Theory & validation of electron-ion thermal relaxation in thermonuclear DT plasma for ICF

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Project Overview

Thermal Relaxation in plasmas

Thermonuclear burn & Ejecta

Opportunities @ LANL

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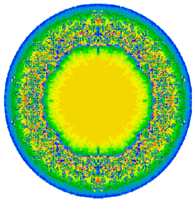
LANL scientists strive to describe physical systems that depend on a wide variety of fundamental processes at various scales

ICF implosion



← m m →

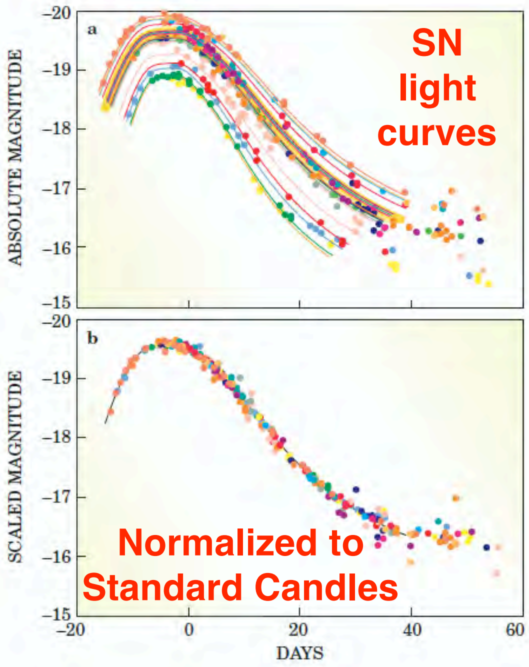
SN explosion

← M m →

- Hydrodynamics
- Solid state properties
- Warm-dense-matter
- Radiation transport
- Nuclear reactions

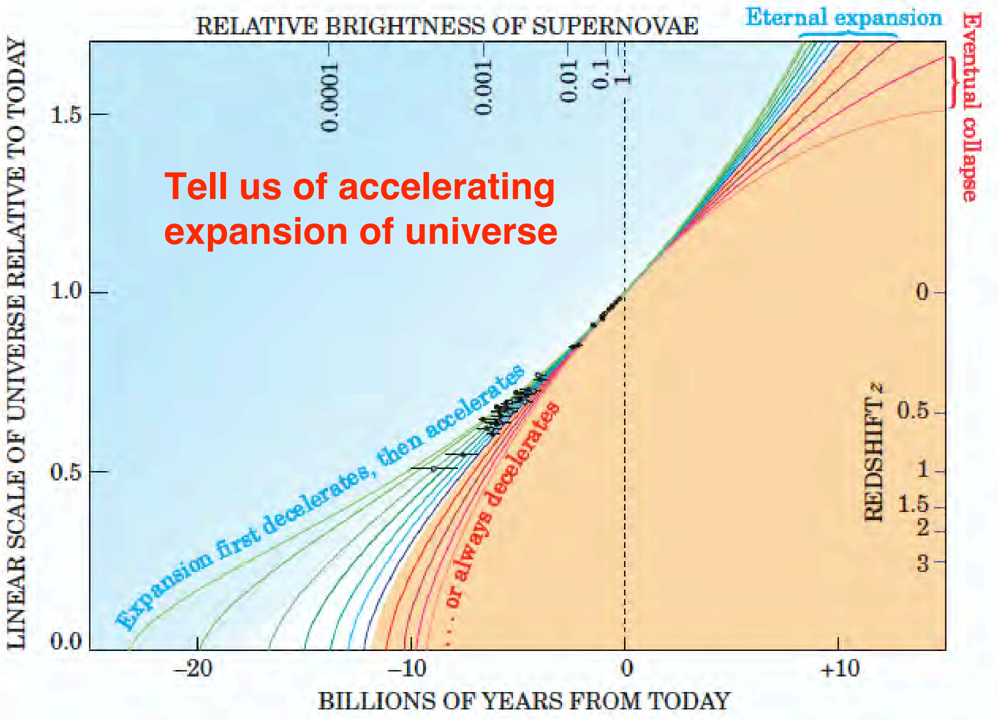
⇒

- Complex EOS
- Fluid turbulence
- Plasma physics
- Opacity
- Hydrodynamics



SN light curves

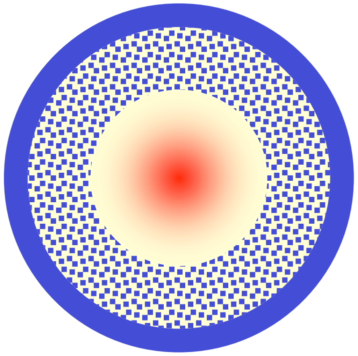
Normalized to Standard Candles



Tell us of accelerating expansion of universe

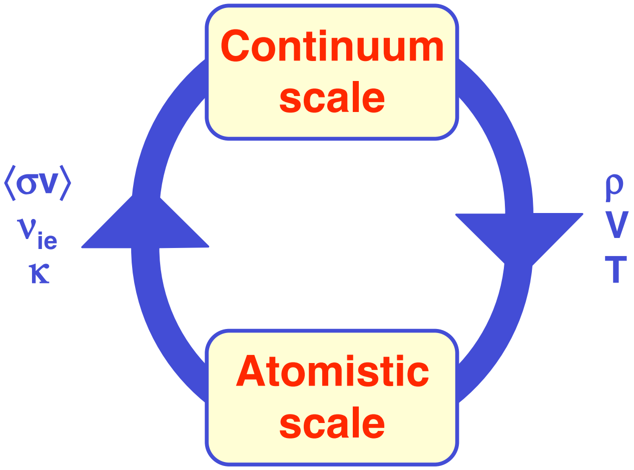
We use high-resolution, 3D single-physics numerical simulations to clarify the physics assumptions in our application codes

- **Multi-physics codes** describe macroscopic (dis-) assembly of applications
  - Combine properties & transport rates for many different processes
    - Hydrodynamic instabilities cause mix & reduce yield
      - Mix can be adjusted to obtain observed yield
      - **But** burn temperature smaller than observed
      - **But** He^3/D results differ from pure gases
      - **But** …



ICF capsule

- **Single-physics simulations** clarify microscopic processes
  - Material properties & transport rates
    - Material strength & damage
    - Transport from turbulent hydrodynamics
    - Atomic mixing rates
    - Electron-ion relaxation rates - ν_{ie}
    - Radiation transport in complex mixtures - κ
    - DT fusion rates - $\langle \sigma v \rangle$
    - Alpha energy deposition
    - …



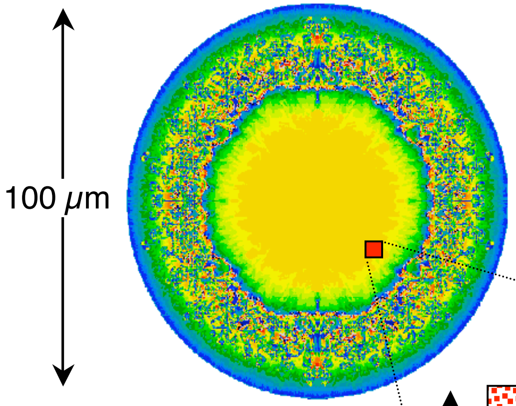
Continuum scale

Atomistic scale

$\langle \sigma v \rangle$
ν_{ie}
κ

ρ
V
T

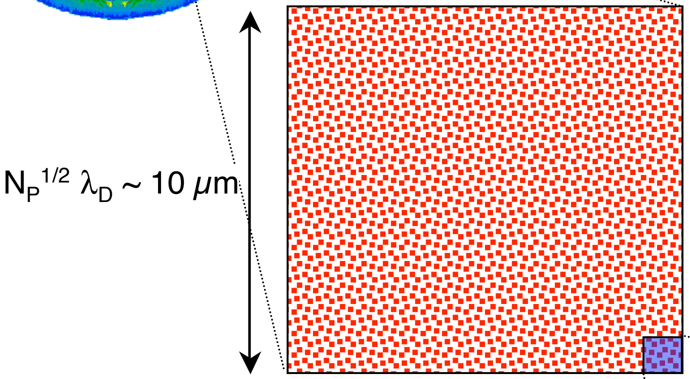
Physics issues are coupled using multi-scale computing up to 1 PetaFlop/s on Roadrunner Computer (LANL)



Continuum simulation of NIF implosion

Hydrodynamics, EOS, radiation transport, nuclear

Assumes Maxwellian fluids & Spitzer collisions



PIC simulation of TN plasma

Macro-particles with TN burn

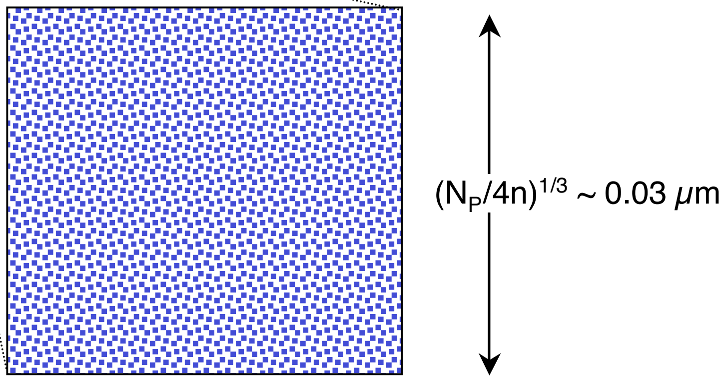
Kinetic & collective effects

Assumes Spitzer collisions

MD simulation of hot plasma

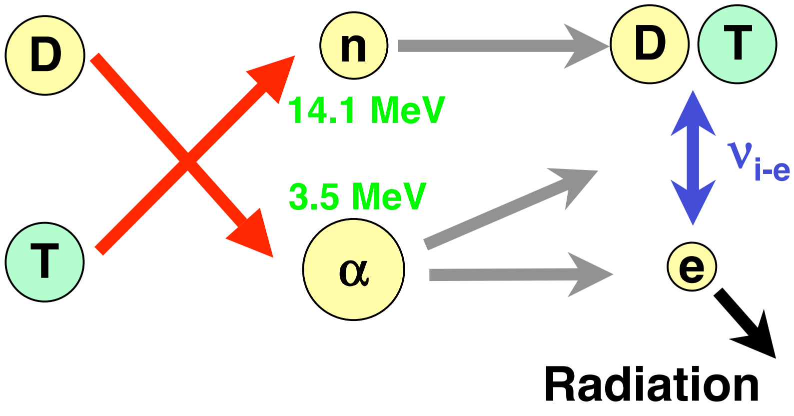
Electrons & ions with Coulomb potential

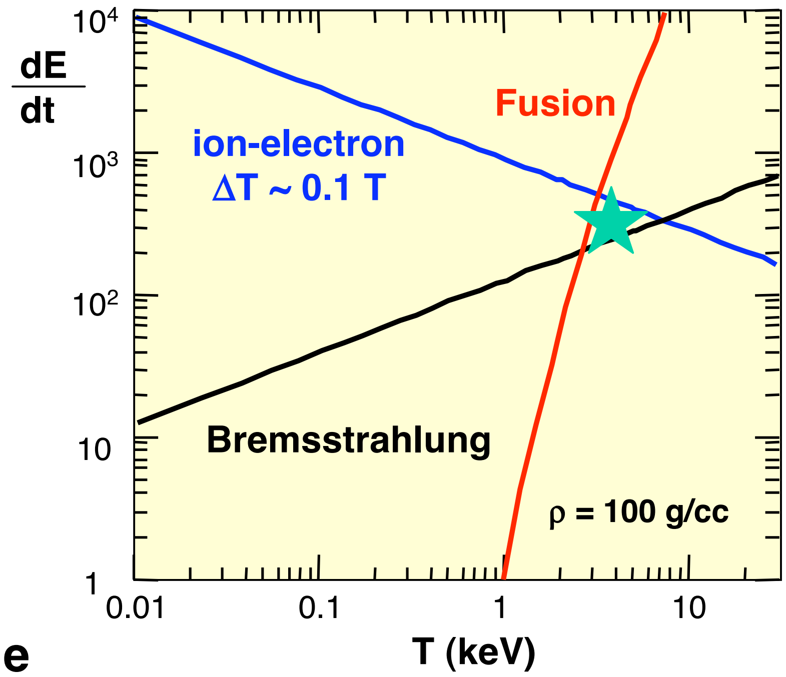
Validates new statistical collision theory



Thermonuclear burn in ICF plasma involves many collisional transport processes whose rates can be improved

Thermonuclear processes in ICF





Transport rates depend on long-range Coulomb collisions

- **Maxwellian electrons & ions**
- **Thermal relaxation** →
- **Thermal conductivity**
- **Electrical conductivity**
- **Radiative**

Uncertainty in Coulomb log

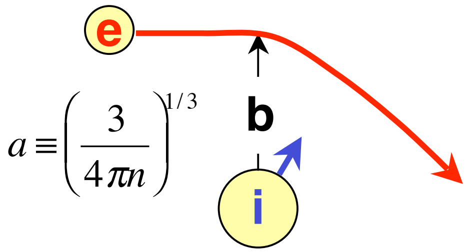
$$\frac{dT_i}{dt} \sim \nu_{ie}\left(T_e - T_i\right)$$

$$\nu_{process} \sim \nu_o \ln \Lambda_{process} \propto \frac{n}{T_e^{3/2}} \ln\left(\frac{b_{\max}}{b_{\min}}\right)$$

Temperature decay not exponential because $\nu \propto T^{-3/2}$

Legacy calculations of temperature relaxation between electrons & ions diverge due to Coulomb force ∝ r^{-2}

Particle collisions can be described by integrating Rutherford cross-section in Boltzman equation, but this diverges due to distant encounters



$$a \equiv \left(\frac{3}{4\pi n}\right)^{1/3}$$

$$\nu_o = \frac{8}{3}\frac{\sqrt{2\pi m}}{M}\frac{e^2 e_i^2}{T^{3/2}}\,n$$

$$\nu_{ie} = \nu_o \int_0^{b_{\max}} \frac{b\,db}{b^2 + \left(Ze^2/mv^2\right)^2}$$

$$\nu_{ie} = \frac{\nu_o}{2}\ln\left(1 + \left(3\frac{b_{\max}}{b_{\min}}\right)^2\right)$$

$$b_{\min} = \frac{Ze^2}{k_B T_e}$$

$$b_{\max} \Rightarrow \infty$$

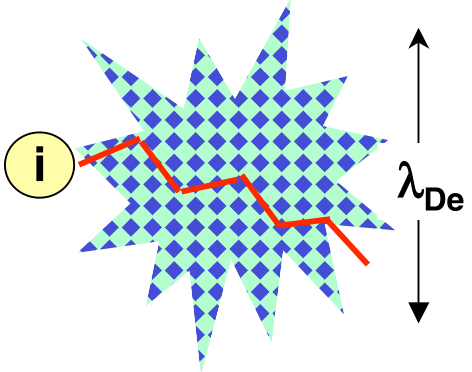
Screening parameter $b_{\max}$

Spitzer: $\lambda_{De} = \sqrt{\frac{k_B T}{4\pi n e^2}}$

Landau: $\lambda_{DH} = \frac{\lambda_{De}}{\sqrt{1+Z}}$

Chandrasekhar: $a = \left(\frac{4\pi n}{3}\right)^{-1/3}$

Plasma fluctuations (ε(k,ω) ~ 0) due to discrete electrons & ions are described by Lenard-Balescu, but this diverges due to close encounters



$$\nu_{ie} = \nu_o \int_0^{k_{\max}} \frac{k^3\,dk}{\left|k \bullet \varepsilon(k,0) \bullet k\right|^2}$$

$$\nu_{ie} = \nu_o \int_0^{k_{\max}} \frac{dk}{k}\frac{k^4}{\left(k^2 + k_{De}^2\right)^2} = \nu_o \ln\left(\frac{\lambda_{De}}{b_{\min}}\right)$$

$$k_{\max} \sim \frac{1}{b_{\min}} \Rightarrow \infty$$

$b_{\min} \sim 1 / k_{\max}$

Landau: $R_L = \frac{Ze^2}{k_B T}$

deBroglie: $\lambda_Q = \frac{\hbar}{\sqrt{m k_B T}}$

Need to capture close & distant encounters self-consistently

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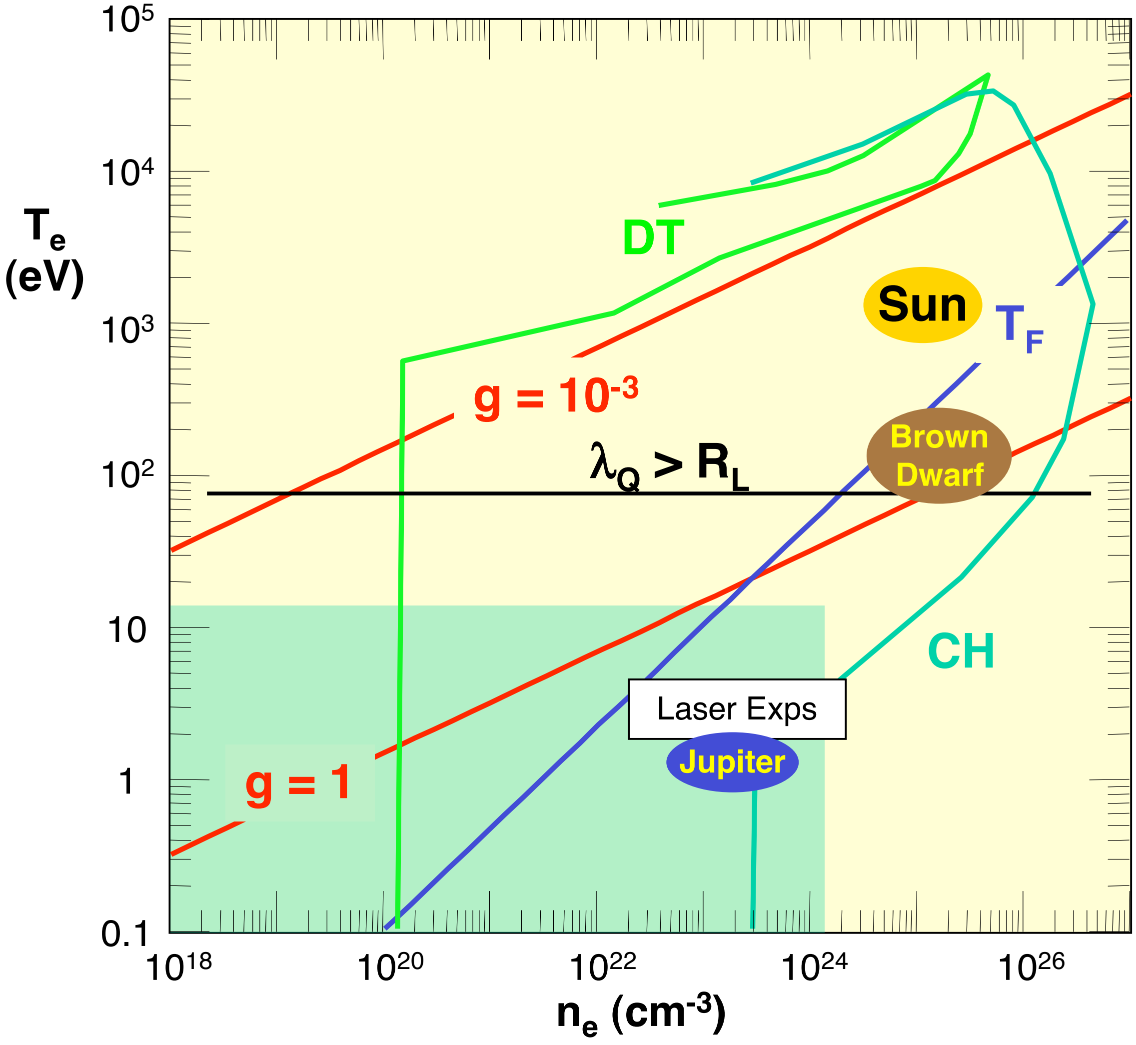
NIF capsule traverses many difficult plasma regimes, but ignition plasma has three simplifying characteristics



Weakly coupled plasma

$$g \equiv \frac{Ze^2}{\lambda_{De} k_B T} = \frac{R_L}{\lambda_{De}} << 1$$

$$R_L = Ze^2 / k_B T_e$$

$$\lambda_{De} = \sqrt{k_B T_e / 4\pi n_e e^2}$$

Quantum diffraction

$$\lambda_Q = \hbar / \sqrt{m k_N T_e} > 1.67 R_L$$

$$T_e > 2.8 \frac{m e^4}{k_B \hbar^2} = 76 eV$$

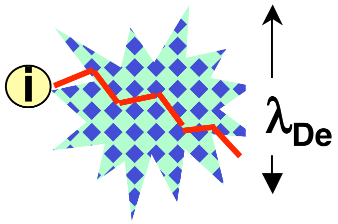
Maxwellian distribution

$$T_e > T_F = \frac{\hbar^2}{2 m k_B} \left(3\pi^2 n\right)^{2/3}$$

ICF codes should treat ALL regimes with unified theory that includes particle correlations (g) & quantum diffraction (λ_Q) & statistics (T_F)

Theory was developed to describe temperature relaxation that includes degeneracy & particle correlations self-consistently

Ion temperature in a spatially uniform, unmagnetized plasma depends on work done on ions (M, n_i, T_i) by electrons (m, $n_e = Z\, n_i$, T_e)



$$\frac{3}{2} n_i k_B \frac{dT_i}{dt} = \left\langle \delta\vec{j}_i \bullet \delta\vec{F}_{ie} \right\rangle$$

Jerome Daligault

Fourier (ω, k) components of fluctuating ion current δj_i & e-i force δF_{ie} are given by

Continuity equation: $\delta\vec{j}_i(k,\omega) = \omega\,\delta n_i(k,\omega)\,\vec{k}/k^2$

Gauss' law: $\delta\vec{F}_{ie}(k,\omega) = i\vec{k}\,V_{ie}(k)\,\delta n_e(k,\omega)$

Fourier transform of interaction potential $V_{ie} \propto 1/k^2$

δj_i & δF_{ie} depend on self-consistent density fluctuations δn_α & plasma susceptibility χ_α for each species α, and we assume a linear response

$$\delta n_\alpha(k,\omega) \equiv n_\alpha - \left\langle n_\alpha \right\rangle = \overset{\text{Spontaneous}}{\delta n_\alpha^s} + \overset{\text{Induced}}{\chi_\alpha \sum_{\beta=e,i} V_{\alpha\beta}\, \delta n_\beta \left[1 - G_{\alpha\beta}(k,\omega)\right]}$$

Mean field assumes particles are allowed everywhere with equal probability
⇒ 'pair distribution' $g_{ie}(r) = 1$

'Local field correction' $G_{\alpha\beta}$ related to Fourier transform of $g_{ie}(r)$
⇒ $G_{\alpha\beta} = 1$ when particles excluded

Coupling between ion & electron subsystems is relatively slow due to small mass ratio m/M & this allows tractable solution

Linear response for density fluctuations introduces total dielectric D(k, ω)

$$\frac{3}{2} n_i \frac{dT_i}{dt} = \pi \int \frac{d^3k}{(2\pi)^3} \int d\omega \frac{V_{ie}(k)}{\left|D(k,\omega)\right|^2} \left[T_i \operatorname{Im} A_{ei}(k,\omega) \operatorname{Im}\chi_i(k,\omega) - T_e \operatorname{Im} A_{ie}(k,\omega) \operatorname{Im}\chi_e(k,\omega)\right]$$

ABSORPTION - EMISSION of plasma fluctuations

where $A_{\alpha\beta} \equiv u_{\alpha\beta}\chi_\alpha\left(1-u_{\beta\beta}\chi_\beta\right), \quad D \equiv \left(1-u_{ee}\chi_e\right)\left(1-u_{ii}\chi_i\right) - u_{ei}u_{ie}\chi_e\chi_i, \quad u_{\alpha\beta} \equiv V_{\alpha\beta}\left(1-G_{\alpha\beta}\right)$

ω-integration is greatly simplified by the small mass ratio m / M << 1

Electron response near $\omega_{pi} \ll \omega_{pe} \Rightarrow \chi_e(k, \omega) \sim \chi_e(k, 0)$

Ion response evaluated using f-sum rule: $\int d\omega \left(f_{abs} - f_{ems}\right) \propto n_e$

Removes i - i interactions
⇒ NO ion screening
Like Bethe stopping power &
TRK sum-rule in spectroscopy

Result reduces to familiar relaxation rate $\nu_{ei} = \nu_o \ln\Lambda$ but with a generalized Coulomb log that includes ALL physics self-consistently

Short-range i-e correlations (pair distribution function ⇒ G_{ie})

$$\ln\Lambda = \int_0^\infty \frac{dk}{k} \frac{1-G_{ie}(k,0)}{\left|\varepsilon_e(k,0)\right|^2} f\left(\frac{k}{2}\right)$$

Quantum Mechanics
Diffraction (λ_Q)
Statistics (E_F)

Electron dielectric (screening modified by e-e correlations ⇒ G_{ee})

Daligault & Dimonte, Phys Rev E 79, 56403 (2009)

We used plasma MD simulations to test comprehensive model

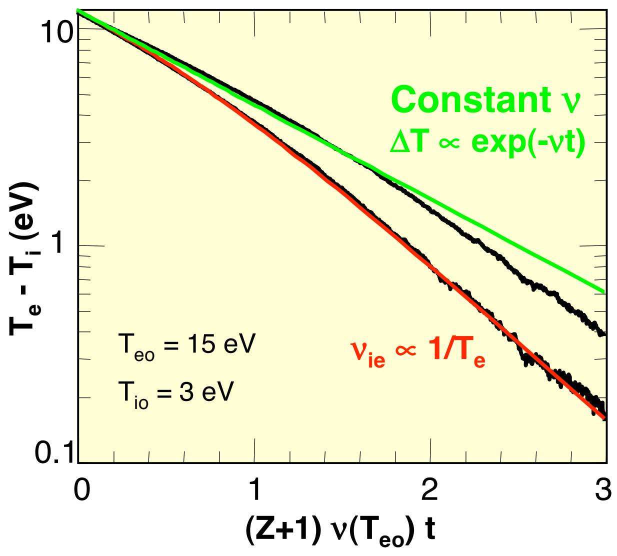
MD simulations provide *ab-initio* transport rates with high accuracy

Classical e's & ions with Coulomb force

$N_{particles} \Rightarrow 10^6$ & $\delta t \Rightarrow 10^{-3}/\omega_{pe}$ for convergence

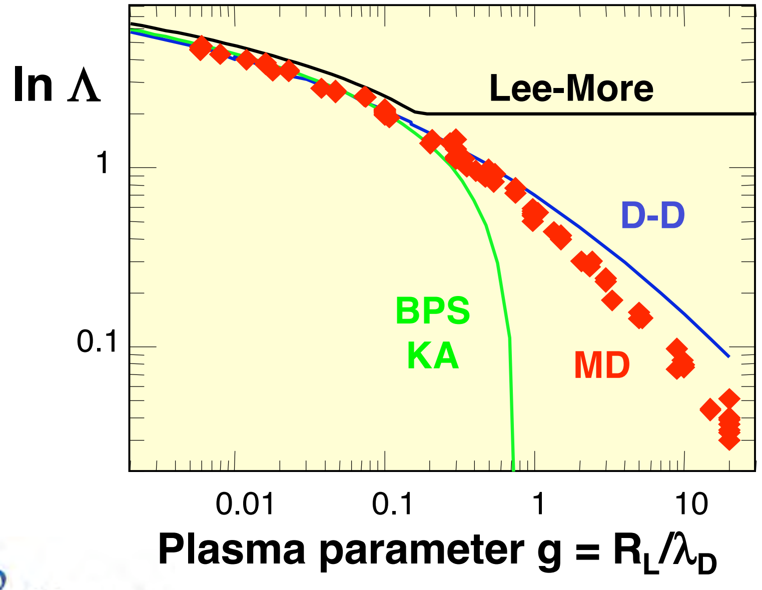
Can discern non-exponential decay due to $\nu(T_e)$

$$(Z+1)\,\nu_{e-i}(T_{eo})\,t = 1 - T + \varepsilon \ln\left(\frac{\varepsilon-1}{\varepsilon-T}\right) \quad \text{where} \quad \varepsilon \equiv \frac{Z+T_{io}/T_{eo}}{1+Z}$$



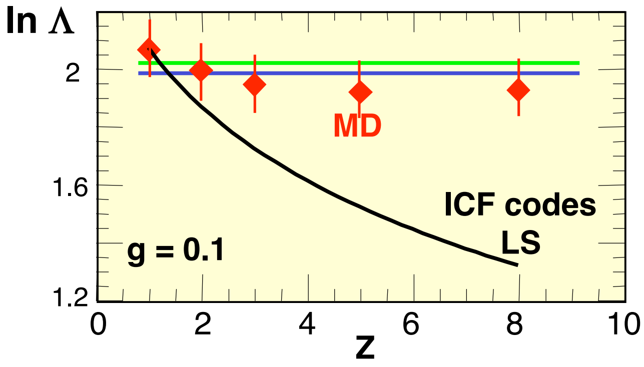
Coulomb log agrees with D & D theory

- Reduces to classical (KA '63, BPS '08) & quantum (Larkin '60) limits for weak coupling
- Extends results to finite coupling g ⇒ 20



NO D-H screening for ν_{ie}

OK for electrical conductivity



Dimonte & Daligault, Phys Rev Lett 101, 135001 (2008)

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Thermonuclear (TN) burn in DT plasma involves many complex processes of comparable time scales that compete with dis-assembly

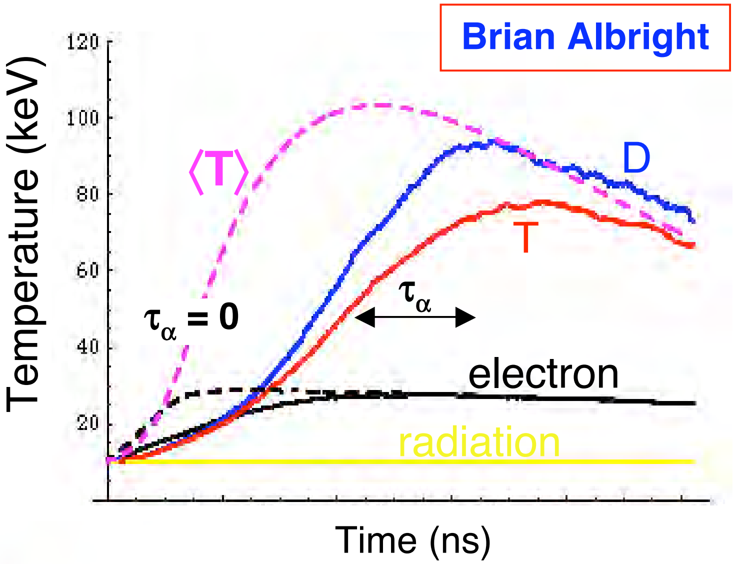
Use VPIC code to simulate infinite D-T plasma @ ρ = 100 g/cc, T = 10 keV

Bowers et al., Phys Plasma **15**, 55703 (08)

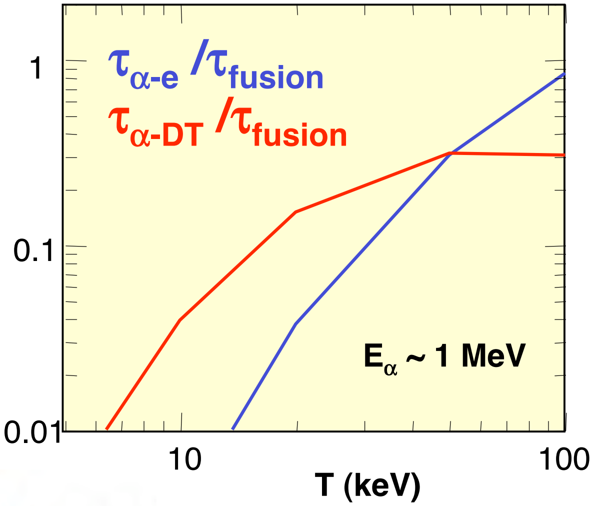
- Kinetic ions, D, T, α's
- Fluid electrons
- Radiation energy sink

α stopping moderates TN burn

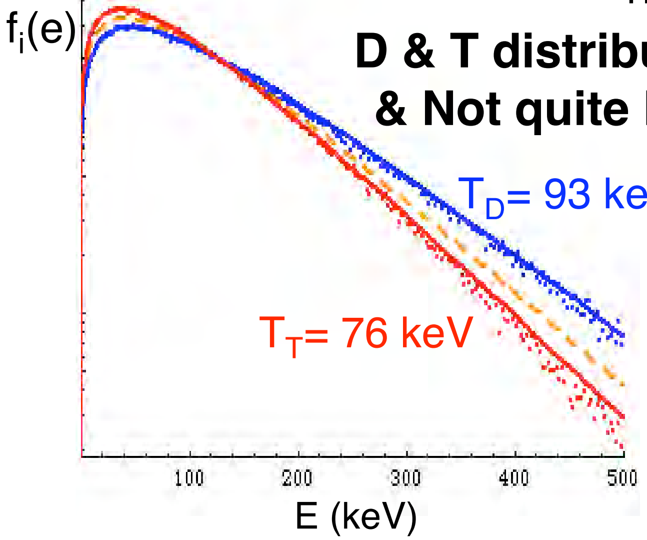
Brian Albright



α's couple first to electrons, then to ions as T increases



D & T distributions differ & Not quite Maxwellian

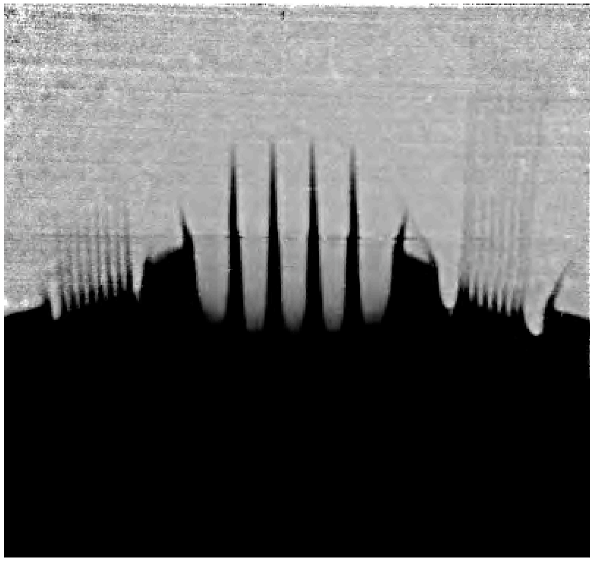


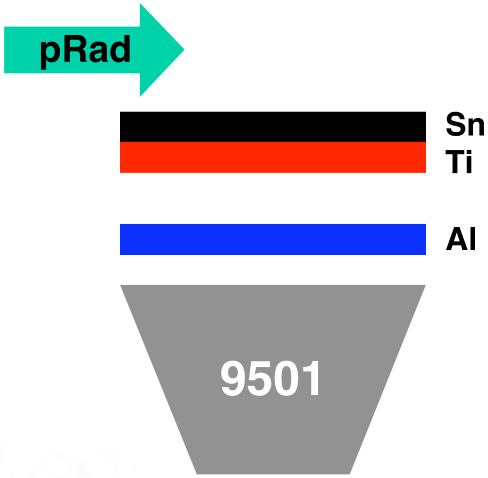
Need to couple results to ICF design code

We couple hydrodynamics & molecular dynamics codes to study Richtmyer-Meshkov instability over variety of scales & conditions

Proton radiography exp's

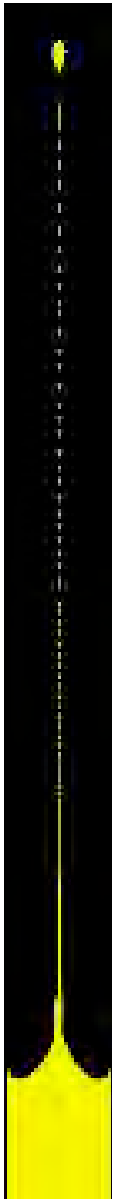
Buttler et al.





Hydro simulations with perfect elastic-plastic,

Terrones

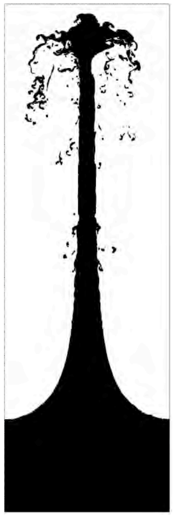


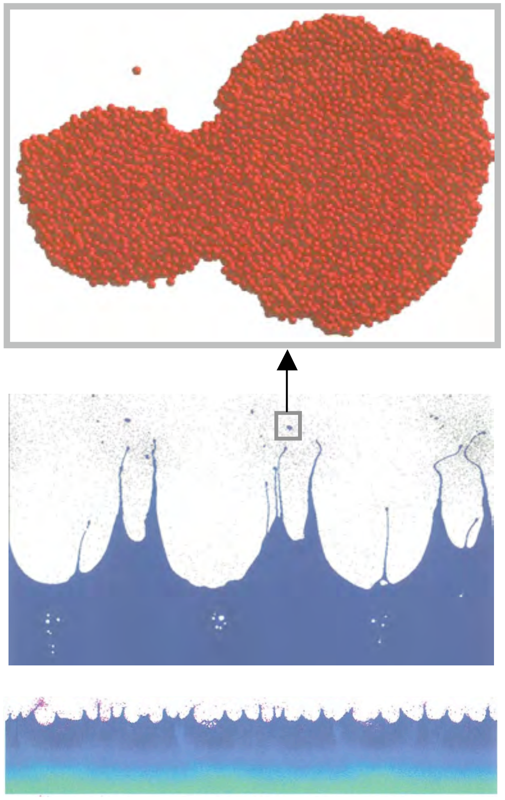
MD simulations to atomic scale

Germann & Cherne

γ-fluids on FLASH (UC)

Ramaprabhu



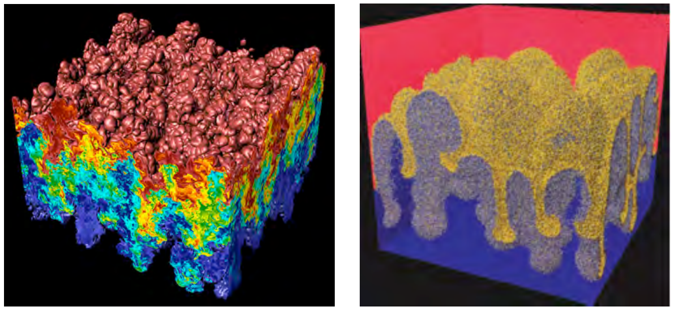


We solve complex physical problems for National Security

Multi-physics codes describe complex physical phenomena in HED regime

- Defense, energy, astrophysics, climate, biology …

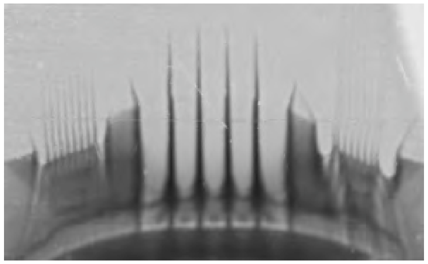
High-resolution, single-physics simulations clarify fundamental properties



- Turbulent hydrodynamics
- Particle-in-cell (collective plasmas)
- Molecular dynamics (HED properties)
- Monte Carlo methods (transport)
- Theory

World-class computing & experimental facilities

- Roadrunner @ 1 PetaFlop/s
- Proton-Radiography
- NIF (LLNL) & Ω (UR)



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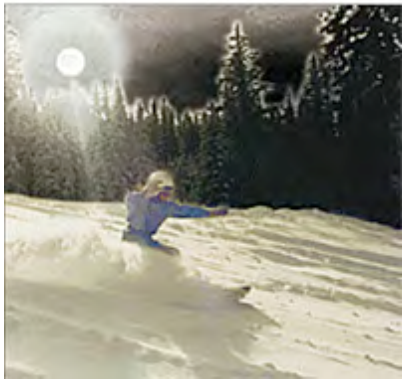
LANL jobs are challenging, relevant, stable & justly compensated



Annualized salaries

Undergraduates	$ 20 - 40 k
Graduates	$ 45 - 60 k
Post-docs	$ 70 - 85 k
Scientist 3	~ $ 112 k
Scientist 5	~ $ 167 k
Management i = 1, 6	+ 25 %

Range ~ ± 25 %

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