasibility of the proposed measurement

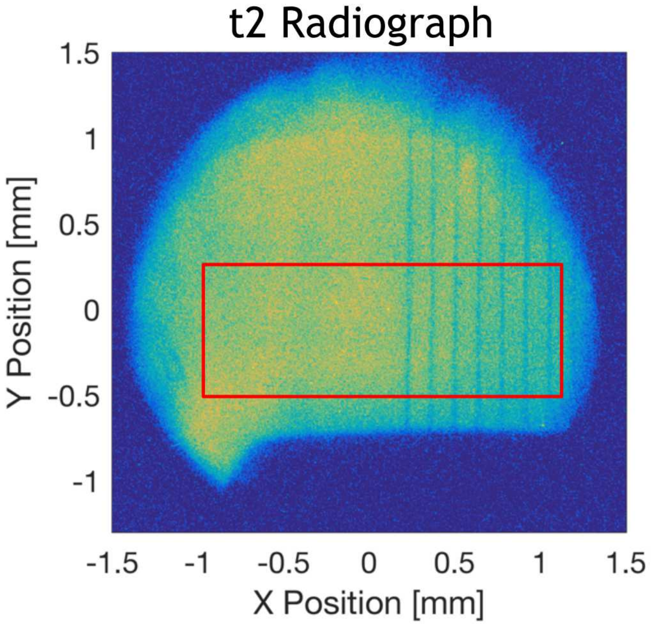
- Executed two experiments in March testing x-ray heating and diagnostics performance
- Demonstrated good contrast of the sample in the radiographs on shot z3220 (6.1 keV backlighter with detector placed at closer focal position)

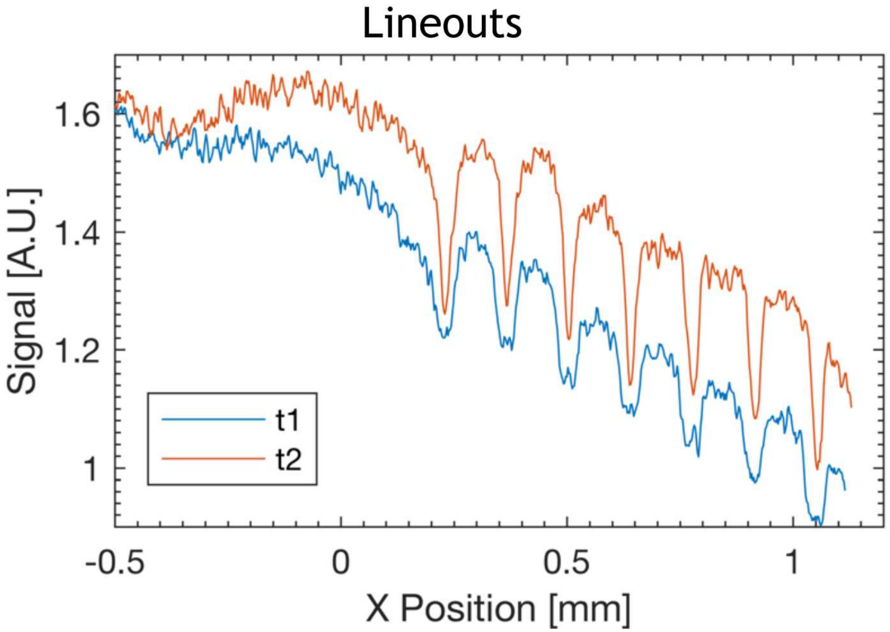


fabricated sample on Si wafer

Al-doped Vanadium Bars







Modeling Blurring of Interface: Need *Predictive* Kinetic Theory

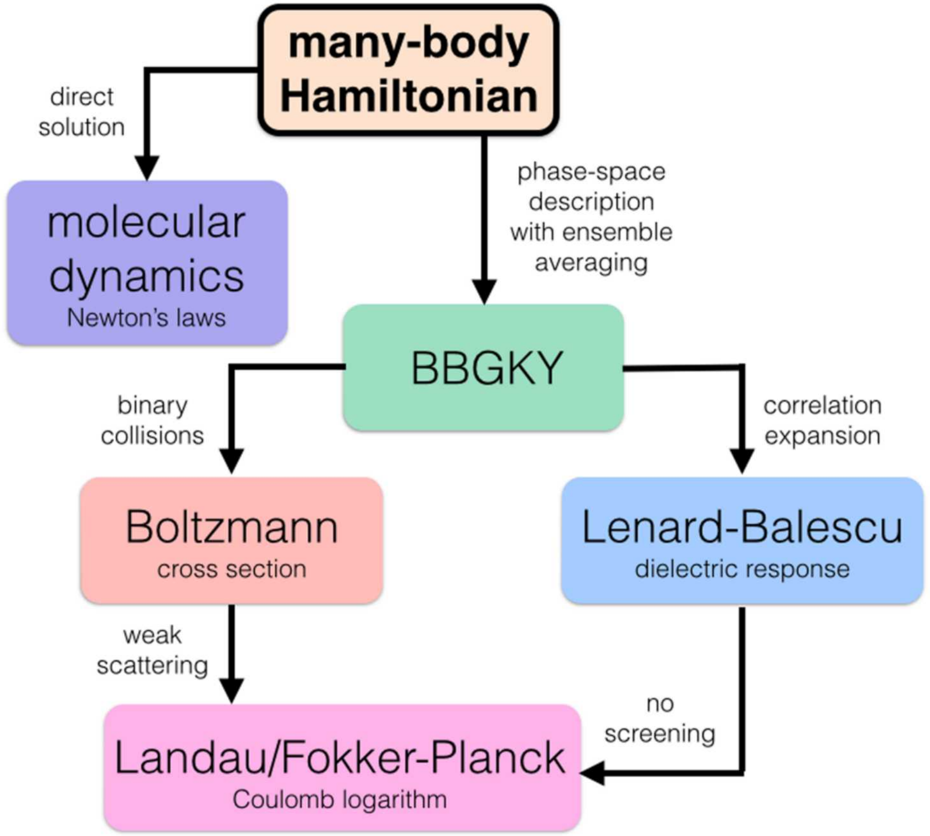
Start from many-body Hamiltonian

Molecular-dynamics treatment:

- direct integration of equations of motion
- expensive for high collision rates, e.g. regimes of interest for HED

BBGKY Hierarchy:

- Binary collision approximation: requires (ad-hoc) effective potential approach, implicitly through limits on range of impact parameter. Weak-scattering approximation *divergent* for zero impact parameter
- Correlation expansion that *includes* screening, i.e. the effective potential arises naturally. While no *upper* limit on impact parameter required, perturbative expansion means that method diverges at *small* impact parameter



Stanton & Murillo (2016): Fig.1
Relevant Structure of Kinetic Theory
[for transport in HED Plasmas]

Boltzmann Equation for HED Plasma Transport

Direct integration of equations of motion:

- *Too* expensive for timescales & length scales of interest for plasma transport experiments

Dense plasmas: strongly collisional and near equilibrium:

- Adopt a *multi-species* Boltzmann model to provide *kinetic* description of plasma transport

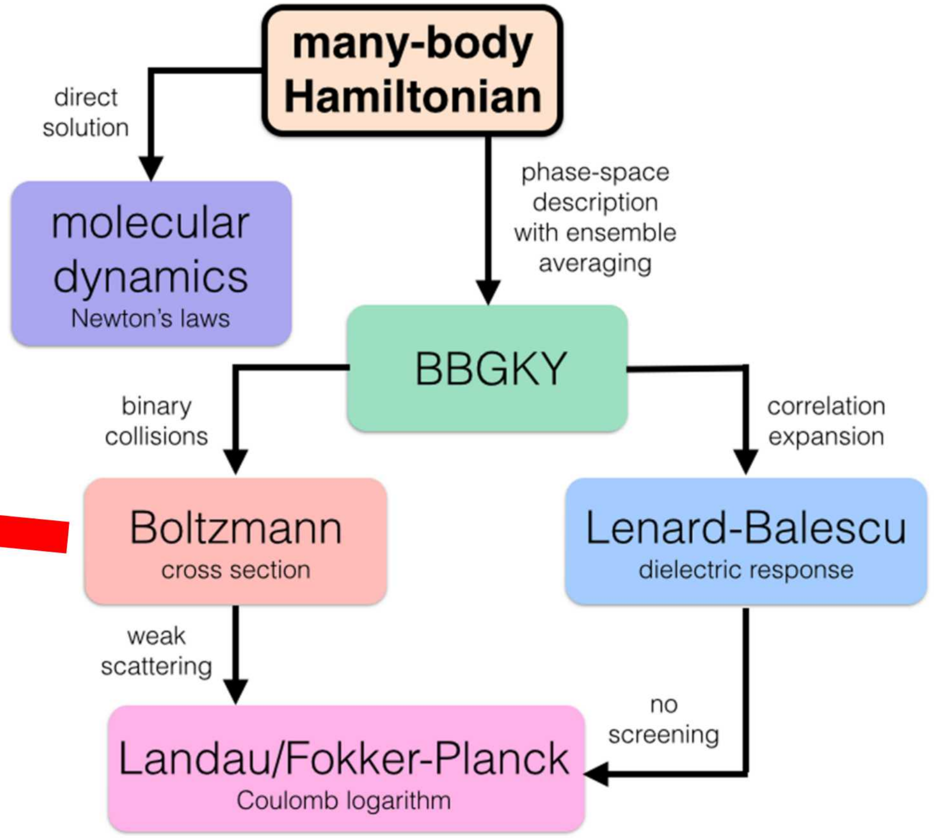
$$\frac{\partial f_i}{\partial t} + \mathbf{c} \cdot \nabla_{\mathbf{x}} f_i + \mathbf{a}_i \cdot \nabla_{\mathbf{c}} f_i = Q_i[\mathbf{f}], \quad i \in \mathcal{S}.$$

Collision operator is critical:

$$Q_i[\mathbf{f}] = \sum_{j \in \mathcal{S}} Q_{ij}[f_i, f_j],$$

$$Q_{ij}[f_i, f_j] = \int (f_i(\mathbf{c}') f_j(\mathbf{c}'_*) - f_i(\mathbf{c}) f_j(\mathbf{c}_*)) g \sigma_{ij} \, d\mathbf{\Omega} d\mathbf{c}_*.$$

- Has to guarantee conservation of mass, momentum and energy and that the entropy is constant to increasing (H-theorem)



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Hydrodynamic Equation for HED Plasma Transport

Dense plasmas: strongly collisional and near equilibrium:

- Adopt a *multi-species* Boltzmann model to provide *kinetic* description of plasma transport:

$$\frac{\partial f_i}{\partial t} + \mathbf{c} \cdot \nabla_{\mathbf{x}} f_i + \mathbf{a}_i \cdot \nabla_{\mathbf{c}} f_i = Q_i[\mathbf{f}], \quad i \in \mathcal{S}.$$

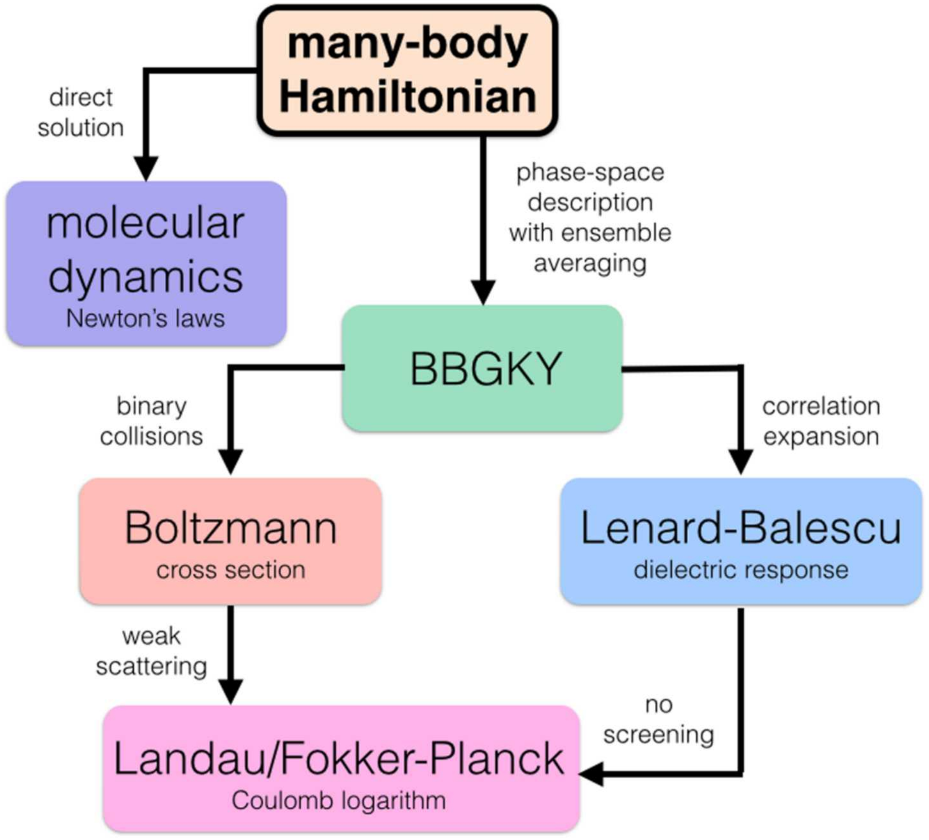
- Hydrodynamics found from taking moments over distribution function:

$$n_i = \int f_i d\mathbf{c}, \quad \rho_i = m_i n_i, \quad \mathbf{v}_i = \frac{1}{\rho} \int m_i \mathbf{c} f_i d\mathbf{c},$$

  - Mass conservation: $\frac{\partial \rho_i}{\partial t} + \nabla_{\mathbf{x}} \cdot (\rho_i \mathbf{v}) + \nabla_{\mathbf{x}} \cdot (\rho_i \mathbf{V}_i) = 0,$
  - Momentum conservation: $\frac{\partial (\rho \mathbf{v})}{\partial t} + \nabla_{\mathbf{x}} \cdot (\rho \mathbf{v} \otimes \mathbf{v}) + \nabla_{\mathbf{x}} \cdot \mathsf{P} = \sum_i \rho_i \mathbf{a}_i,$
  - Energy conservation: $\frac{3}{2}\left(\frac{\partial (nT)}{\partial t} + \nabla_{\mathbf{x}} \cdot (nT\mathbf{v}) \right) + \nabla_{\mathbf{x}} \cdot \mathbf{q} + \mathsf{P} : \nabla_{\mathbf{x}} \mathbf{v} = \sum_i \rho_i \mathbf{V}_i \cdot \mathbf{a}_i,$

- Closures:

$$\mathbf{V}_i = \frac{1}{n_i} \int \mathbf{C} f_i d\mathbf{c} = \mathbf{v}_i - \mathbf{v}. \qquad \mathsf{P} = \sum_{i \in \mathcal{S}} \int m_i \mathbf{C} \otimes \mathbf{C} f_i d\mathbf{c} = \sum_{i \in \mathcal{S}} \mathsf{P}_i. \qquad \mathbf{q} = \sum_{i \in \mathcal{S}} \int \frac{m_i}{2} C^2 \mathbf{C} f_i d\mathbf{c} = \sum_{i \in \mathcal{S}} \mathbf{q}_i.$$



Stanton & Murillo (2016): Fig.1
Relevant Structure of Kinetic Theory
[for transport in HED Plasmas]

BGK Collision Operator for HED Plasma Transport

Dense plasmas: strongly collisional and near equilibrium:

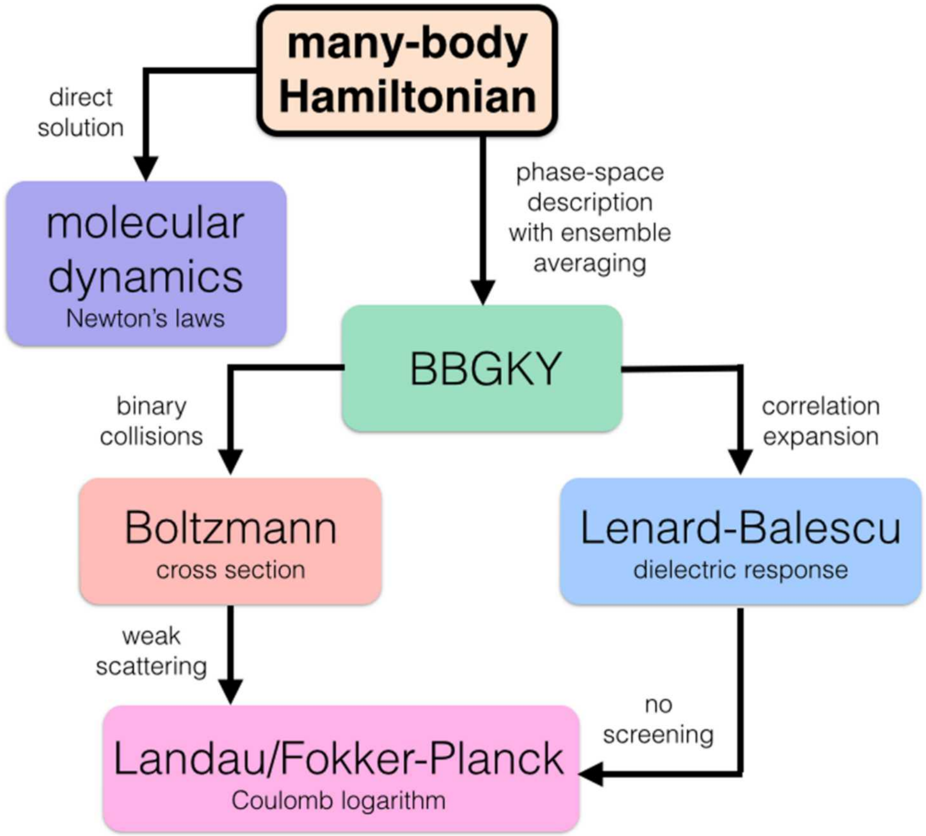
- Expand collision operator about equilibrium: BGK-like approach (Haack et al., 2017a)
- Replace Boltzmann collision operator with a relaxation operator that (Haack et al., 2017a):
  - Conserves particle number, momentum and energy
  - Satisfies the H-theorem

$$Q_i[\mathbf{f}] = \sum_{j\in\mathcal{S}} Q_{ij}[f_i, f_j], \quad Q_{ij}^{\mathrm{BGK}} = \nu_{ij}(\mathbf{c})(\mathcal{M}_{ij} - f_i),$$

$$\mathcal{M}_{ij}[f_i, f_j] = n_i \left(\frac{m_i}{2\pi T_{ij}}\right)^{3/2} \exp\left[-\frac{m_i(\mathbf{c}-\mathbf{v}_{ij})^2}{2T_{ij}}\right].$$

$$\mathbf{v}_{ij} = \frac{\rho_i \nu_{ij}\mathbf{v}_i + \rho_j \nu_{ji}\mathbf{v}_j}{\rho_i \nu_{ij} + \rho_j \nu_{ji}}, \quad T_{ij} = \frac{n_i \nu_{ij} T_i + n_j \nu_{ji} T_j}{n_i \nu_{ij} + n_j \nu_{ji}} + \frac{\rho_i \nu_{ij}(v_i^2 - v_{ij}^2) + \rho_j \nu_{ji}(v_j^2 - v_{ij}^2)}{3(n_i \nu_{ij} + n_j \nu_{ji})}.$$

  - Cross distribution depends on single species density, mass and cross velocity, temperatures and interspecies collisions rates
    - **Unknown: how to compute collision rates?**

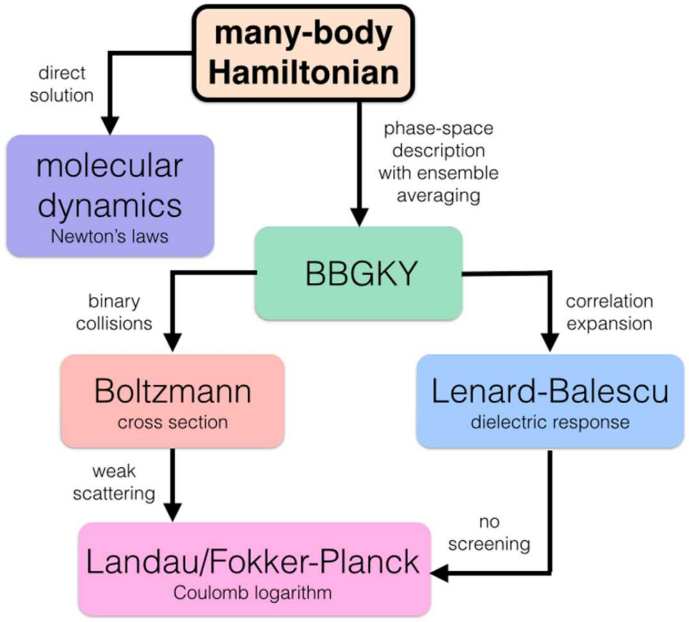


Stanton & Murillo (2016): Fig.1
Relevant Structure of Kinetic Theory
[for transport in HED Plasmas]

Collision Rates for HED Plasma Transport

Dense plasmas: strongly collisional and near equilibrium:

- Expand collision operator about equilibrium: BGK-like approach (Haack et al., 2017a)
- Requires knowledge of interspecies collision rates. Aren't we back where we started?
- No!
  - Use Landau/Fokker-Planck Theory (Haack et al., 2017a; Stanton & Murillo, 2016)
  - Dense plasma: ion-ion interaction screened by electrons
  - Use *screened* interaction in cross-section calculation that *avoids* ad-hoc cutoffs
  - Allows direct computation of self/inter-species diffusivity, viscosity, thermal conductivity and collision rates



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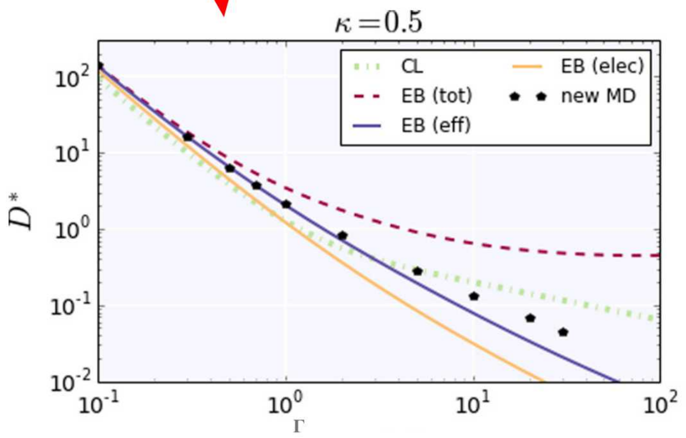
Stanton & Murillo (2016): Fig.10
Dimensionless self-diffusion coefficient computed using screened interaction



BGK Theory *Predicts Non-Fluid-like* Plasma Transport at CHO-DT Interface

Haack et al. (2017b):

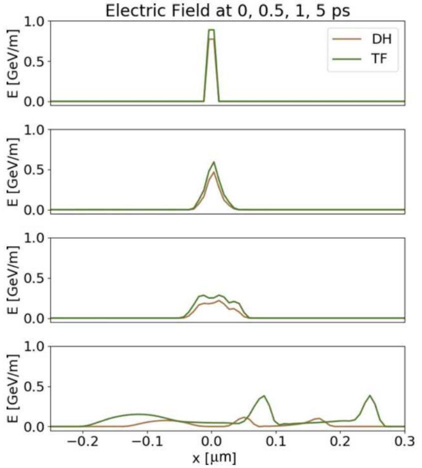
- Utilize multi-species Vlasov-Poisson-BGK system to study plasma transport at CHO-DT interface
- Electric field computed as:

$$-\frac{1}{4\pi}\nabla_x^2\phi = \sum_i Z_i e n_i - e n_e, \quad \mathbf{E} = -\nabla_\mathbf{x}\phi,$$

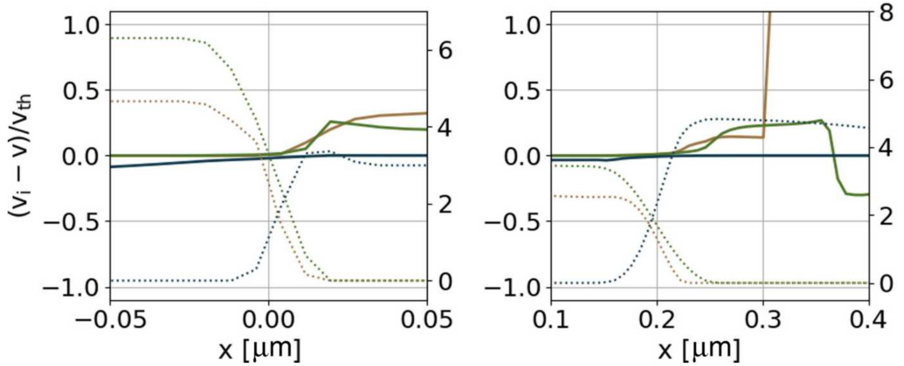
- Thomas-Fermi electron model: strong electric fields form at interface (~GeV/m).

$$n_e = \frac{2(2\pi m_e T_e)^{3/2}}{(2\pi\hbar)^3}\mathcal{F}_{1/2}[(e\phi + \mu)/T_e].$$

- Hydrogen can separate from the plastic and mix into the fuel (also dependent on the electron heating model).
- Ion diffusion velocities sufficiently large c.f. ion thermal speed to invalidate assumptions used in deriving Navier-Stokes-like fluid equations from VBGK-system
  - Predictions made with hydrodynamic models should be falsifiable

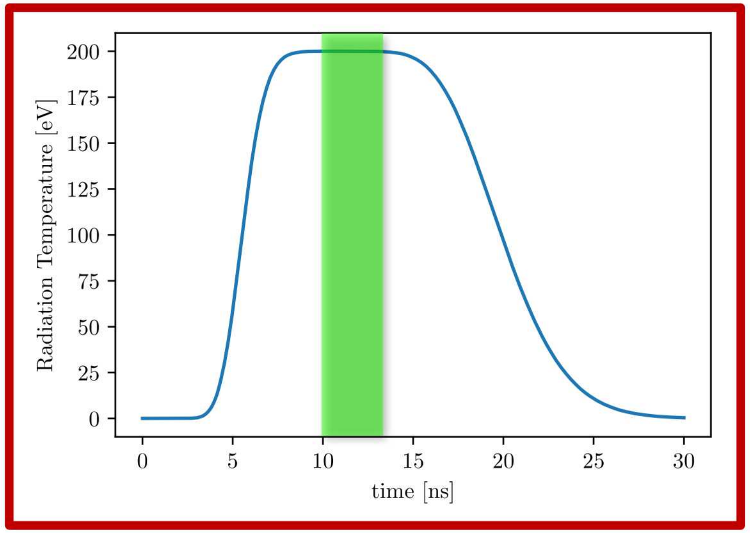


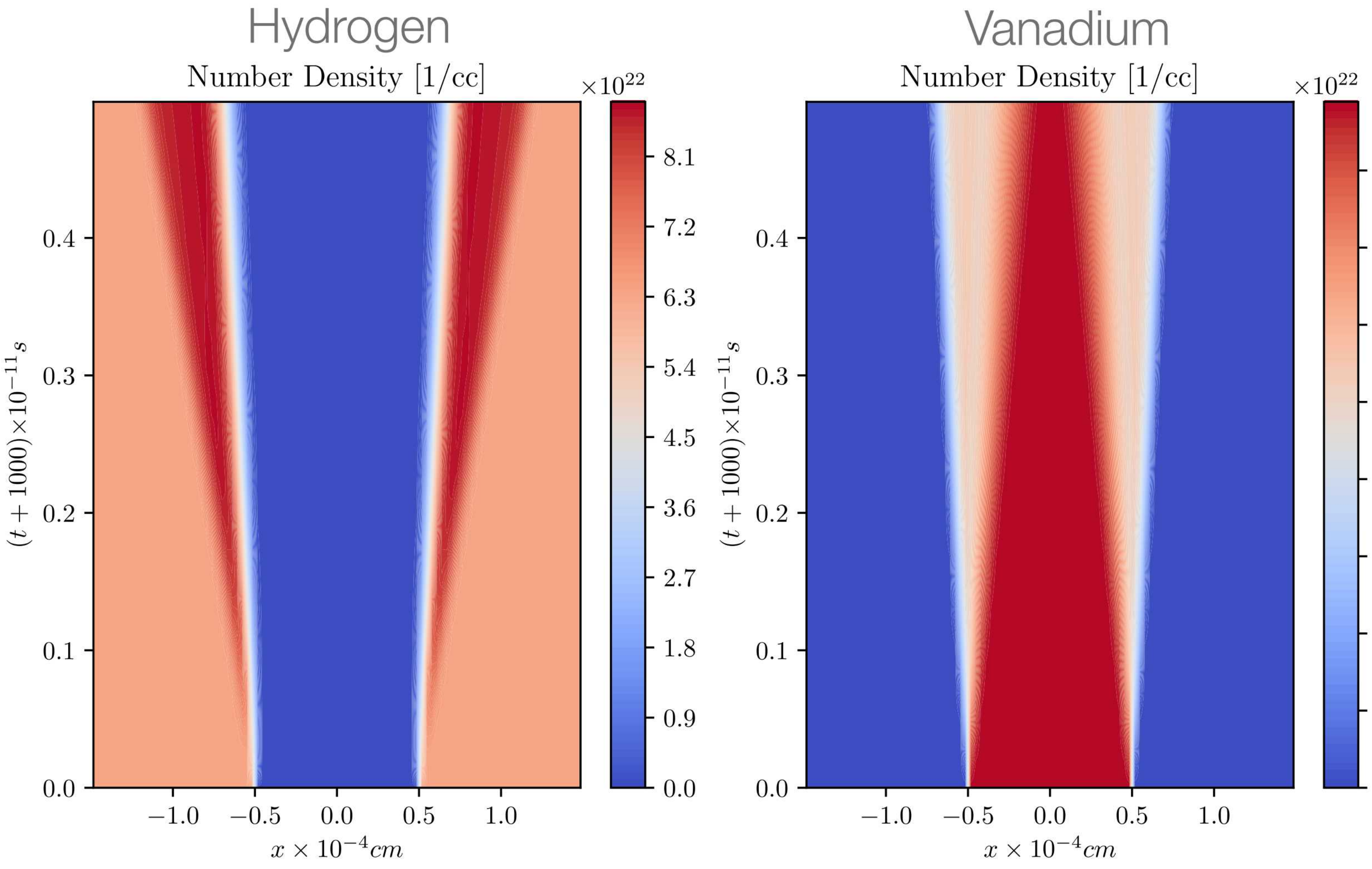
Haack et al. (2017b): Fig. 3. (left); Interfacial electric fields for CHO-DT interface computed using Debye-Huckel & Thomas-Fermi models. These electric fields drive the evolution of hydrogen at the interface



Haack et al. (2017b): Fig. 5. (above); Number densities (10-22/cc, dotted lines) and diffusion velocities (solid lines) for H (green), C (brown) and D (black) at 500fs (left) and 10 ps (right). Note the separation between the C,H distributions at the interface and that the H has diffusion velocities ~ thermal velocity

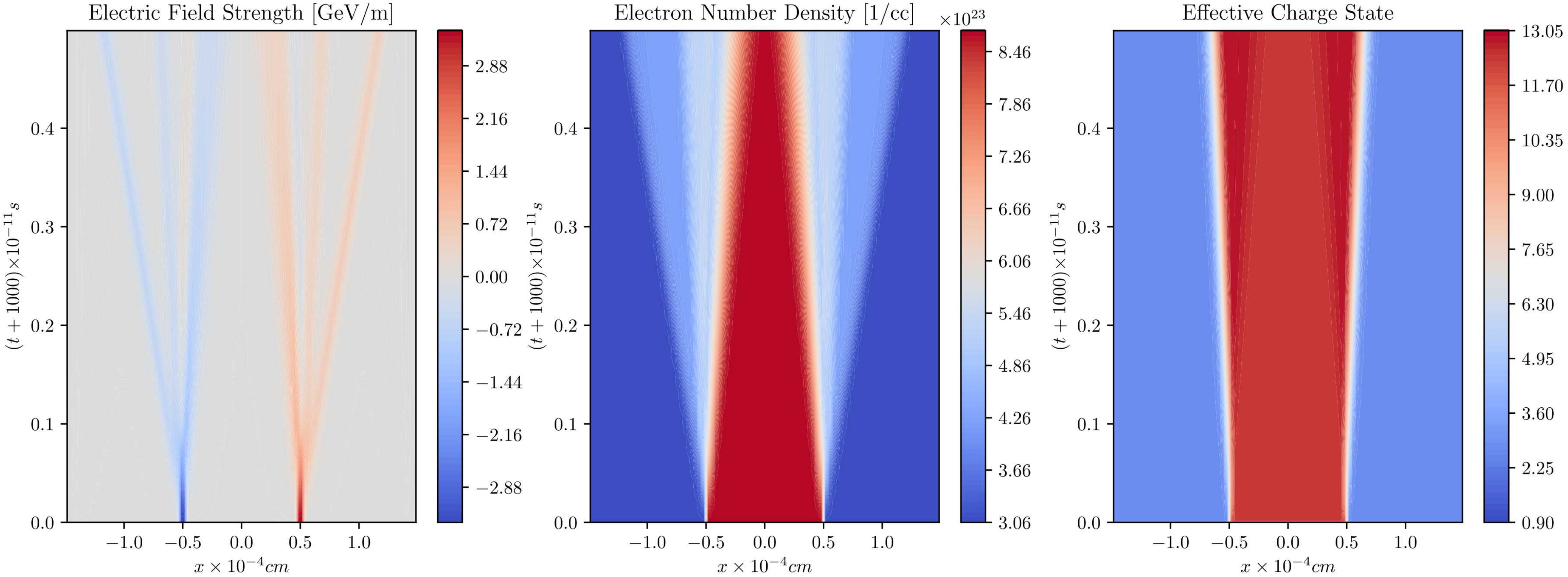
VPBGK Modeling of V/CH Interface: Evolution @Constant Temperature





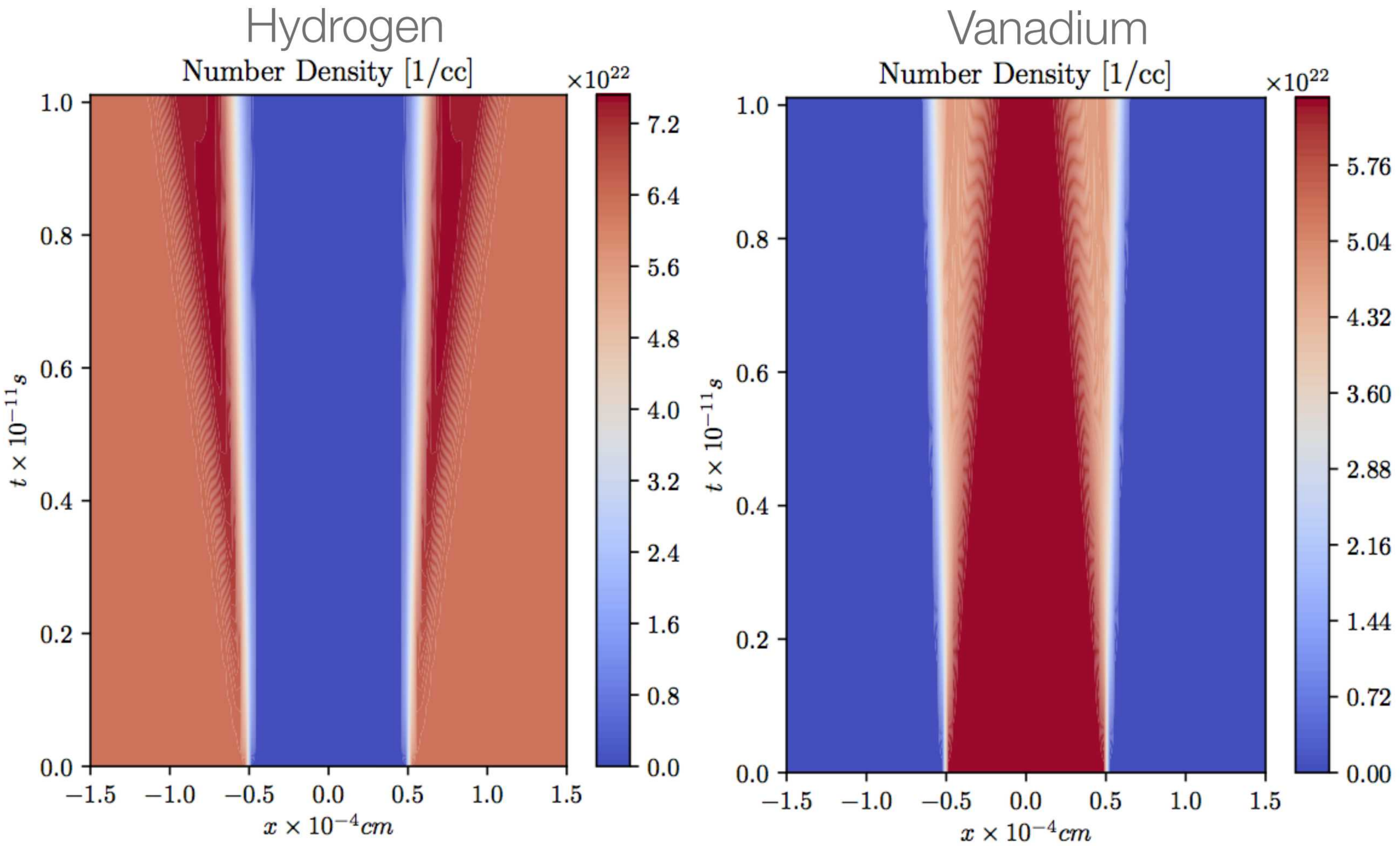
- Utilize multi-species VPBGK code to study plasma transport at CHO-VAl interface
  - Thomas-Fermi Average Atom model for ionization state
  - Fermi-Dirac statistics for electrons
- Simulation setup: replace DT-mix with V at 90% solid density with 10% Al doping
  - Fix electron temperature at 200eV, initialize ions at 200eV

VPBGK Modeling of V/CH Interface: Electrostatic Fields



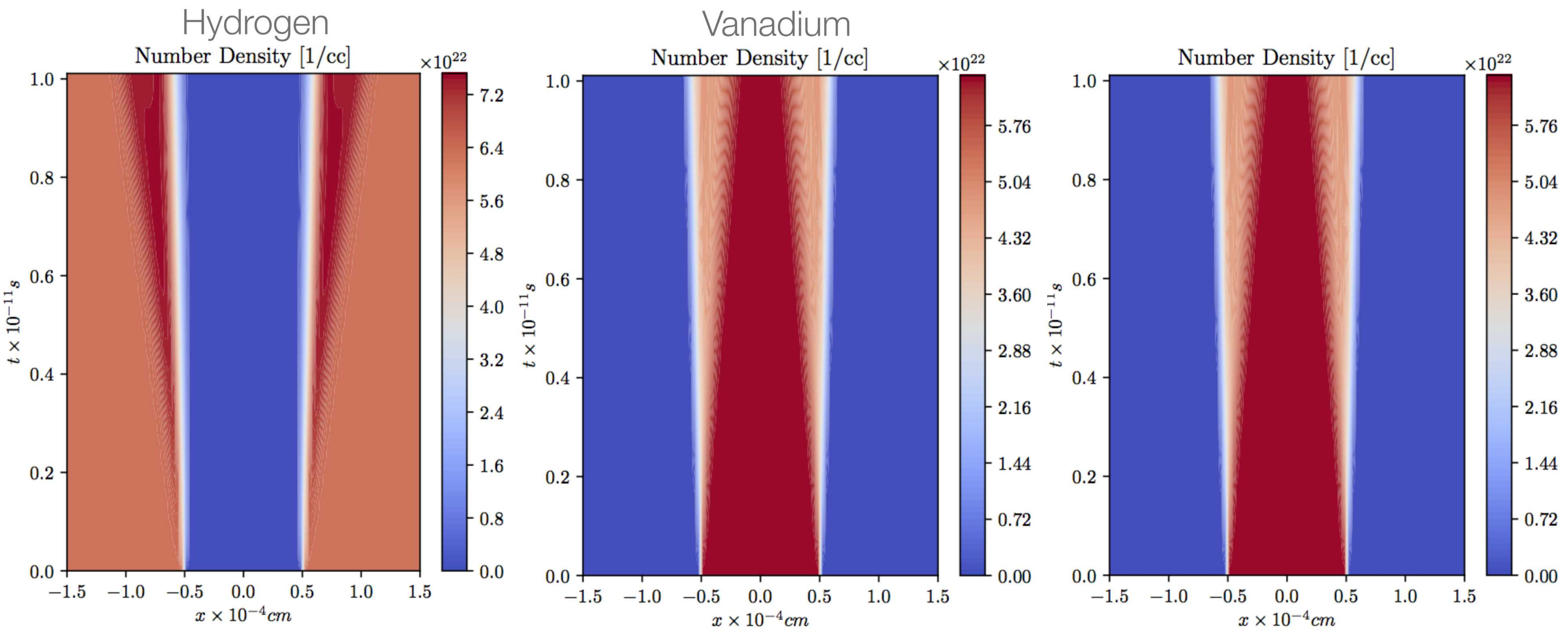
- Utilize multi-species VPBGK code to study plasma transport at CHO-VAl interface
- Simulation setup: replace DT-mix with V at 90% solid density with 10% Al doping
- Fix electron temperature at 200eV, initialize ions at 200eV
- Similar to CHO-DT case, observe strong electric fields that spread into plasma with time
  - Electrons are concentrated within the V/Al plasma and spread into plastic with time

VPBGK Modeling of V/CH Interface: Interface Tracking



- Initial evolution: Vanadium expands into plastic
  - Position of CHO-V interface moves
- The position of the interface can be tracked through (e.g.) the reduced mass
  - Allows measurement of interface properties

VPBGK Modeling of V/CH Interface: Interface Tracking



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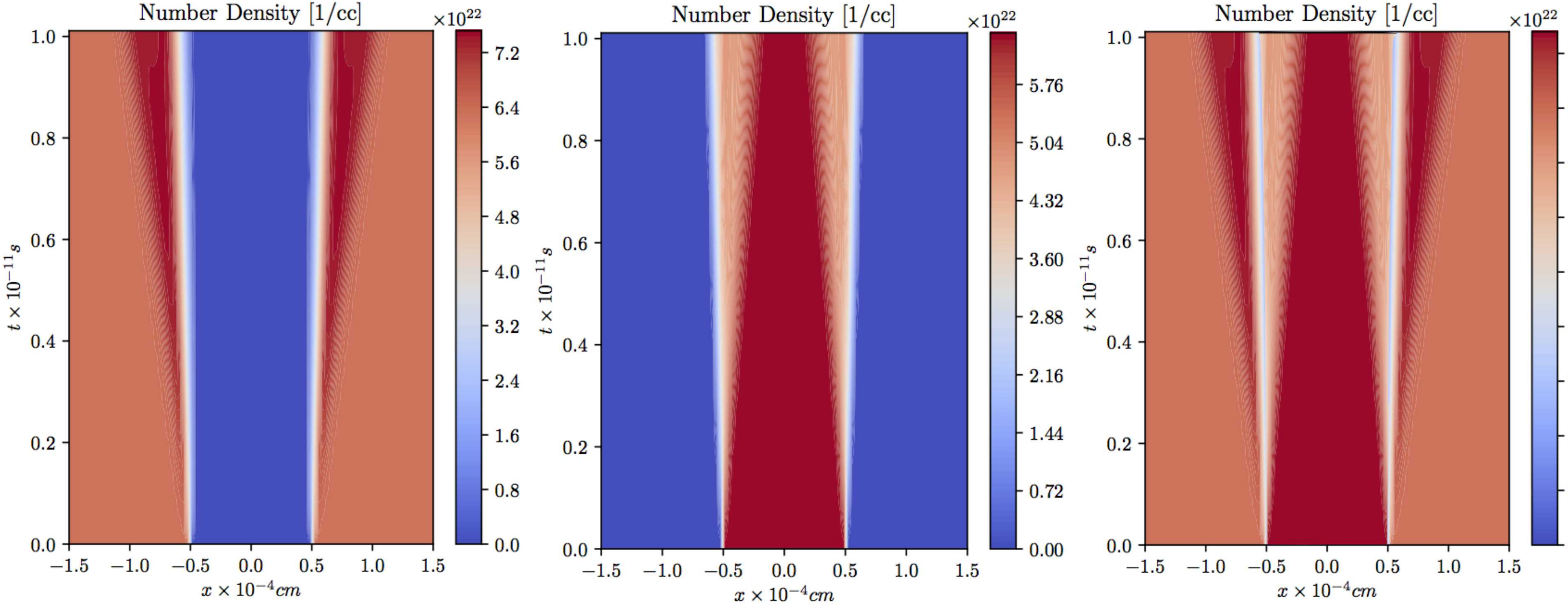
VPBGK Modeling of V/CH Interface: Interface Tracking

Hydrogen

Vanadium



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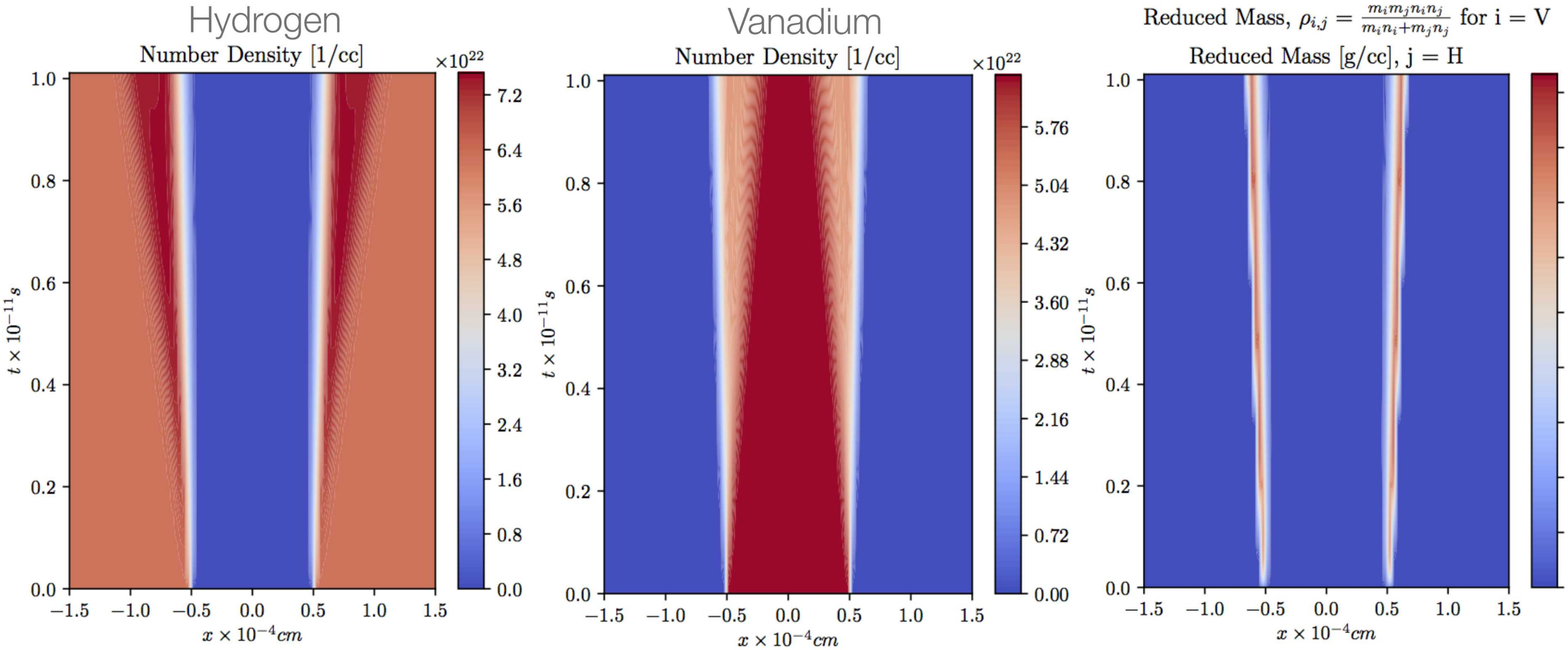

- Initial evolution: Vanadium expands into plastic
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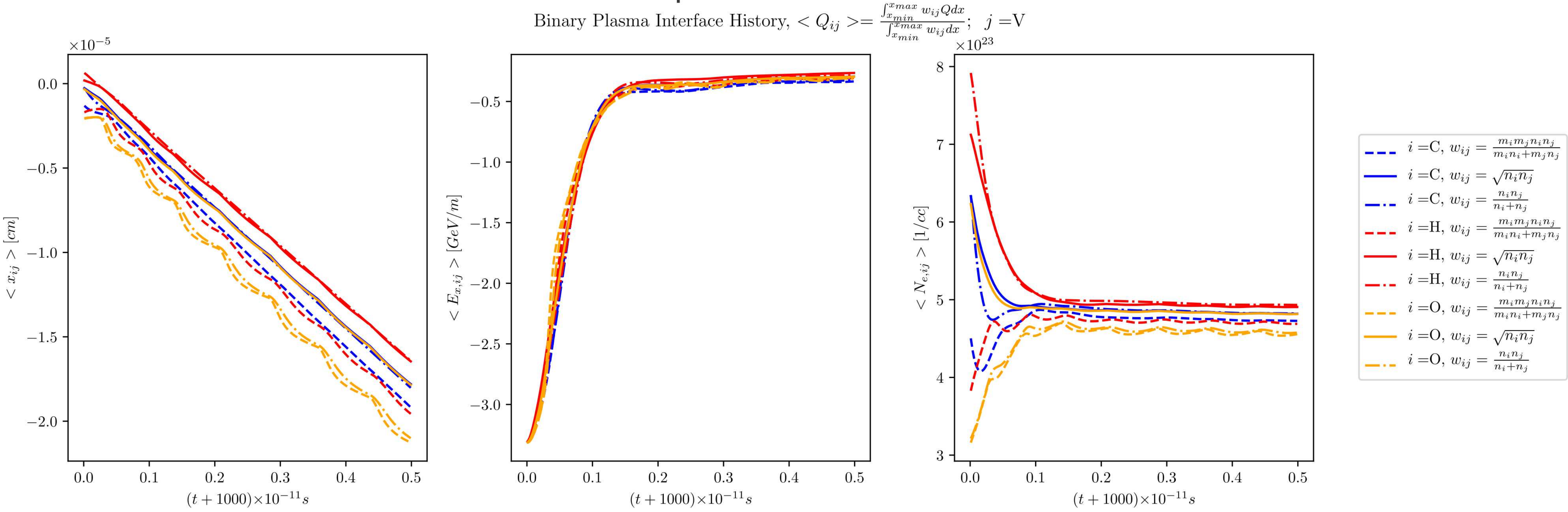
- The position of the interface can be tracked through (e.g.) the reduced mass
  - Allows measurement of interface properties

VPBGK Predictions of Plasma Transport at CHO-V Interface: Plasma Conditions



Utilize multi-species VPBGK code to study plasma transport at CHO-V/Al interface

- Initial setup: replace DT with V at 90% solid density with 10% Al doping
- Fix electron temperature at 200eV, initialize ions at 200eV

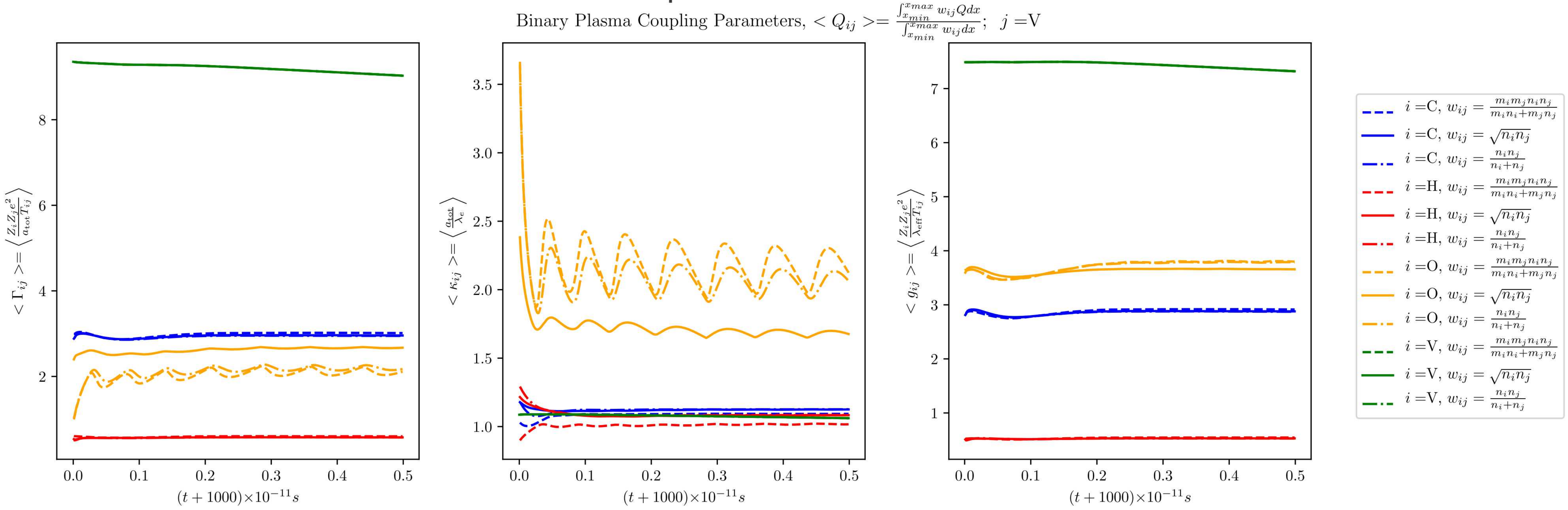
Developed analysis tools that probe:

- Plasma regimes probed during experiment
- Average single species diffusion coefficients
- Interfacial properties: position, electric field, interspecies diffusion

Preliminary conclusions:

- If V/Al plasma contains majority of electrons, then V/Al moves into the CHO
- Electric field evolution is approximately the same at each interface
- However, if the majority of charge is contained in the plastic, then evolution is more complex…

VPBGK Predictions of Plasma Transport at CHO-V Interface: Plasma Parameters



Utilize multi-species VPBGK code to study plasma transport at CHO-V interface

- Initial setup: replace DT with V at 90% solid density with 10% Al doping
- Fix electron temperature at 200eV, initialize ions at 200eV

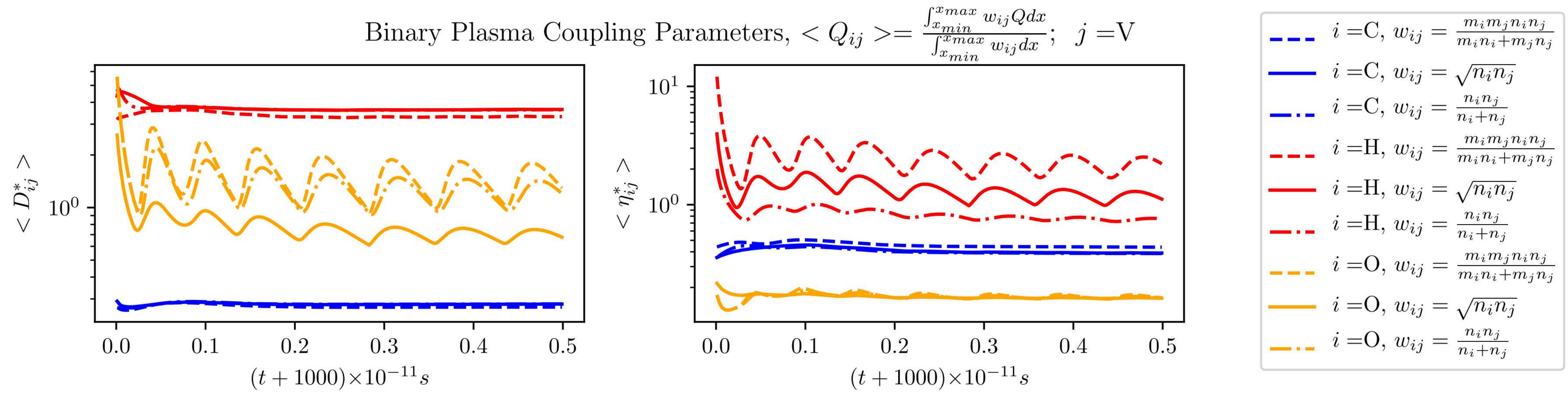
Developed analysis tools that probe:

- Plasma regimes probed during experiment
- Average single species diffusion coefficients
- Interfacial properties: position, electric field, interspecies diffusion

Preliminary conclusions:

- Vanadium plasma is strongly coupled, hydrogen plasma weakly coupled
- Little self-diffusion within the Vanadium
- Weakly coupled hydrogen exhibits strong self-diffusion

VPBGK Predictions of Plasma Transport at CHO-V Interface: Plasma Diffusion



Utilize multi-species VPBGK code to study plasma transport at CHO-V interface

- Initial setup: replace DT with V at 90% solid density with 10% Al doping
- Fix electron temperature at 50eV, initialize ions at 10eV

Developed analysis tools that probe:

- Plasma regimes probed during experiment
- Average single species diffusion coefficients
- Interfacial properties: position, electric field, interspecies diffusion

Hydrodynamic closures require knowledge of interspecies diffusion coefficient, along with viscous and thermal conductivities:

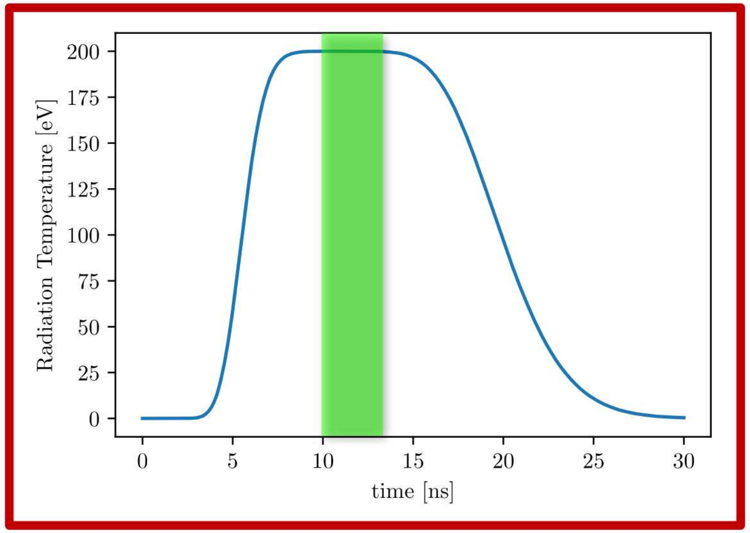
$$\mathsf{P} = pT - \eta[(\nabla \mathbf{v} + (\nabla \mathbf{v})^T] - 2/3(\nabla \cdot \mathbf{v})\mathsf{I}$$

$$\mathbf{d}_i = \nabla x_i + (x_i - y_i)\nabla \log p + \frac{\rho_i}{p}\left(\frac{Z_i e}{m_i} - \sum_j y_j \frac{Z_j e}{m_j}\right)\mathbf{E}.$$

$$\mathbf{V}_i = \sum_j D_{ij}\mathbf{d}_j \qquad \mathbf{q} = -K\nabla T + \frac{5T}{2}\sum_i n_i \mathbf{V}_i$$

- Utilize hydrodynamic model to interpret competing physics in the full VPBGK simulation
  - In principle, will allow us to understand the physics that the plasma transport experiments probe.

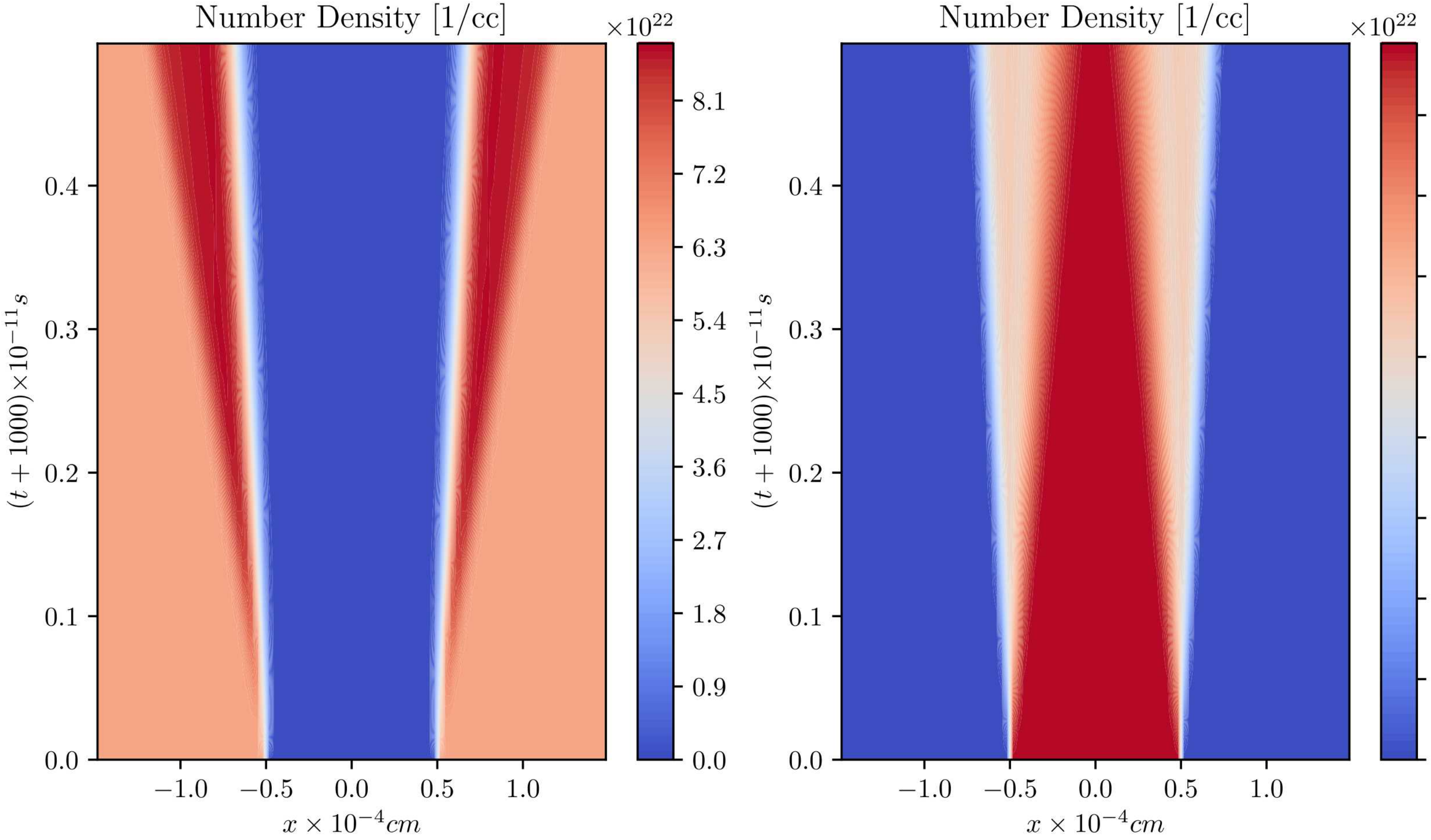
VPBGK Modeling of V/CH Interface: Impact of Slow Heating



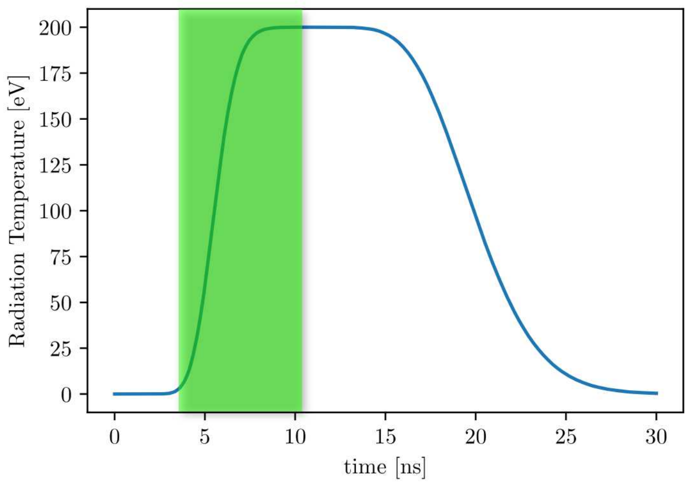
- Utilize multi-species VPBGK code to study plasma transport at CHO-VAl interface
  - Thomas-Fermi Average Atom model for ionization
  - Fermi-Dirac statistics for electrons
- Account for gradual heating of the interface:
  - Collision timescale << rise time
  - Sample at discrete points on temperature curve:
    - Assume that ions equilibrate with electrons on timescales << rise time
    - Allow ions to relax to equilibrium state
    - Use equilibrium state as initial condition for next discrete temperature sample

Ion, Electrons initialized to 200eV at 10ns

Hydrogen | Vanadium



VPBGK Modeling of V/CH Interface: Impact of Slow Heating



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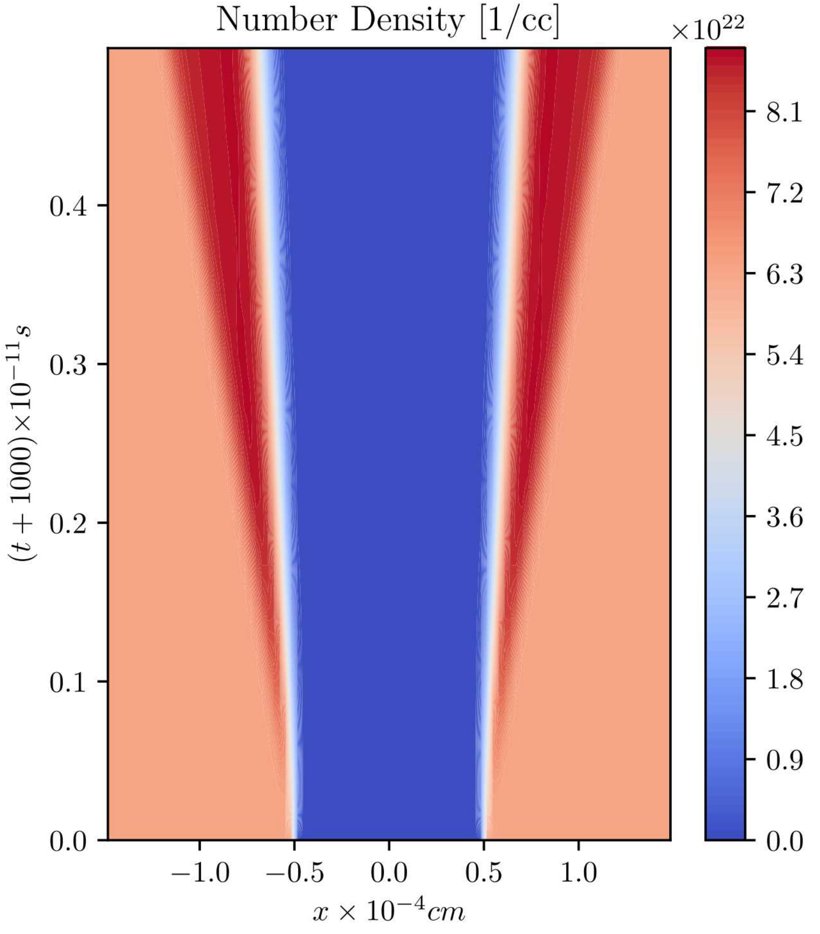
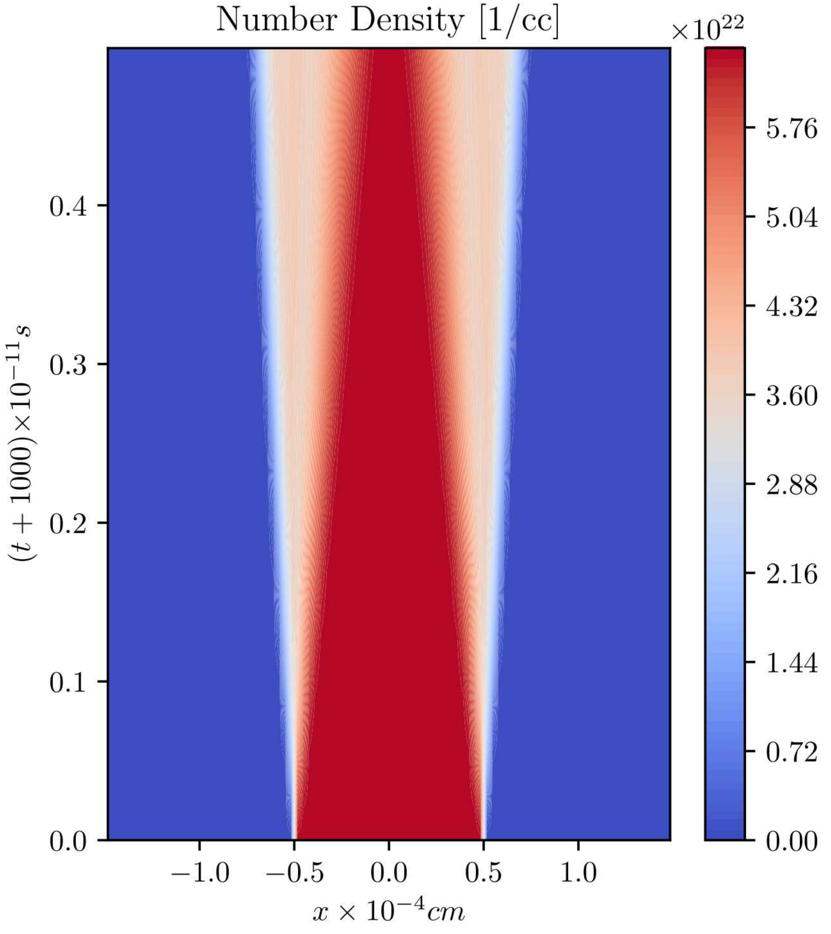
Ion, Electrons initialized to 200eV at 10ns

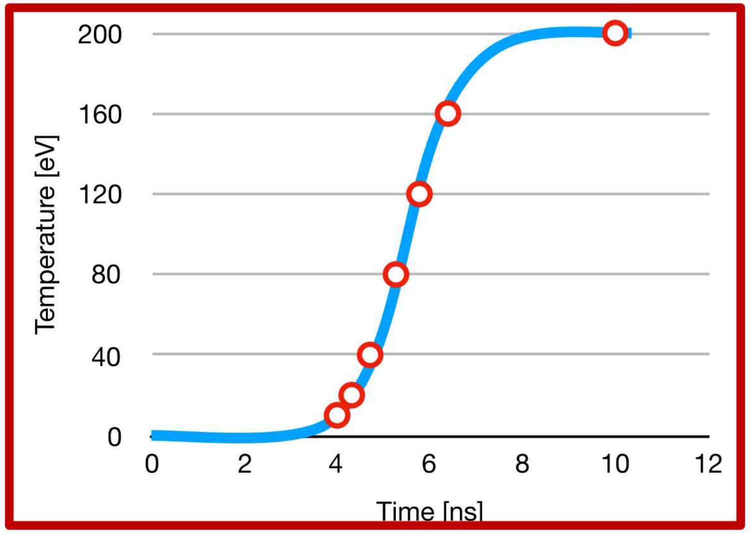
Hydrogen



Vanadium



VPBGK Modeling of V/CH Interface: Impact of Slow Heating



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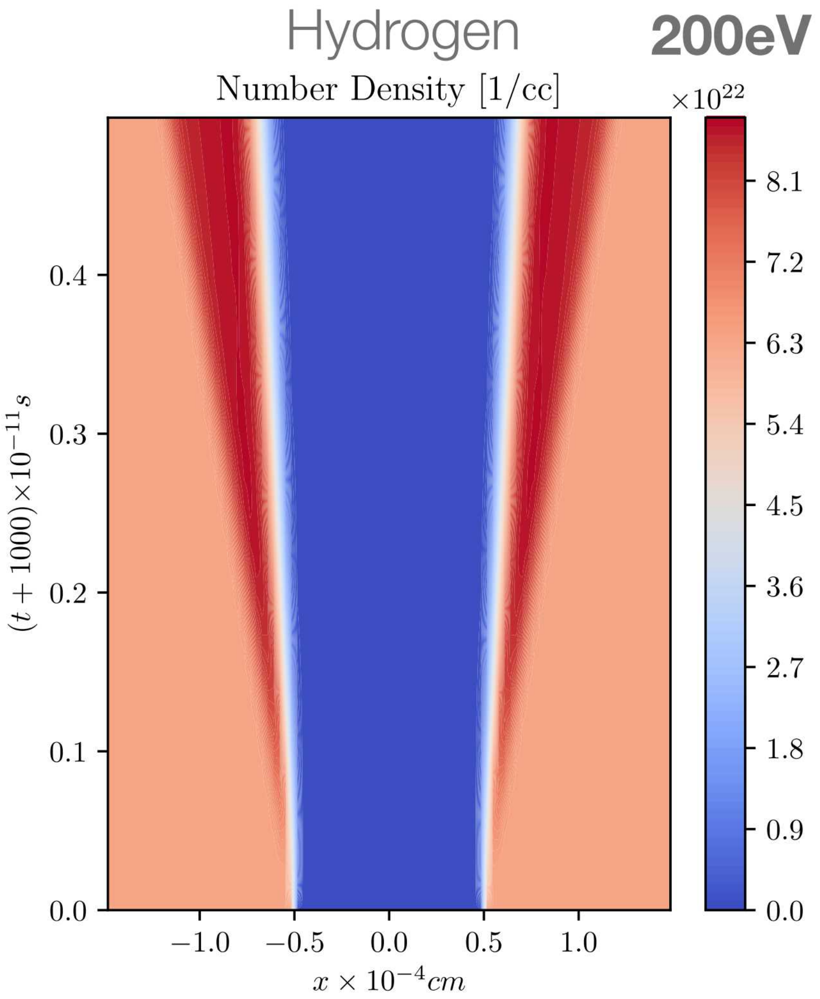
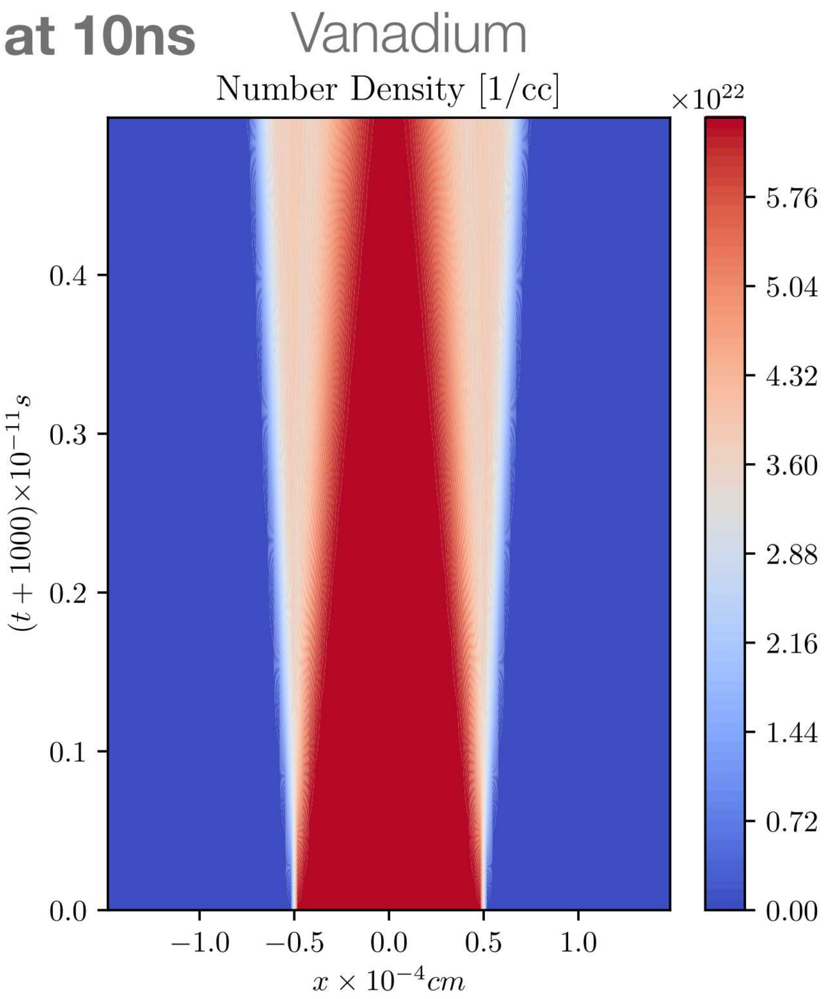
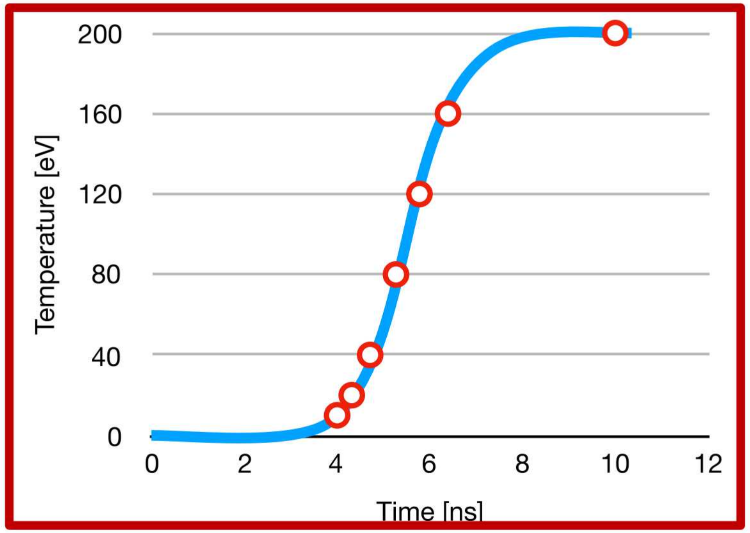




VPBGK Modeling of V/CH Interface: Impact of Slow Heating



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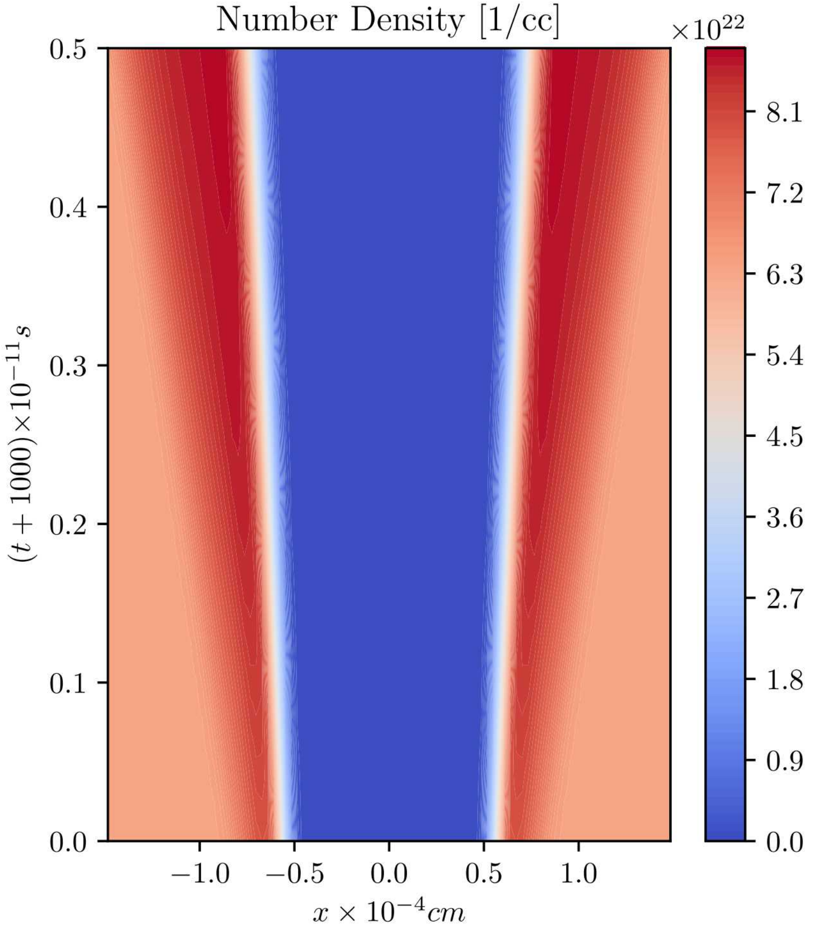
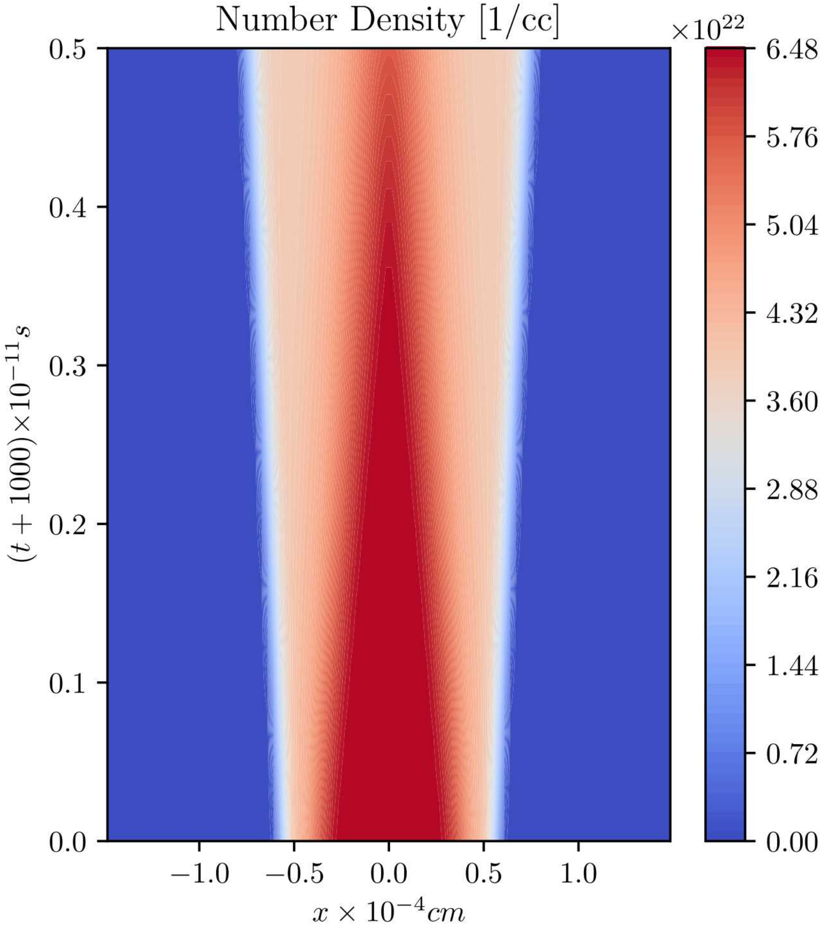
Ion, Electrons heated to 200eV over 10ns

Hydrogen

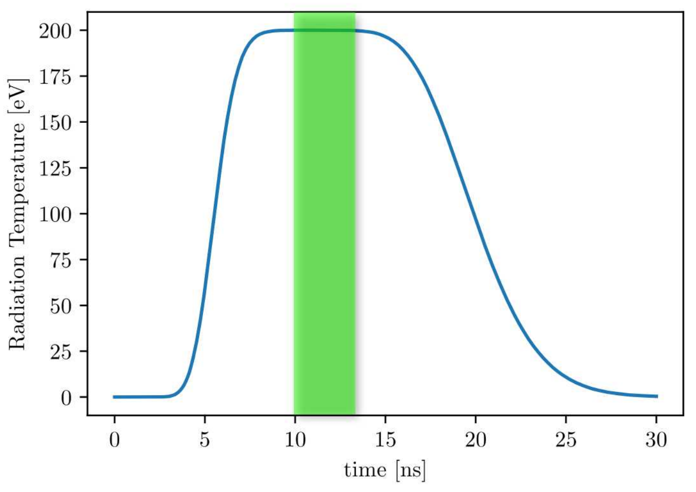


Vanadium



Vanadium has already begun to diffuse into plastic @10ns

VPBGK Modeling of V/CH Interface: Impact of Slow Heating



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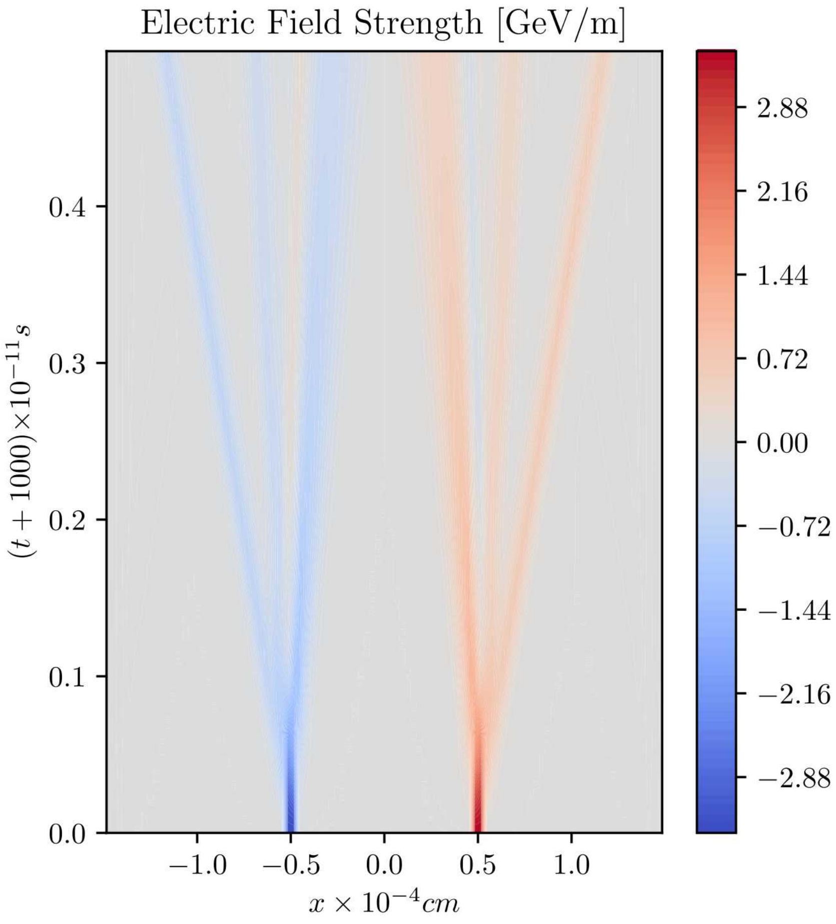
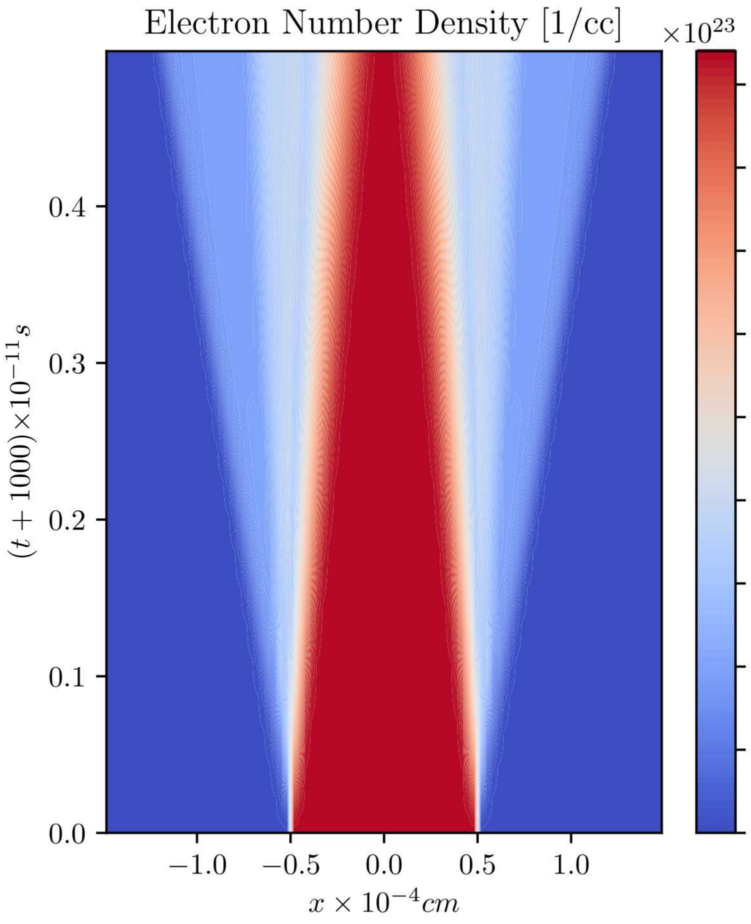
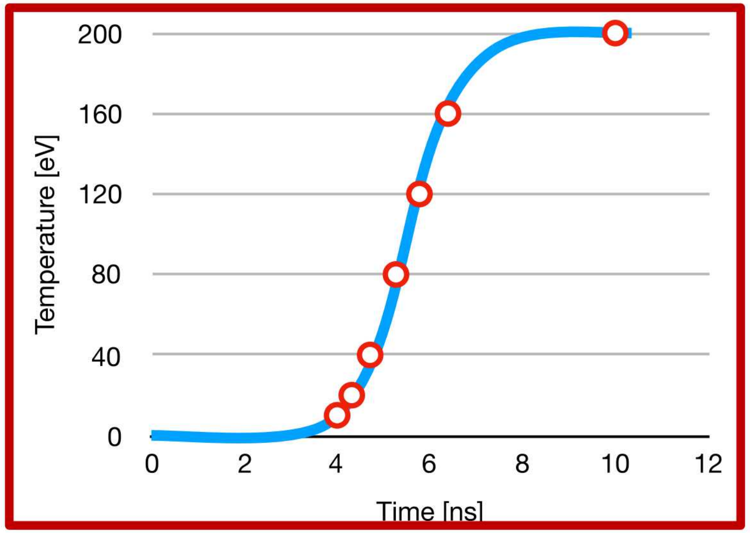
Ion, Electrons initialized to 200eV at 10ns





VPBGK Modeling of V/CH Interface: Impact of Slow Heating



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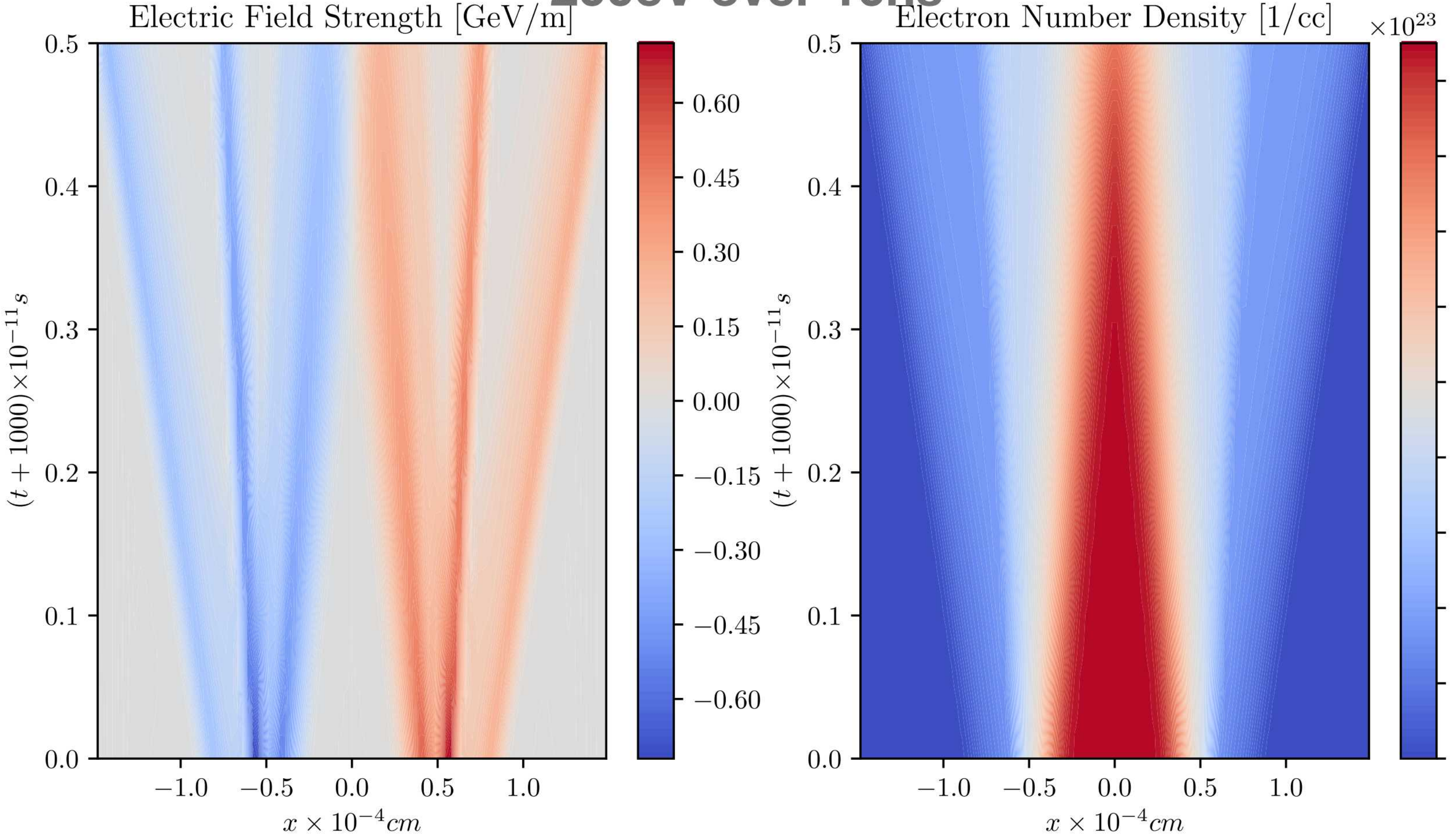
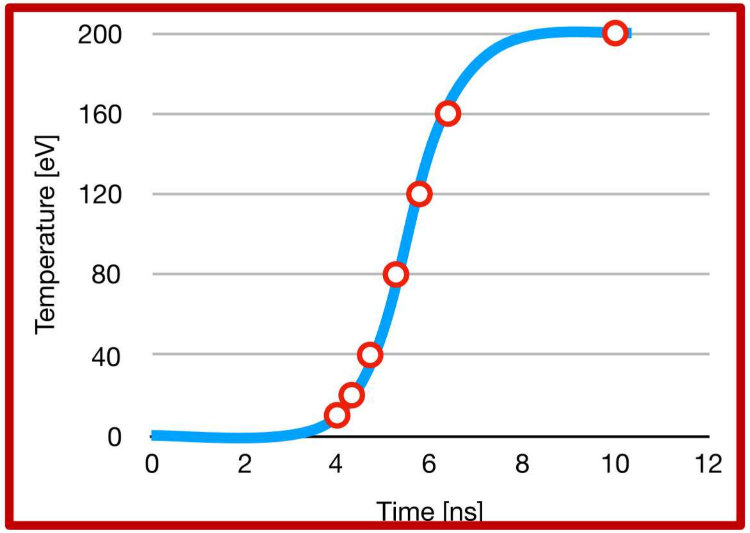
Ion, Electrons heated to 200eV over 10ns



Weaker electric field; diffused into bulk material

VPBGK Modeling of V/CH Interface: Impact of Slow Heating



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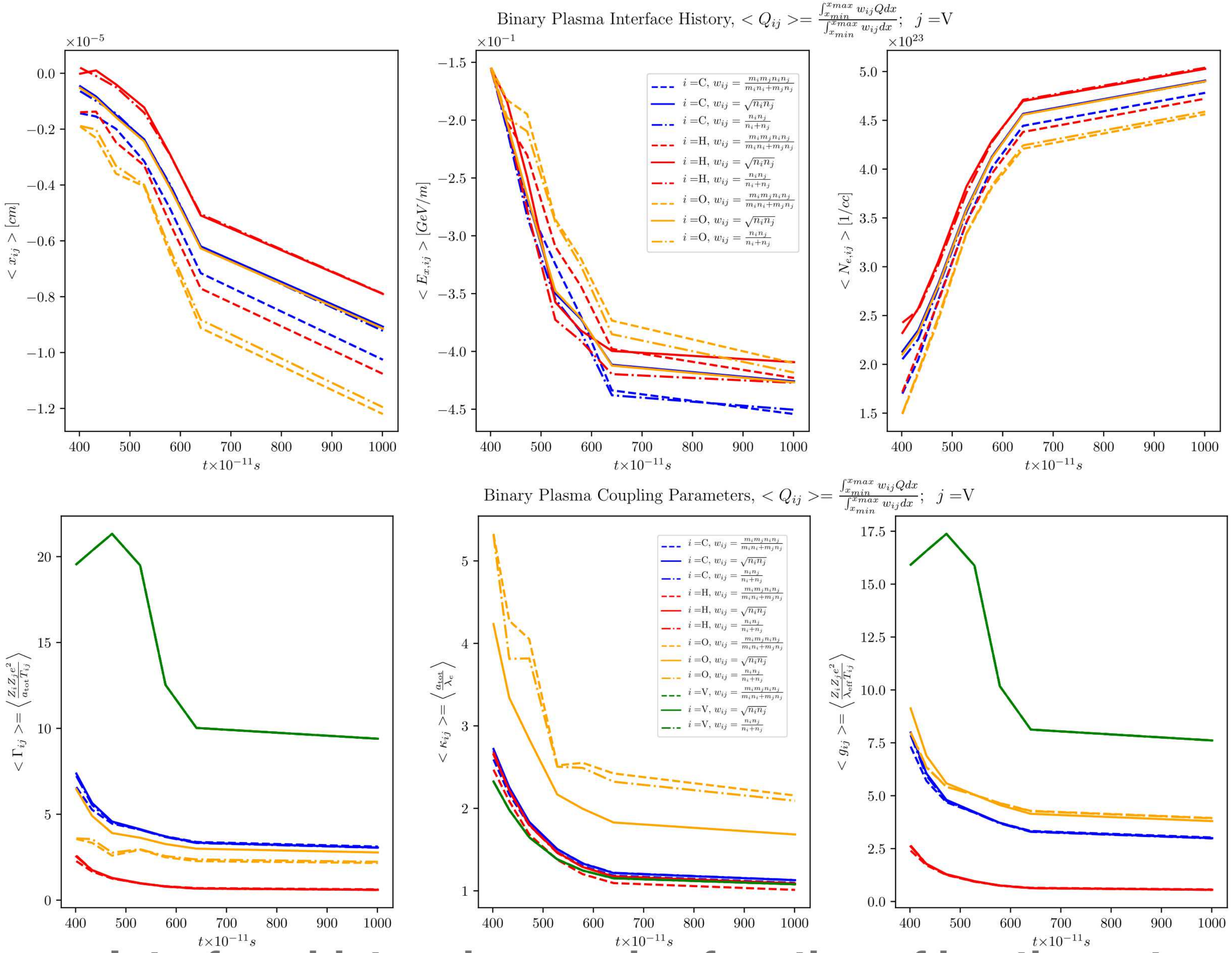

Interface history is complex function of heating rate

Conclusions & References

Z-Machine provides a unique capability to study plasma transport

- Initial series of experiments have examined diffusion of a Vanadium/Plastic interface
- Modeling is challenging: broad range of timescales and temperatures
- Initial modeling efforts have utilize Vlasov-Poisson BGK Multi-species BGK code (Haack et al., 2017a, 2017b) with cross-sections that span weak-to-strong coupling regimes (Stanton & Murillo, 2016)

Initial modelling effort:

- Ions and electrons are instantaneously heated to 200eV, multi-GeV electric fields are observed at interface
- Slowly heating the interface (200eV over 10ns) leads to weaker electric fields that penetrate into bulk material
- Plasma transport regime probed is a complex function of heating history

Open physics questions:

- Is the use of Landau/Fokker-Planck Theory to compute collision rates valid for the Vanadium-Aluminum plasmas considered here?
- How would a more physically complete picture of electron transport (incorporating radiation and magnetic fields) influence the interface evolution?
- Ionization model is incomplete for low Z material (i.e. plastic). Worthwhile to examine (e.g.) Li/V-Al or Be/V-Al interfaces or C-Au interface to make contact with LANL experiments.

References:

- VPBGK code available at: https://github.com/lanl/Multi-BGK
- Stanton & Murillo (2016): 10.1103/PhysRevE.93.043203
- Haack et al. (2017a): 10.1007/s10955-017-1824-9
- Haack et al. (2017b): 10.1103/PhysRevE.96.063310