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Temperature Equilibration in Strongly Coupled Plasma

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A laser-driven experiment investigating electron-ion equilibration in strongly coupled plasma was performed in 1995 [1]. At that time, standard estimates for the electron-ion equilibration time were two-to-three orders of magnitude faster than observed experimentally. As a result, the electron-ion equilibration time was taken as a fitting parameter to understand the experimental results. Based upon guidance from nonequilibrium molecular dynamics mixture calculations [2] and comparison with strongly coupled resistivity experiments, we have developed a consistent binary collision model to understand the electron-ion equilibration experiment. The model has been implemented in a newly developed multi-species, multi-temperature physics code, which was used for simulation of the experiment. The resulting electron-ion exchange rate is close to the experiment, which is about three orders-of-magnitude slower than given by standard estimates, most of which is the result of a modified coulomb logarithm.

1. A. Ng, P. Celliers, G. Xu, and A. Forsman, Phys. Rev. E **52**, 4299 (1995).

2. L. E. Thode, W. S. Daughton, M. S. Murillo, and K. Y. Sanbonmatsu, Los Alamos National Laboratory Memorandum X-1:99-02 (October 14, 1999).

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TEMPERATURE EQUILIBRATION IN STRONGLY COUPLED PLASMA

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Poster Session VII: Non-Equilibrium Dense Plasmas

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ABSTRACT

A laser-driven experiment investigating the electron-ion coupling coefficient in a strongly coupled plasma was performed in 1992. At that time, standard estimates for the electron-ion coupling coefficient, based on a cut-off coulomb logarithm, were two-to-three orders of magnitude faster than inferred from the experiment. As a result, the electron-ion coupling coefficient was used as a fitting parameter to understand the experimental results.

Based upon guidance from non-equilibrium molecular dynamics calculations of light-heavy-ion-mixtures, as well as comparison with strongly coupled resistivity experiments, we have used a consistent strongly-screened-binary-collision collision model to understand the electron-ion equilibration rate experiment. The model has been implemented in a newly developed multi-species, multi-temperature hydrodynamic code, which was subsequently validated against the experiment. There are a number of issues concerning the equation of state, but the electron-ion coupling coefficient appears close to the fitted value used in the 1992-1995 evaluation of the experiment.

The electron-ion coupling coefficient obtained from a Kogan integral formulation with a screened interaction potential obtained from an average atom model also appears close to the fitted electron-ion coupling coefficient. The dynamic range of the experiment is insufficient to differentiate between the two models. Both models predict an electron-ion coupling coefficient of 2-3 times the fitted coefficient.

Electron-Ion Equilibration in a Strongly Coupled Plasma

P. Celliers, A. Ng, G. Xu, and A. Forsman, *Phys. Rev. Lett.* 68, 2305 (1992)

A. Ng, P. Celliers, G. Xu, and A. Forsman, *Phys. Rev.* E 52, 4299 (1995)

Shock Heating with $T_i >> T_e$

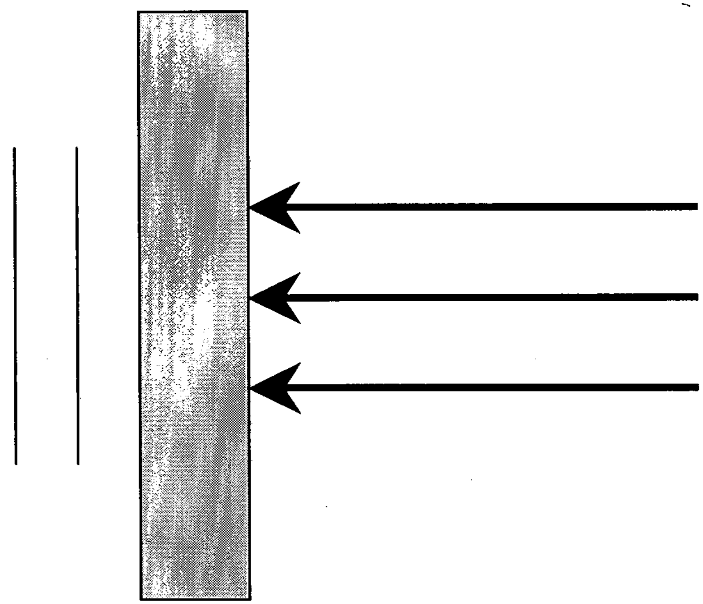
Ablation with $T_e >> T_i$

Shock Breakout Time

and

430 nm and 560 nm

Shock Emission Data



0.5 μm laser ,$10^{13} - 10^{14}$ W/cm^{2,} 65 – 85 mm Si wafers

A fixed electron-ion coupling coefficient was used in a hydro code to compare with shock speed and emission data

Calculation of Interaction Potential

Average Atom Model

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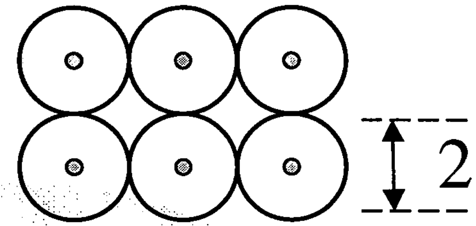
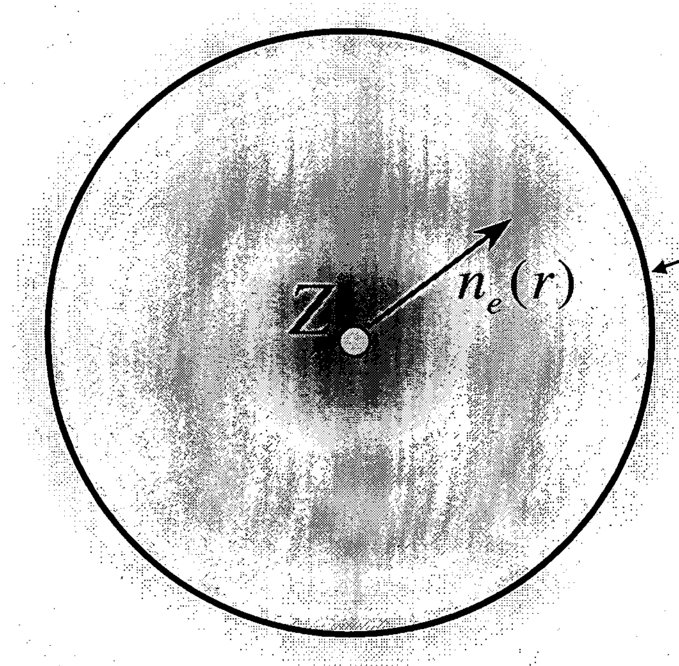
Standard Approach - Ion cell model

Confine each ion to a cell



$$2a = 2\left(\frac{3}{4\pi n_i}\right)^{1/3}$$

Each cell contains Z electrons and is charge neutral



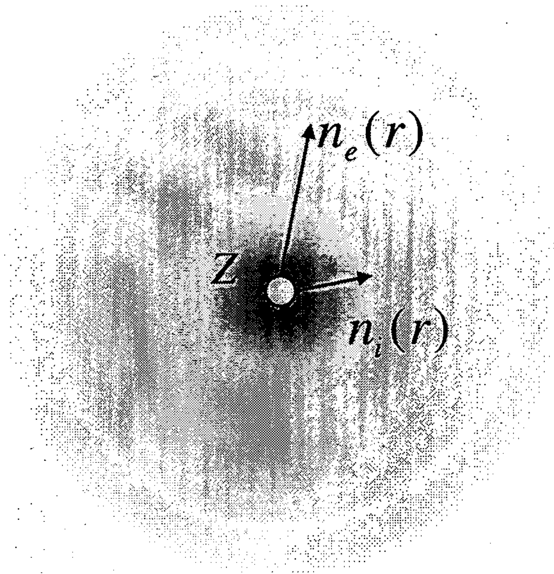
$$E = -\frac{\partial V}{\partial r} = 0$$

Function of V(r)
1. Thomas-Fermi
SESAME
2. Kohn-Sham
INFERNO

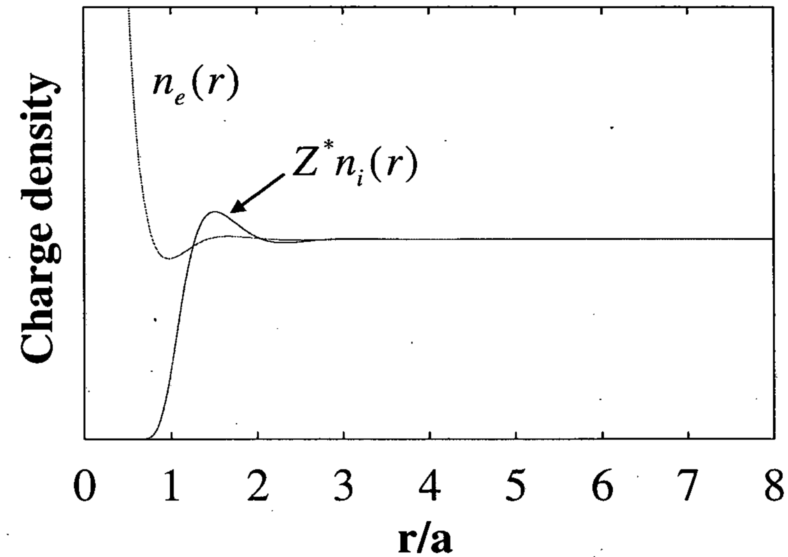
Solve for self-consistent potential

$$-\nabla^2 V(r) = 4\pi Ze\,\delta(r) - 4\pi e n_e(r)$$

More recent approach - Ion Correlation Model



The statistical distributions of both ions and electron are computed around the test ion



$$-\nabla^2 V(r) = 4\pi Z e\,\delta(r) + 4\pi e\left[Z^* n_i(r) - n_e(r)\right]$$

$Z^* n_i(r)$	$n_e(r)$
1. HNC	1. Thomas-Fermi
2. Mean Field	2. Kohn-Sham

Hypernetted Chain Theory

Ornstein-Zernike relation:

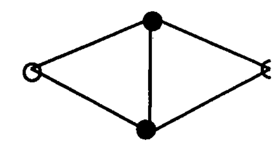
$$h(r) = c(r) + n_{io} \int c(|\mathbf{r} - \mathbf{r}'|)\, h(r')\, d^3\mathbf{r}'$$

Pair correlation function

Direct correlation function

Closure relation:

HNC approximation
B(r)=0



$$g(r) = 1 + h(r) = \exp[-\beta u(r) + h(r) - c(r) + B(r)]$$

Radial distribution function

$$\beta \equiv \frac{1}{k_B T}$$

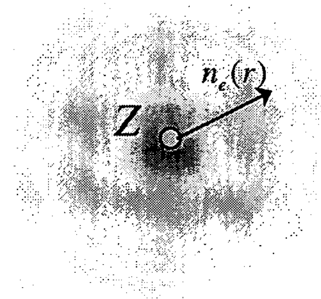
Pair interaction potential

Bridge function

New Model

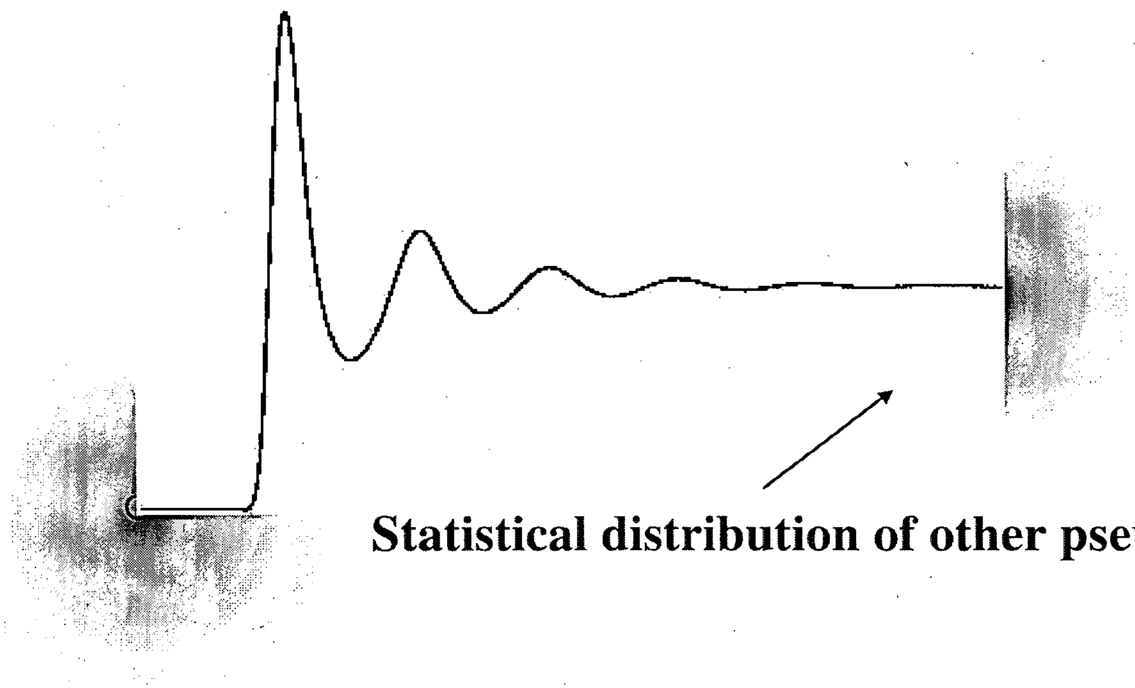
Inspired by L. Dagens, 1972
Neutral pseudo-atom model

Decompose plasma into N identical charge neutral clouds ⇨



$$\int n_e(r)\,d\mathbf{r} = Z$$

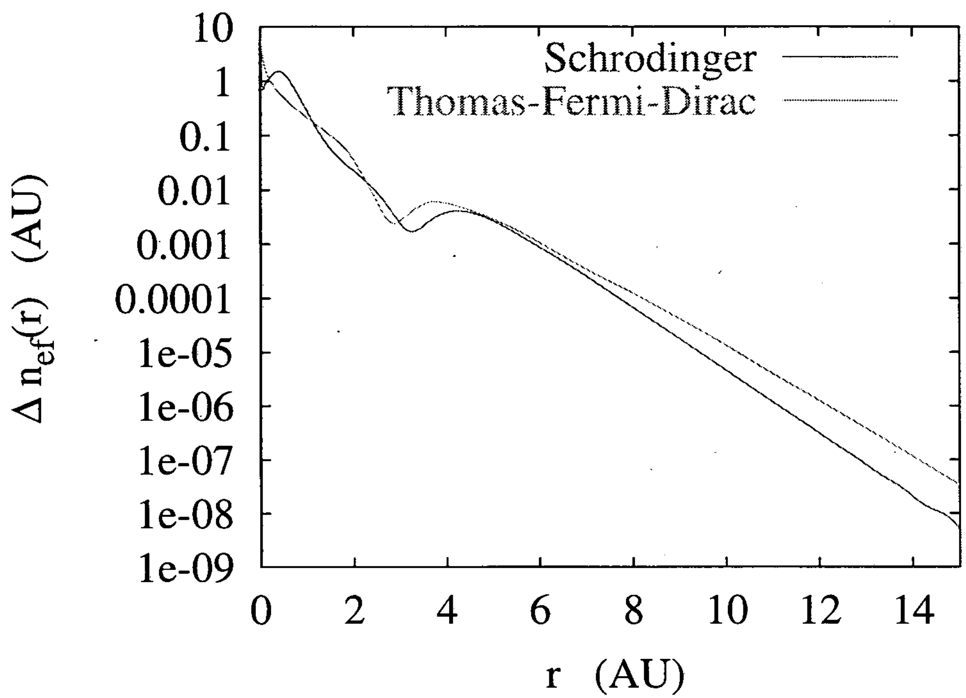
Central Pseudo-Atom ⇨



Statistical distribution of other pseudo-atoms

$$V_{atom}(r) = -\frac{Z}{r} + \int \frac{n_e(r')}{|\mathbf{r}-\mathbf{r}'|}d\mathbf{r}' \qquad V_{ext}(r) = n_i \int g(r')\,V_{atom}(|\mathbf{r}-\mathbf{r}'|)\,d\mathbf{r}'$$

New Model Used to Calculate Free Electron Distribution



$$\Delta n(r) = n_e^{free}(r) - n_e^{\infty}$$

$$\Delta n(q) = 4\pi \int_0^R r \frac{\sin(qr)}{q} \Delta n(r) dr$$

Energy Equilibration Rate

Using

Kogan Integral Formulation

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Kogan Formula for Energy Equilibration Rate of a Two-Temperature Plasma is Based on Fermi Golden Rule

$$\frac{dE_{rlx}}{dt} = \int_0^{\infty} \frac{d\omega}{2\pi} \int \frac{d^3 q}{(2\pi)^3} |U_{ei}|^2 \Delta N_{ei} A^e A^i$$

$$\Delta N_{ei} = N(\omega / T_e) - N(\omega / T_i)$$

$$N(\omega / T) = \left(e^{\omega / T} - 1\right)^{-1}$$

$$A^e = -2\,\mathrm{Im}[\chi_{ee}(q, \omega, T_e)]$$

$$A^i = -2\,\mathrm{Im}[\chi_{ii}(q, \omega, T_i)]$$

χ_{ee} dynamic linear response function for electron subsystem

χ_{ii} dynamic linear response function for ion subsystem

U_{ei} effective interaction or pseudopotential

Several Models Investigated for the Interaction Potential

Empty Core Potential

$$U_{ei}^{ec}(q) = -\frac{4\pi Z^*}{q^2}\cos(qR_c) \text{ where } R_c \approx \frac{1}{2}a_0$$

Screened Empty Core Potential

$$U_{ei}^{ecs}(q) = \frac{U_{ei}^{ec}(q)}{\varepsilon(q)} \quad \text{where } \varepsilon(q,\omega,T_e) = 1 - \frac{4\pi}{q^2}[1-G_e(q)]\chi_{ee}(q,\omega,T_e)$$

Yukawa Potential

$$U_{ei}^{y}(q) = -\frac{4\pi Z^*}{(q^2+q_e^2)} \quad \text{where } q_e = \frac{1}{\lambda_e}$$

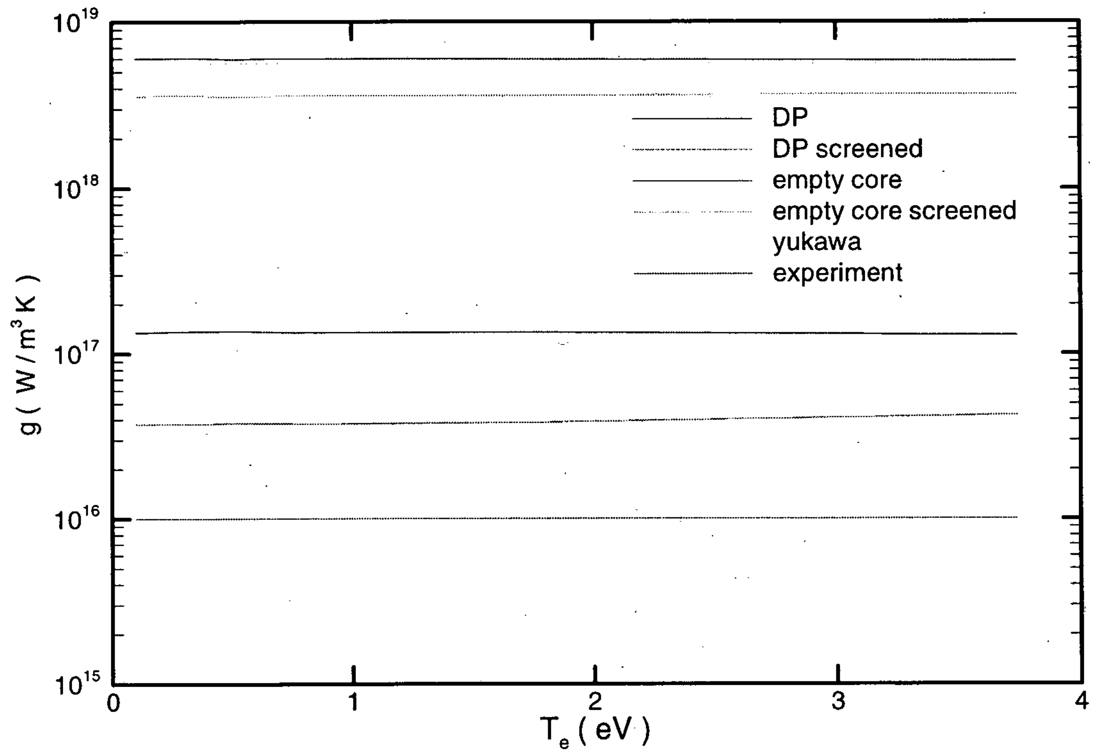
Dharma – wardana – Perrot Potential

$$U_{ei}^{DP}(q) = -\frac{\Delta n(q)}{\chi_{ee}(q)} \text{ where } \Delta n(q) = \mathrm{n}_{\mathrm{e}}^{\mathrm{free}}(q) - n_e^{\infty} \quad \text{is from average atom model}$$

Screened Dharma – wardana – Perrot Potential

$$U_{ei}^{DPs}(q) = \frac{U_{ei}^{DPs}}{\varepsilon(q)}$$

Kogan Integral with Different Potentials Yields Significantly Different Coupling Coefficient Rates



6 g/cm^3

Screened Dharma-wardana-Perrot (DP) Potential Near Matched Experimental Result

Energy Equilibration Rate

Using

Strongly-Screened Binary-Collision (SSBC) Model

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Multi-Species MD Compared with Strongly-Screened Binary-Collision (SSBC) Energy Relaxation Rate Model

$$\frac{\partial n_i T_i}{\partial t} = \frac{2}{3} g(T_I - T_i)$$

$$\frac{\partial n_I T_I}{\partial t} = \frac{2}{3} g(T_i - T_I)$$

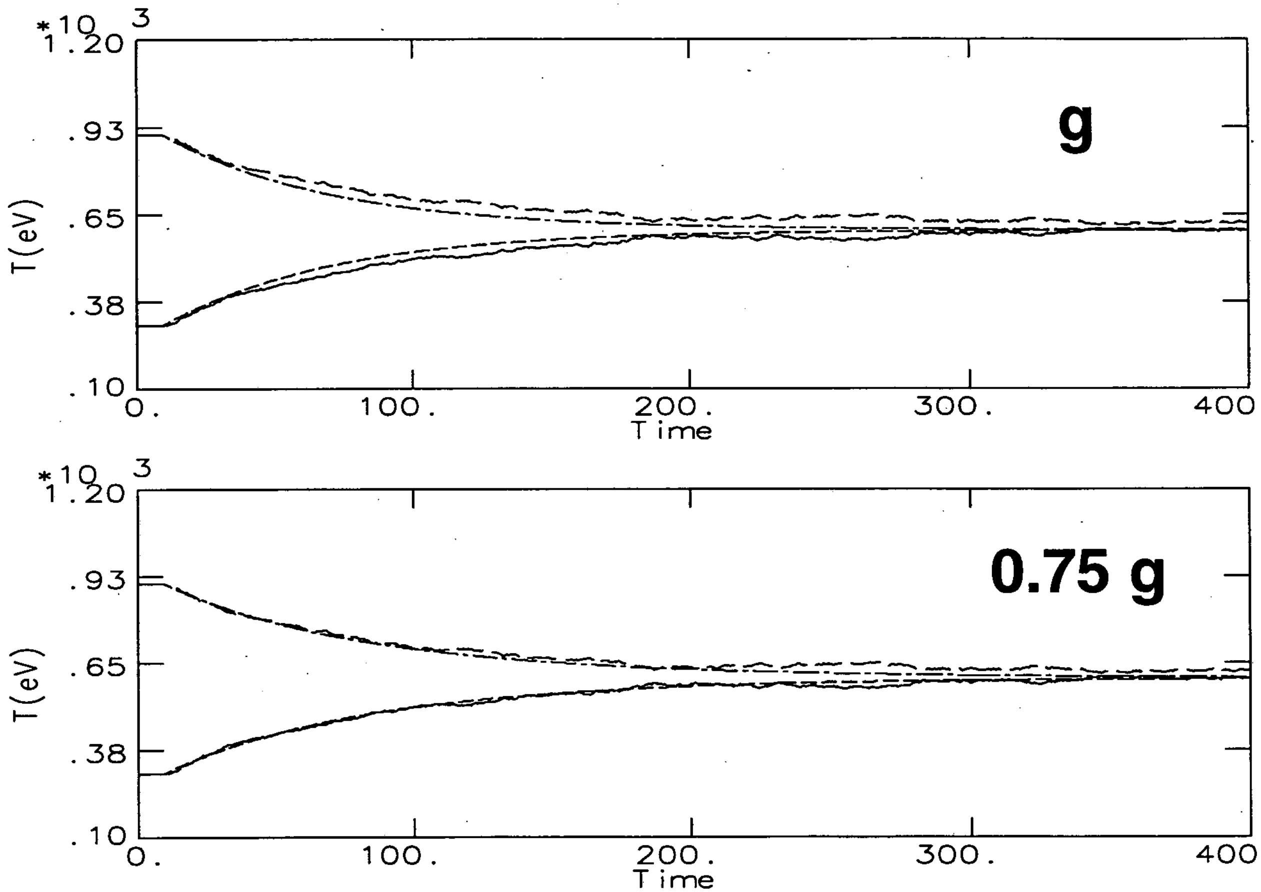
$$g = \frac{\omega_\alpha^2 \omega_\beta^2}{\left(\pi\left\langle v_\alpha^2\right\rangle + \pi\left\langle v_\beta^2\right\rangle\right)^{3/2}} \ell n\Lambda$$

$\omega_\alpha^2 = \dfrac{4\pi n_\alpha e^2}{m_\alpha}$ is the plasma frequency

$\left\langle v_\alpha^2 \right\rangle = \dfrac{2k_B T_\alpha}{M_\alpha}$ is the average thermal velocity

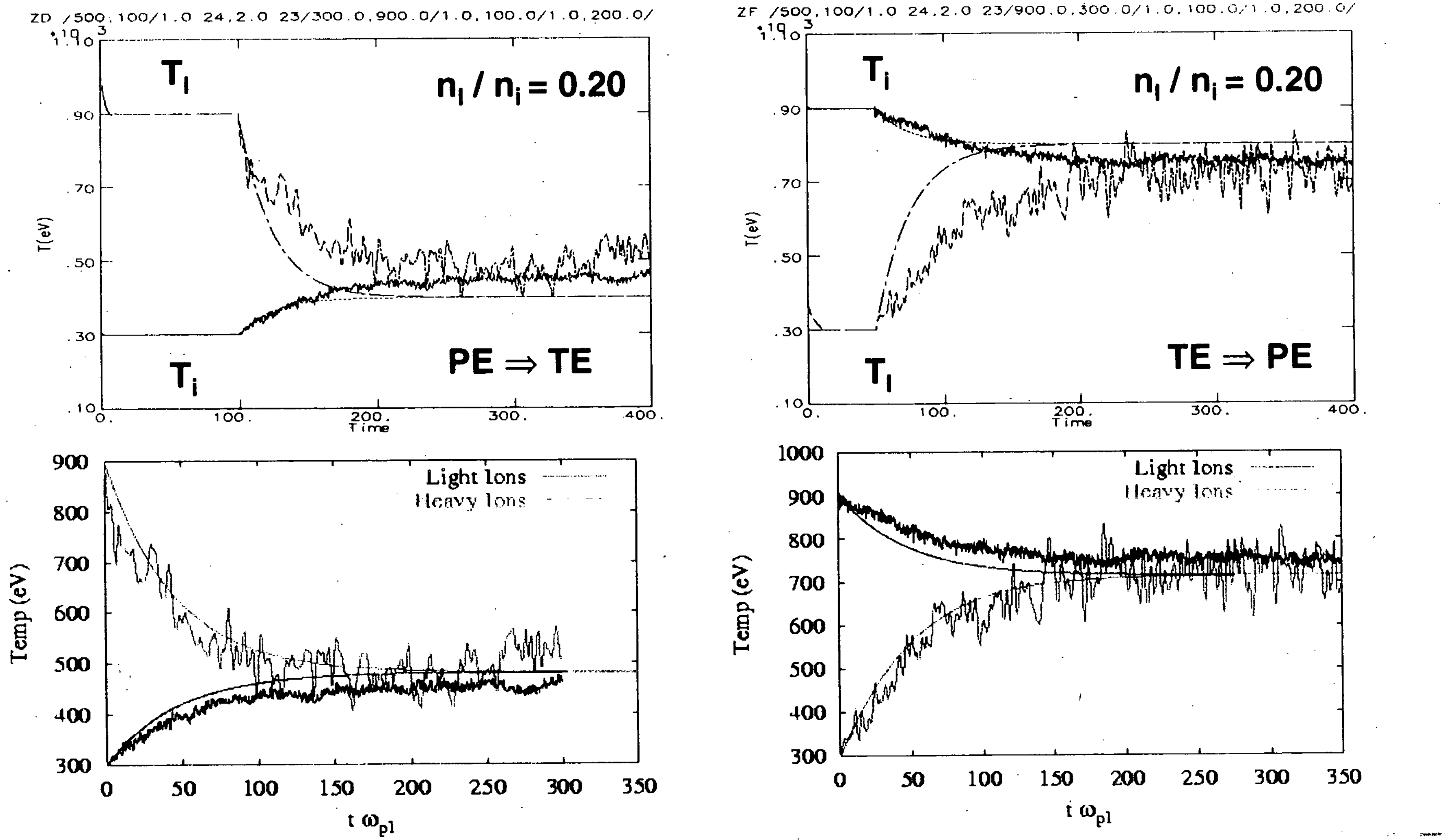
$\ell n\Lambda = \dfrac{1}{2}\ell n\left[1 + \left(\dfrac{\lambda_{screen}}{\lambda_{\alpha\beta}}\right)^2\right] << 1$ when strongly screened

Multi-Ion-Species MD in Good Agreement with SSBC Energy Equilibration Rate – Weakly Coupled Plasma



D-T at 10^{24} cm^{-3}

Multi-Ion-Species MD in Good Agreement with SSBC Energy Equilibration Rate – Moderately Coupled Plasma



SSBC Model Extended to Degenerate Regime

H. Brysk, *Plasma Physics* 16, 927 (1974)

$$g_{e,i} = g_{i,e} = D\left(\frac{\mu_e}{k_B T_e}\right)\frac{\omega_e^2 \omega_i^2}{\left(\pi\left\langle v_e^2\right\rangle + \pi\left\langle v_i^2\right\rangle\right)^{3/2}}\ell n\Lambda$$

$$\ell n\Lambda = \frac{1}{2}\ell n\left[1+\left(\frac{\lambda_{screen}}{\lambda_{ei}}\right)^2\right]$$

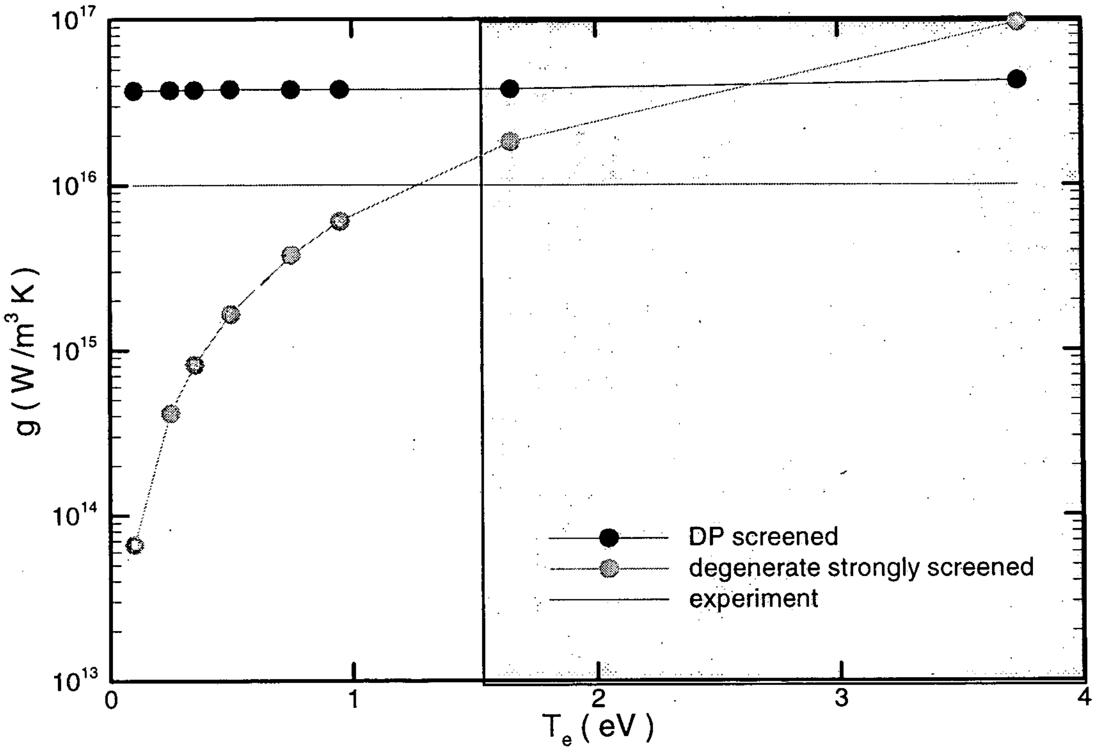
$$\lambda_{screen} = \left(\frac{k_B (T_e + T_F)^{1/2}}{4\pi n_e e^2}\right)^{1/2}$$ where T_F is the Fermi temperature

$$\lambda_{ei} = \max\left(\frac{Z^* e^2}{3k_B T_e}, \frac{h}{2(3m_e k_B T_e)^{1/2}}\right)$$

$$D\left(\frac{\mu_e}{k_B T_e}\right) = \frac{\pi^{1/2}}{2\left[1+\exp\left(-\frac{\mu_e}{k_B T_e}\right)\right]}F_{1/2}\left(\frac{\mu_e}{k_B T_e}\right)$$ where $\frac{\mu_e}{k_B T_e} = g(T/T_F)$

Kogan with Screened Dharma-wardana-Perrot Potential
Degenerate SSBC Model

Near Fitted Electron-Ion Coupling Coefficient



6 g/cm^3

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Hydrodynamic Code Comparison With Laser Driven Electron-Ion Equilibration Experiment

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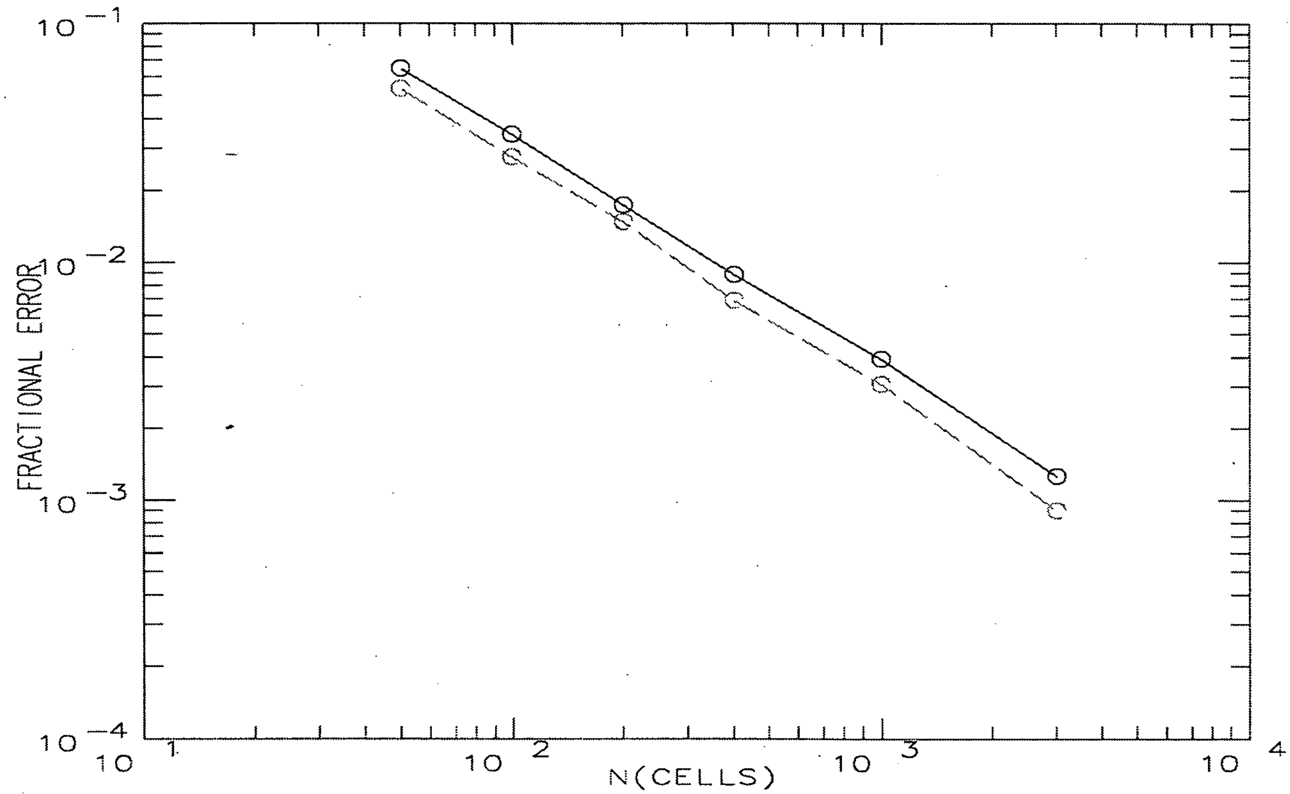
Multi-Species Hydrodynamic Code Validated Against Published Calculations and Experimental Data

- One-Dimensional Planar, Cylindrical, or Spherical
- Separate Electron and Ion Species
- Ambipolar Diffusion
- Matrix Heat Capacity for Strongly Coupled Plasma
- Non-Equilibrium Equation of State
- Lagrangian Covariant Formulation of Artificial Viscosity
- Strongly Screened Transport Coefficients

- Extensively Tested Against Analytic Problems - Verification
- Laser Shock Experiment - Validation

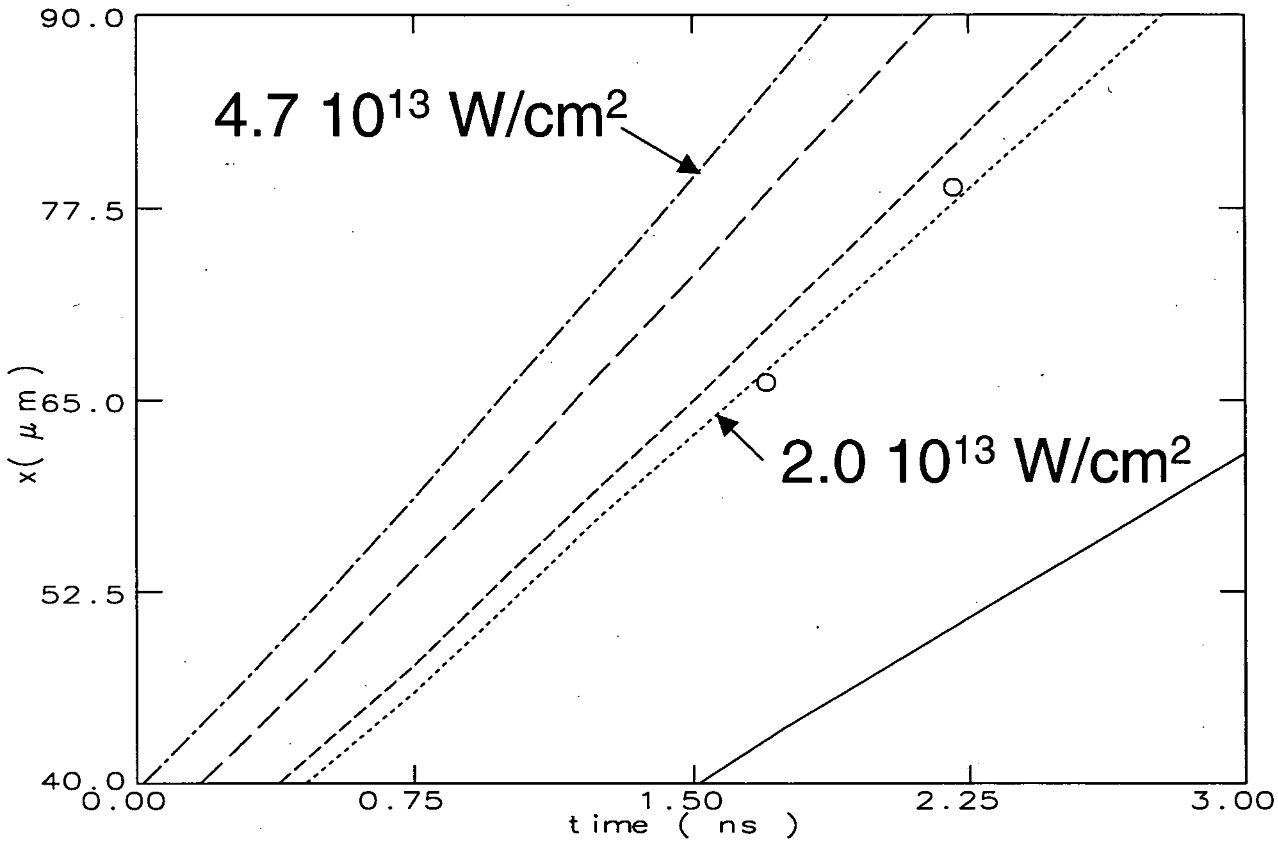
Code Extensively Verified Against Analytic Problems
Uniform Convergence Observed for Noh Shock Problem

Total
Internal
Energy



Covariant Artificial Viscosity Against Scalar Artificial Viscosity

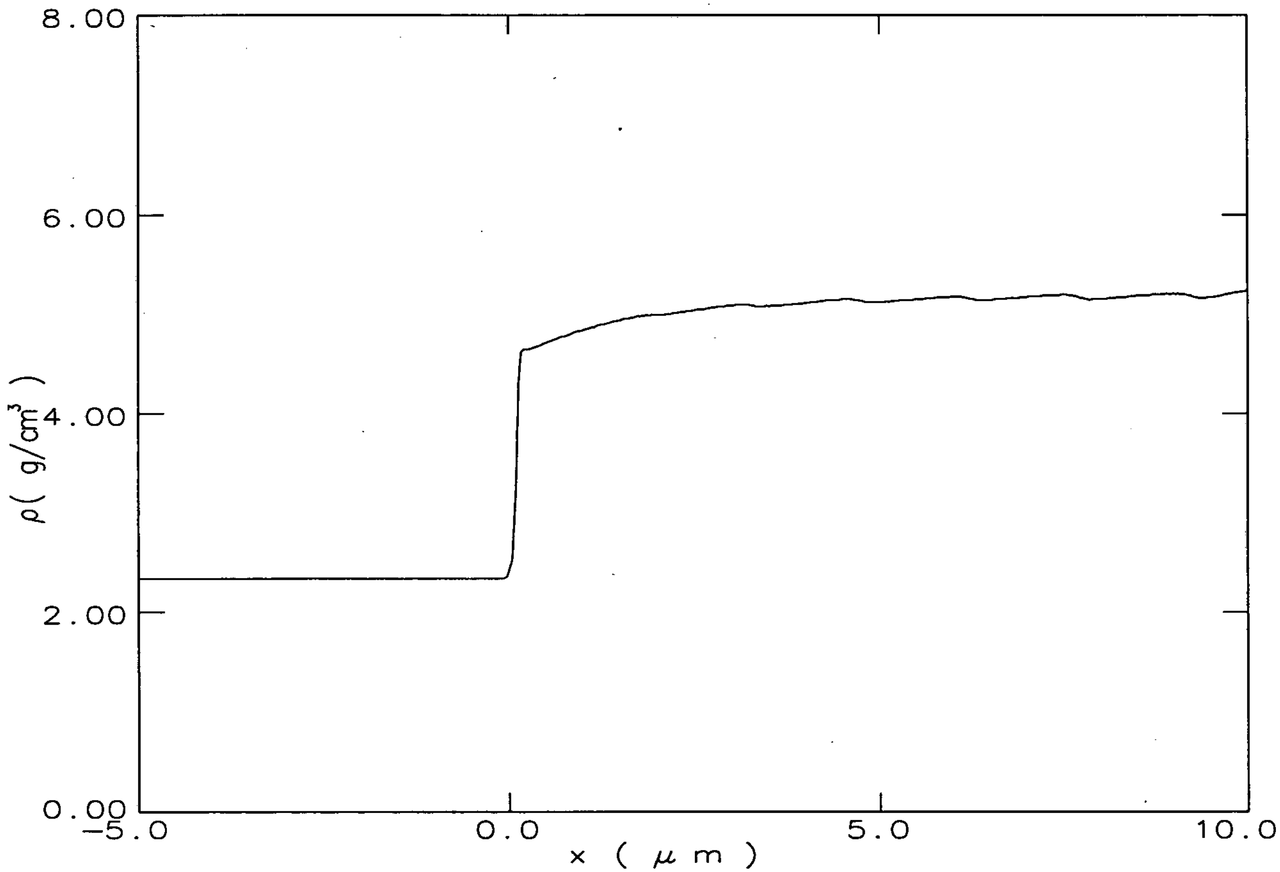
Observed Shock Breakout Time with Laser Intensity Inconsistent with Published Results



EOS Discrepancy with Sesame 3810 and QEOS?

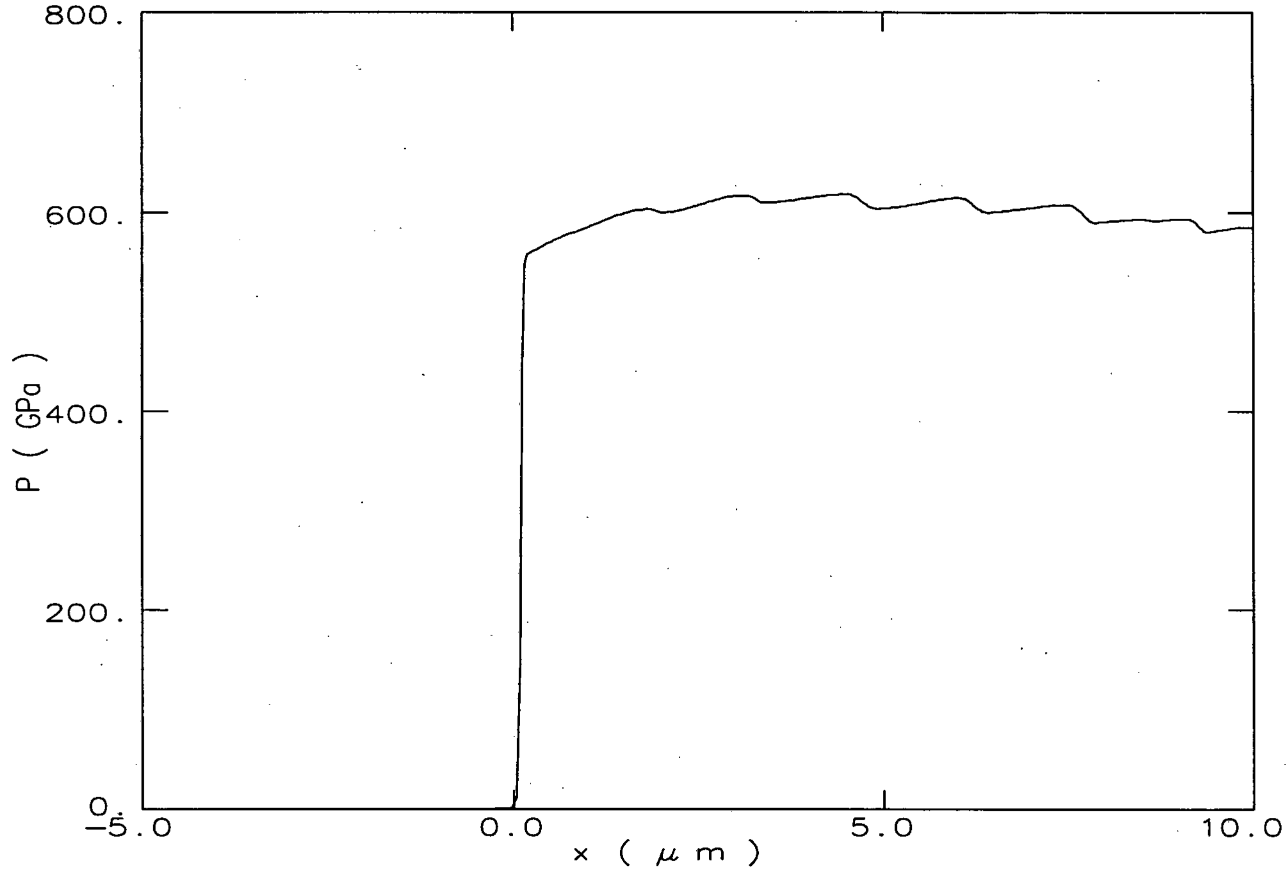
Laser-Matter Interaction Model?

Shock Parameters Consistent with Published Hydrodynamic Results if Shock Breakout Time is Matched



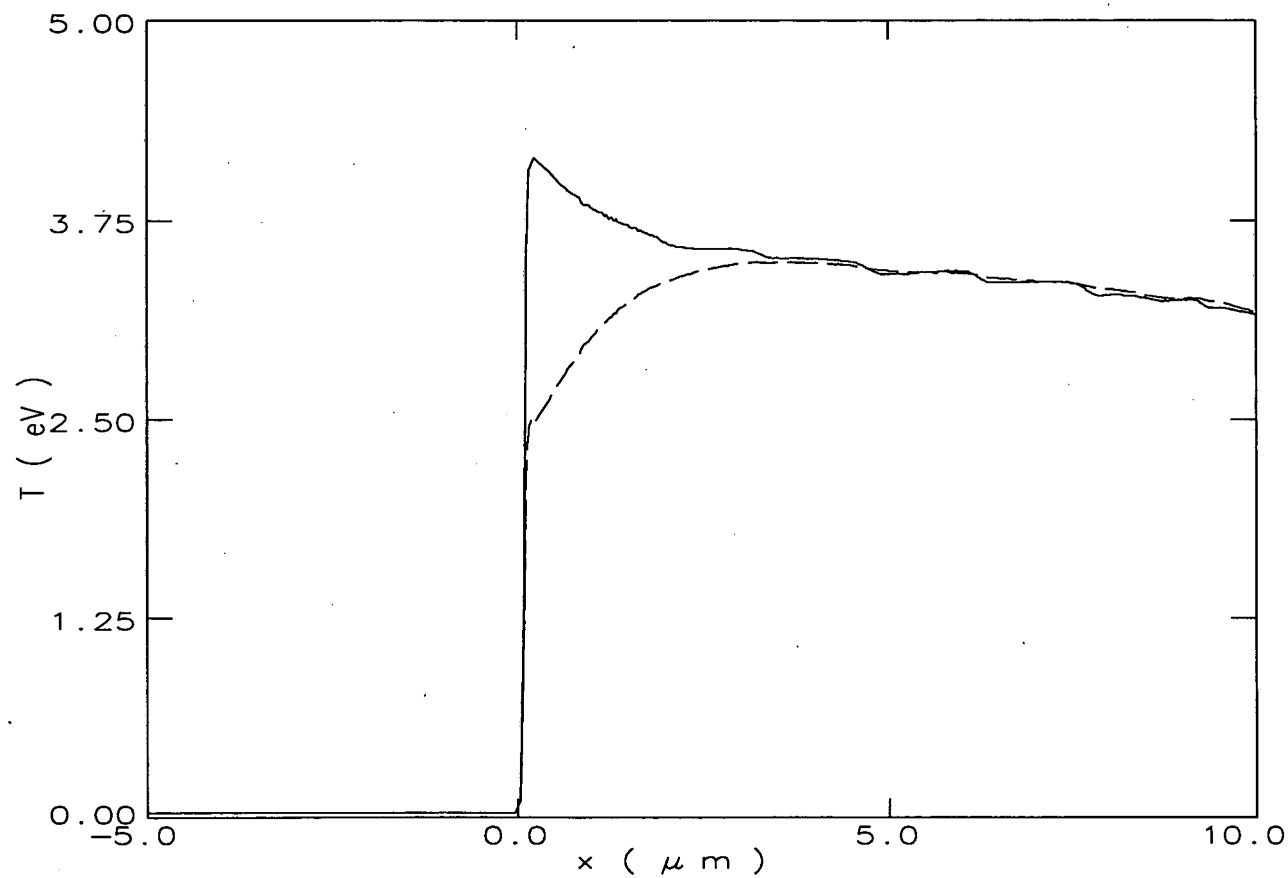
Shock Density at 1.5 ns Past Peak Laser Intensity

Shock Parameters Consistent with Published Hydrodynamic Results if Shock Breakout Time is Matched



Shock Pressure at 1.5 ns Past Peak Laser Intensity

Electron-Ion Equilibration Distance within 2 - 3 of Fitted Distance of 10 μm



Electron-Ion Temperate Separation One-Half of Published Result

EOS Discrepancy with Sesame 3810 and QEOS?

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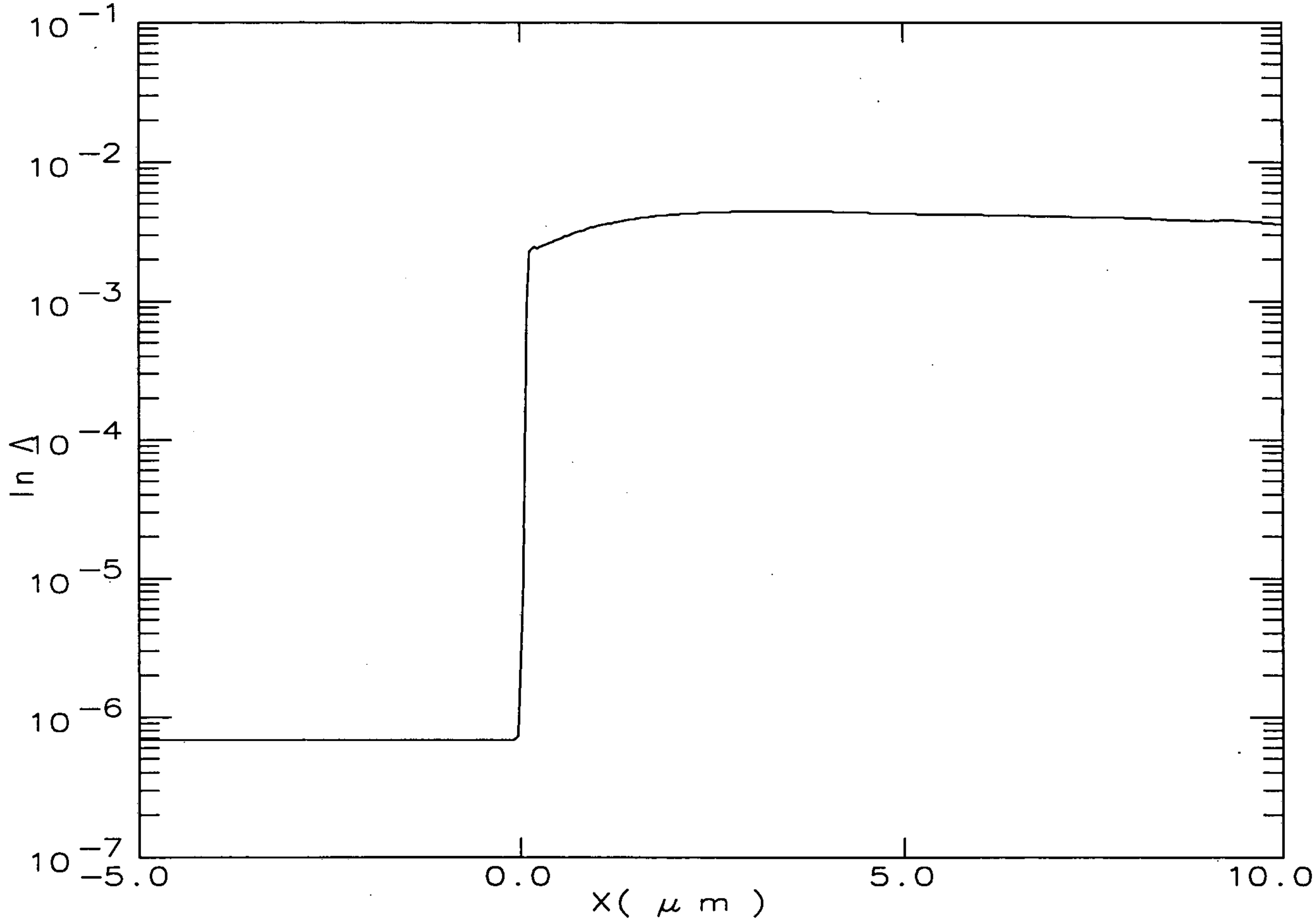
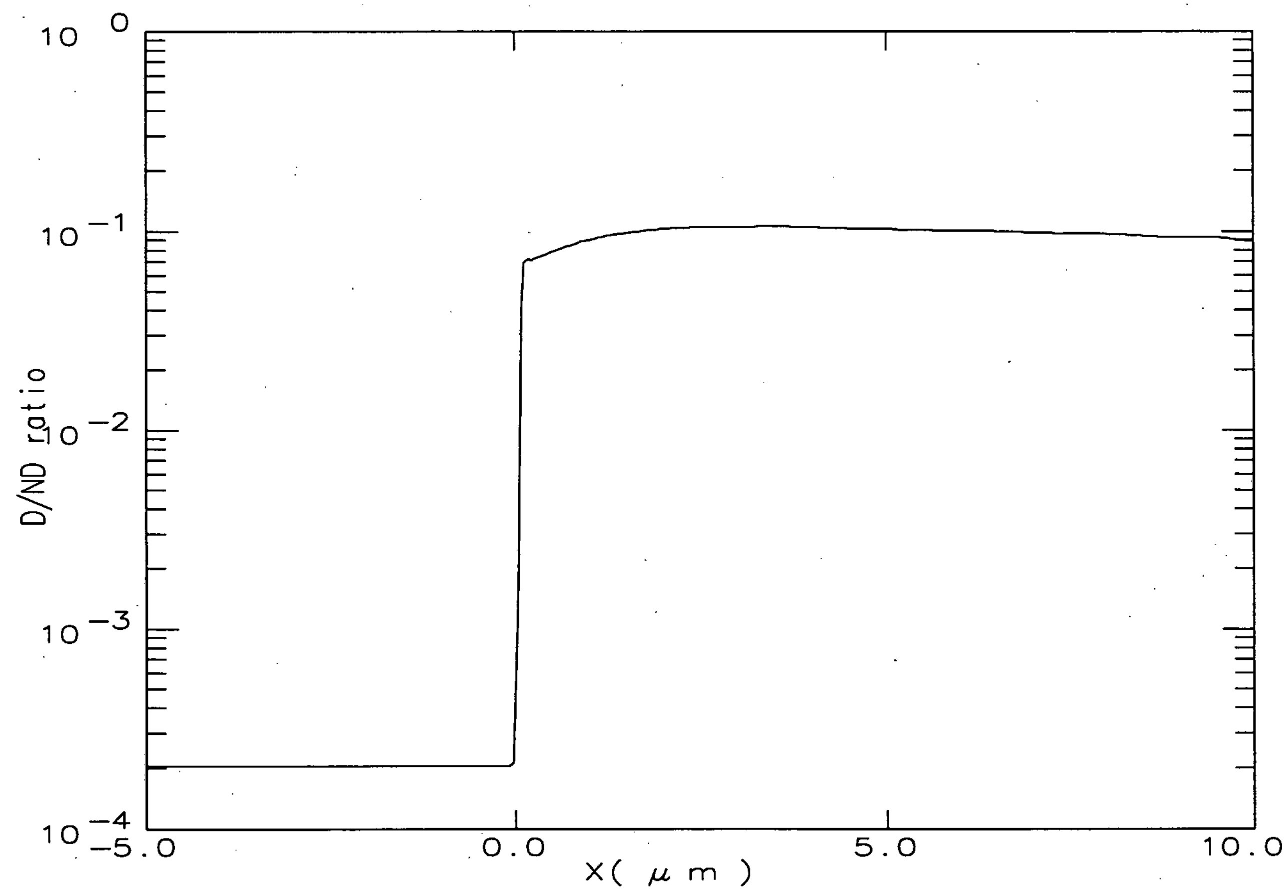
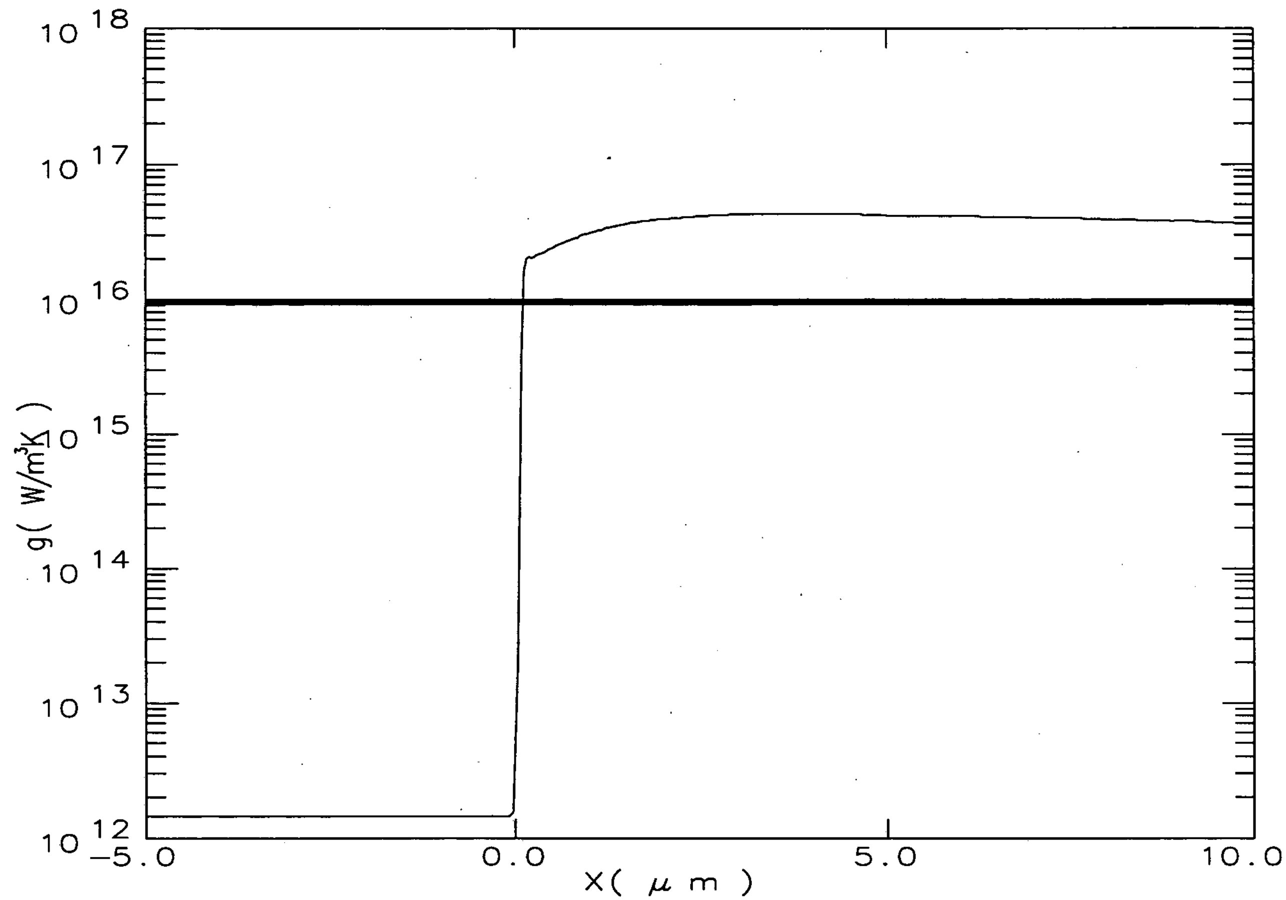
Coulomb Logarithm is Two Orders-of-Magnitude Below Standard Cutoff



Plasma Moderately Degenerate, Which Further Slows Energy Equilibration Rate



Electron-Ion Equilibration Rate is 2 - 3 Times Fitted Rate of 10^{16} W / m^3 K



SUMMARY

- **Two Electron-Ion Coupling Constant Models Close to Experiment**
  - Degenerate Strongly-Screened Binary-Collision Model
  - Kogan Integral with Screened Dharma-wardana-Perrot Potential

- **Models Orders-of-Magnitude Smaller Than Coulomb Cutoff Model**

- **Multi-Species, Multi-Temperature Code Extensively Verified**

- **Code-Experiment Comparison may be Improved**
  - Laser Intensity verses Shock Breakout Time Inconsistent
  - EOS Inconsistencies
  - Kogan Integral Model