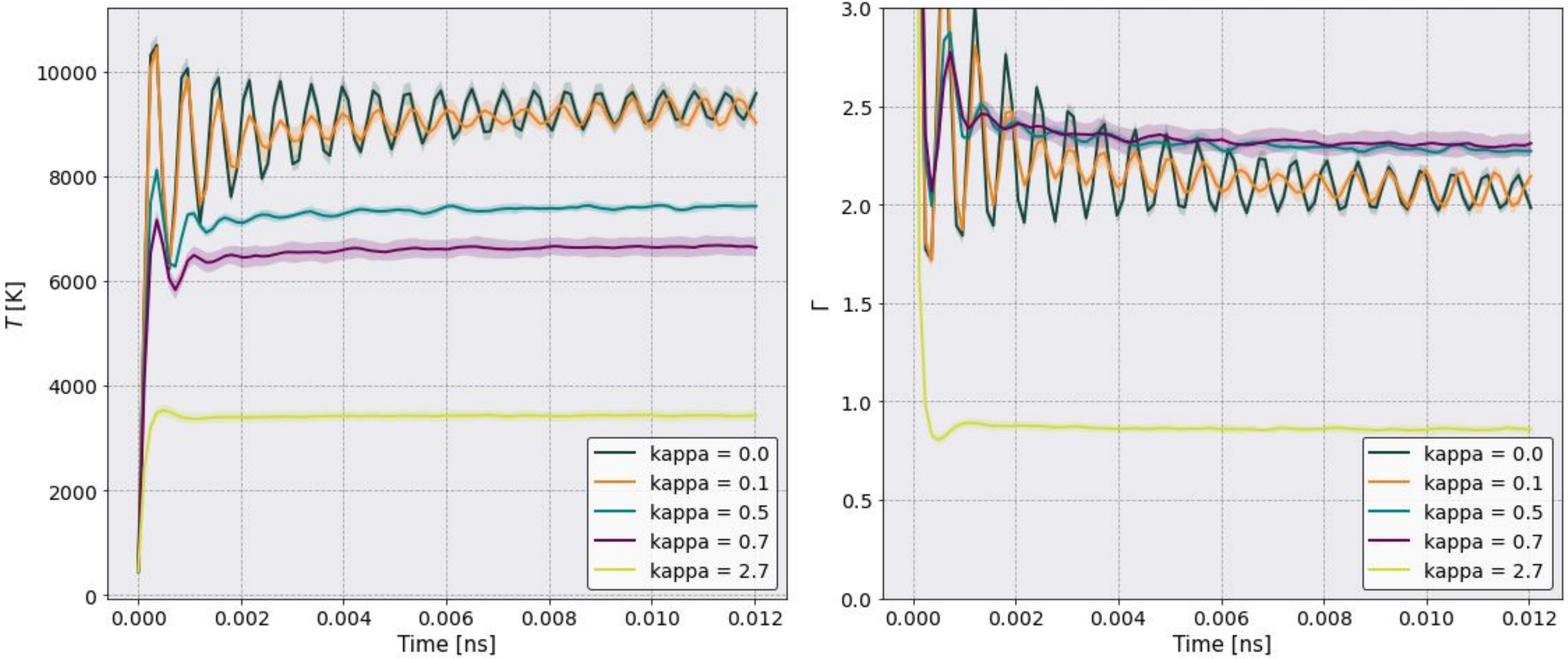
MD Results



T [K]
10000
8000
6000
4000
2000
0
0.000
0.002
0.004
0.006
0.008
0.010
0.012
Time [ns]
kappa = 0.0
kappa = 0.1
kappa = 0.5
kappa = 0.7
kappa = 2.7
Γ
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0.000
0.002
0.004
0.006
0.008
0.010
0.012
Time [ns]
kappa = 0.0
kappa = 0.1
kappa = 0.5
kappa = 0.7
kappa = 2.7

CLAMS

Controlled Laser-Assisted Microplasma Studies

Team MSU

MICHIGAN STATE
UNIVERSITY

Plan

- The CLAMS model
- Where to find codes
- Values of physical parameters
- Code base (Results)
- Extensions

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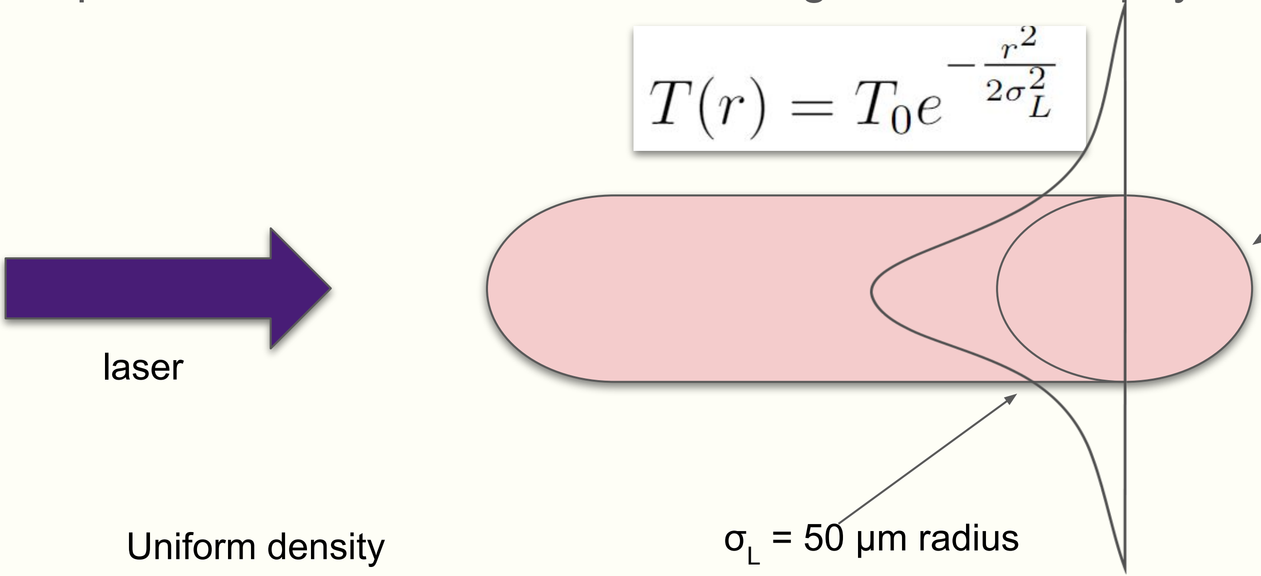
Current Understanding of the Plasma

The plasma is assumed to have these geometric and physical properties:

$$T(r) = T_0 e^{-\frac{r^2}{2\sigma_L^2}}$$



Uniform density profiles *(electrons and ions)*

$$\bar{Z}(T_e)$$

$$T_i^{exp} = T_0$$

or

$$T_i^{exp} = \frac{\int d^3r \; n_i T_i}{\int d^3r \; n_i}$$

Current Model of the Plasma

Implemented

- Gaussian initial temperature profiles $T_e(r), T_i(r)$
- $\bar{Z} = 1$ (everywhere!)

Not Implemented

- Density profile $n_e(r), n_i(r)$
- Neutrals
- TF ionization $\bar{Z}(T_e)$

Two-Temperature Model (TTM)

A TTM can be defined as:

energy sources
(e.g., laser, rad. loss)

$$c_e \frac{\partial T_e}{\partial t} = \nabla \cdot (k_e \nabla T_e) - G(T_e - T_i) + S_e$$

$$c_i \frac{\partial T_i}{\partial t} = G(T_e - T_i)$$

+ possible ionic thermal conduction

Parameters are: $\{c_e, c_i, k_e, G\}(T_e, T_i, n_e, n_i)$

initial conditions $n_e(r), n_i(r), T_e(r), T_i(r)$

TTM and Transport Literature

Improved Two-Temperature Model and Its Application in Ultrashort Laser Heating of Metal Films

Lan Jiang
Hai-Lung Tsai[1]

Laser-Based Manufacturing Laboratory, Department of Mechanical and Aerospace Engineering, University of Missouri-Rolla, Rolla, MO 65409

The two-temperature model has been widely used to predict the electron and phonon temperature distributions in ultrashort laser processing of metals. However, estimations of some important thermal and optical properties in the existing two-temperature model are limited to low laser fluences in which the electron temperatures are much lower than the Fermi temperature. This paper extends the existing two-temperature model to high electron temperatures by using full-run quantum treatments to calculate the significantly varying properties, including the electron heat capacity, electron relaxation time, electron conductivity, reflectivity, and absorption coefficient. The proposed model predicts the damage thresholds more accurately than the existing model for gold films when compared with published experimental results. [DOI: 10.1115/1.2035113]

Keywords: Ultrashort Laser, Quantum Mechanics, Metal Thin Film, Two-Temperature Model

PHYSICAL REVIEW E, VOLUME 65, 036418

Dense plasma temperature equilibration in the binary collision approximation

D. O. Gericke* and M. S. Murillo
Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545

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(Received 28 August 2001; published 7 March 2002)

Efficient model for electronic transport in high energy-density matter

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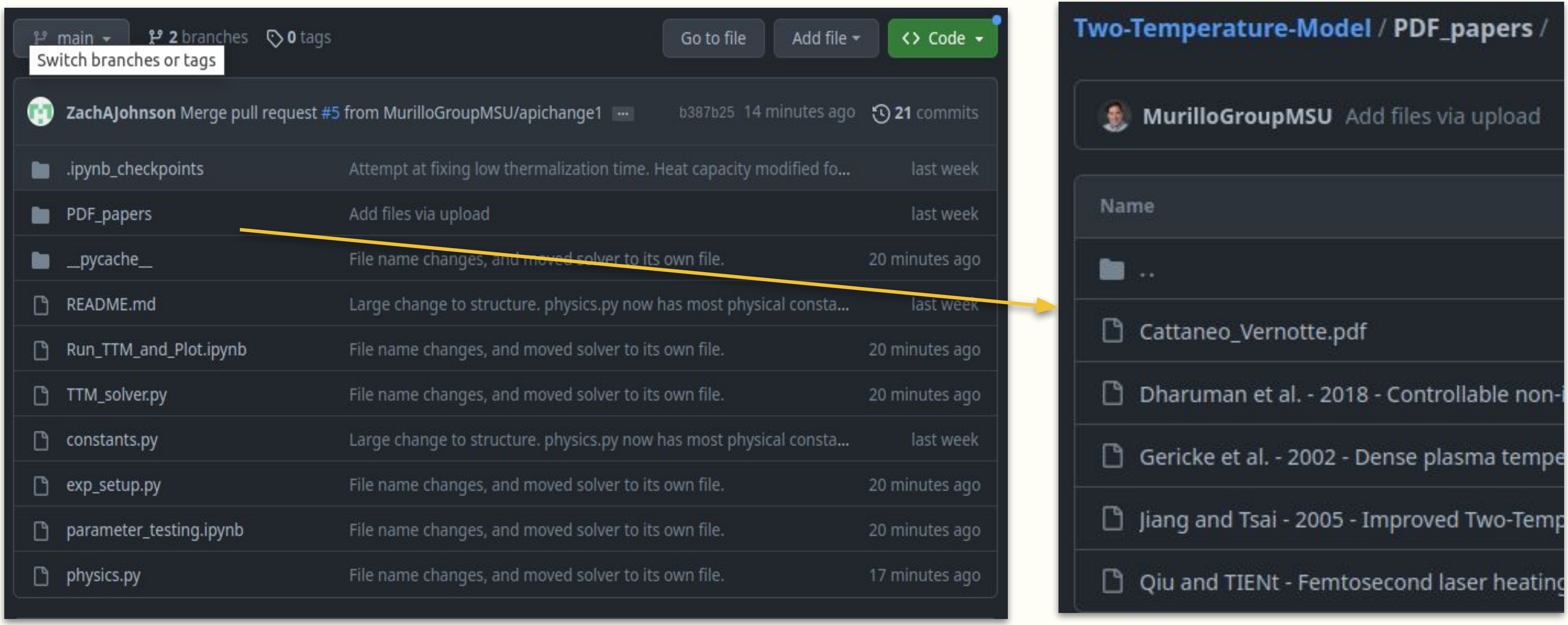
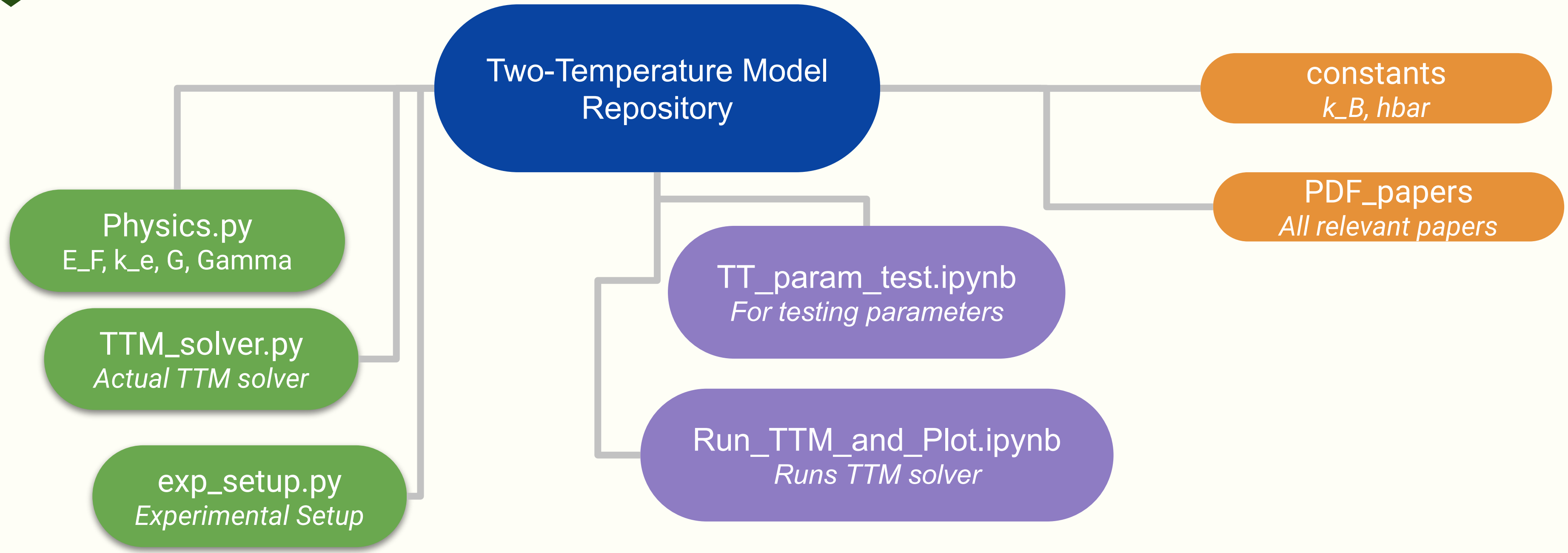
Where are we: GitHub

A GitHub repo for CLAMS. <github.com/MurilloGroupMSU/Two-Temperature-Model>



GitHub Layout



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Where are we: Physical Parameters

The physical properties of the plasma are captured by 7 parameters:

1. electron specific heat
2. ion specific heat
3. temperature relaxation rate
4. electron thermal conductivity
5. ion thermal conductivity
6. electron-electron collision rate
7. ion-ion collision rate

EOS and Heat Capacities

Specific Heat:

$$c_{e,i} = \frac{\partial U}{\partial T_{e,i}}$$

Currently ideal gas:

$$U_{\text{ideal}} = \frac{3}{2} T_e n_e + \frac{3}{2} T_e n_e$$

Future classical, strongly coupled EOS:

$$U = U_{\text{ideal}} + U_{\text{ex}}$$

$$U_{\text{ex}} = \frac{e^2}{\pi} n_e \int dq \left(S_{ee}(q) + Z S_{ii}(q) - 2\sqrt{Z} S_{ei}(q) - (Z+1) \right)$$

Temperature Relaxation Rate

Temperature relaxation through classical scattering trajectories

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- Electron-Ion coupling:

$$G = c_e/\tau_{ei}$$

- Electron temperature relaxation time:

$$\tau_{ei} = \frac{3 m_i m_e}{4\sqrt{2\pi} n_i \bar{Z}^2 e^4 \lambda} \left(\frac{k_B T_e}{m_e} + \frac{k_B T_i}{m_i} \right)^{3/2}$$

- Ion temperature relaxation time

$$\tau_{ie} = \frac{c_i}{c_e} \tau_{ei}$$

Thermal Conductivities

What is the electron conductivity?

$$k_e = \frac{1}{3} v_{the}^2 \tau_{ee} c_e \qquad k_e = \frac{1}{3} v_{the}^2 \tau_{ei} c_e$$

Very different!

If using left equation, modify i->e in earlier τ_{ei}

$$\tau_{ee} = \frac{3 m_e^2}{4\sqrt{2\pi} n_i e^4 \lambda_{ee}} \left(2 \frac{k_B T_e}{m_e} \right)^{3/2}$$

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Keywords: Ultrashort Laser, Quantum Mechanics, Metal Thin Film, Two-Temperature Model

Used in Plots

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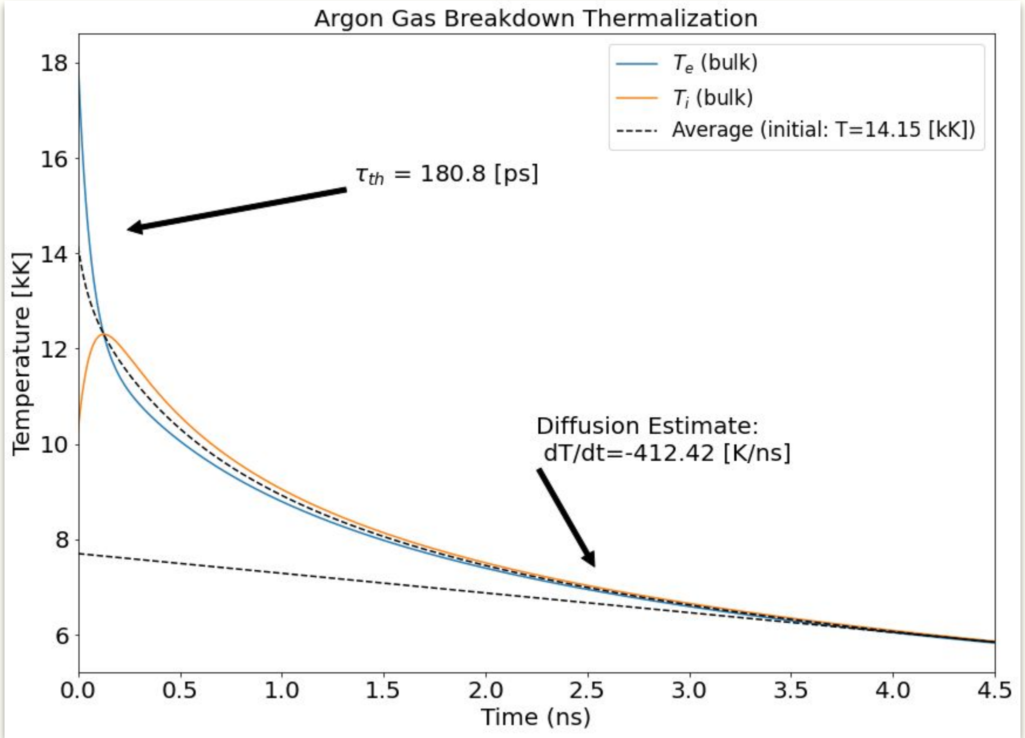
Where are we: Numerical Results

Our preliminary model has been solved (i.e., forward Euler, finite-volume).



Bulk definition of temperature

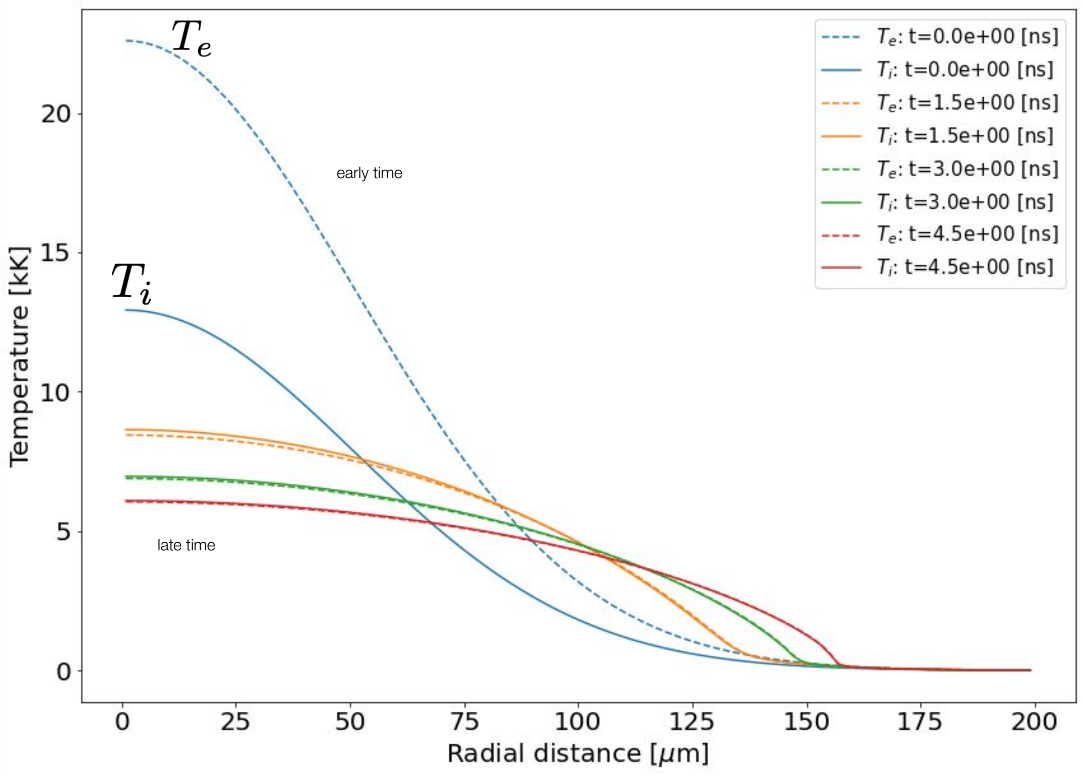
$$T(r) = T_0 e^{-\frac{r^2}{2\sigma_L^2}}$$

$$T_i^{exp} = \frac{\int d^3r \; n_i T_i}{\int d^3r \; n_i}$$

This plot is based on class `JT_GMS_Physics` in `physics.py` (Jiang et al., Gericke et al.)

Where are we: Numerical Results

We see the temperatures diffusing, and relaxing.



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Extensions: Cattaneo-Vernotte Heat-Flux Response

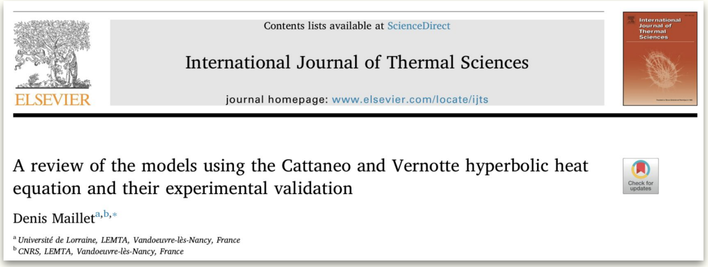
Fourier's Law assumes a steady-state heat flux ***Q*** driven by a linear gradient in temperature. In reality, there is a PDE that describes the spatiotemporal evolution of Q. (And, in principle, that PDE couples to a hierarchy of higher-order moments.)

Fourier's Law terms

$$\tau_{ee}\frac{\partial \mathbf{Q}}{\partial t} + \underbrace{\kappa\nabla T_e + \mathbf{Q}}_{\text{Fourier's Law terms}} = 0$$

?

More thinking about this model and its importance is needed.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A review of the models using the Cattaneo and Vernotte hyperbolic heat equation and their experimental validation

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