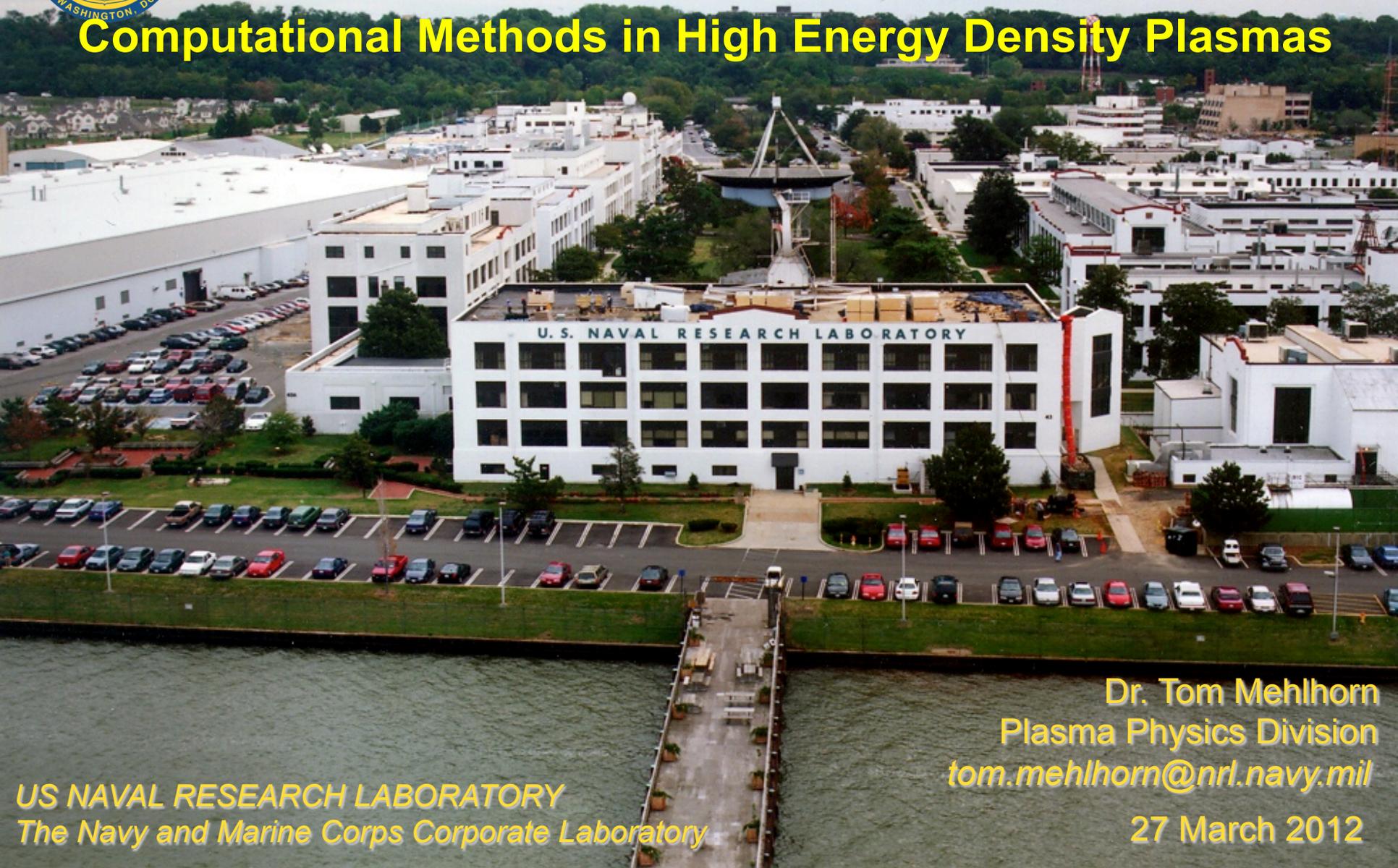


The Role of Non-Local and Non-Equilibrium Physics in High Energy Density Plasmas



IPAM - UCLA

Computational Methods in High Energy Density Plasmas



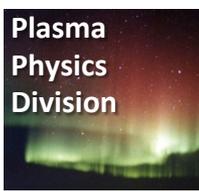
Dr. Tom Mehlhorn
Plasma Physics Division
tom.mehlhorn@nrl.navy.mil

27 March 2012

US NAVAL RESEARCH LABORATORY
The Navy and Marine Corps Corporate Laboratory



Thanks to the many NRL researchers who have contributed to this talk



1. Non-LTE in radiation-dominated K-shell Z-pinches:

Dr. Arati Dasgupta

Dr. John Giuliani

Dr. Ward Thornhill

Ref: J.W. Thornhill, J.L. Giuliani, A. Dasgupta, et al., IEEE Trans. Plasma Sci., 38, 606 (2010).

2. Non-local electron transport in laser fusion

Dr. Wally Mannheimer

Dr. Andy Schmitt

Ref: W. Manheimer, D. Colombant and V. Goncharov, Phys. Plasmas, **15**, 083103, 2008

3. Non-equilibrium physics in clusters irradiated by ultra-short pulsed laser (USPL)

Dr. Jack Davis

Dr. George Petrov

Dr. Lina Petrova

Ref: G.M Petrov, J. Davis, Phys. Plasmas 15, 056705 (2008)

Atomic physics and non-LTE Effects

J. Davis, R. Clark, M. Blaha, & J. Giuliani, Lasers & Part Beams 19, 557-577 (2001)



NRL has a distinguished history



THOMAS A. EDISON

“GOVERNMENT SHOULD MAINTAIN A GREAT RESEARCH LABORATORY TO DEVELOP GUNS, NEW EXPLOSIVES AND ALL THE TECHNIQUE OF MILITARY AND NAVAL PROGRESSION WITHOUT ANY VAST EXPENSE.”

THOMAS A. EDISON,
THE NEW YORK TIMES MAGAZINE
SUNDAY, MAY 30, 1915

A WORLD-CLASS LABORATORY

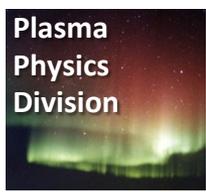
- Idea followed the sinking of the Lusitania in 1915
- Secretary Josephus Daniels Established Naval Consulting Board with Edison Chair, meeting October 7, 1915
- August 29, 1916 Congress appropriates funds to establish the Lab
- Delayed by WW-I, Assistant Secretary of the Navy, Theodore Roosevelt, Jr. Commissions the Lab at Bellevue site on July 2, 1923

Primarily In-house Research to support Navy and Marine Corps needs



Plasma Physics is one of 18 NRL Research Divisions

Plasma
Physics
Division



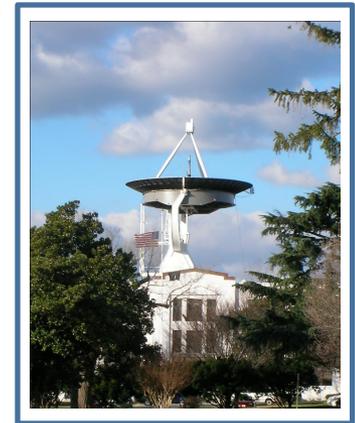
Ocean & Atmospheric S&T
Acoustics
Remote Sensing
Oceanography
Marine Geosciences
Marine Meteorology
Space Science

VXS-1, Patuxent River, MD



Systems Directorate
Radar
Information Technology
Optical Sciences
Tactical Electronics Warfare

Material Science & Component Technology
Chemistry
Material Science and Technology
Laboratory for Computational Physics &
Fluid Dynamics
Plasma Physics
Electronics Science Technology
Center for Bio/Molecular Science and
Engineering



Electra Laser Facility



Naval Center for Space Technology
Space Systems Development
Spacecraft Engineering

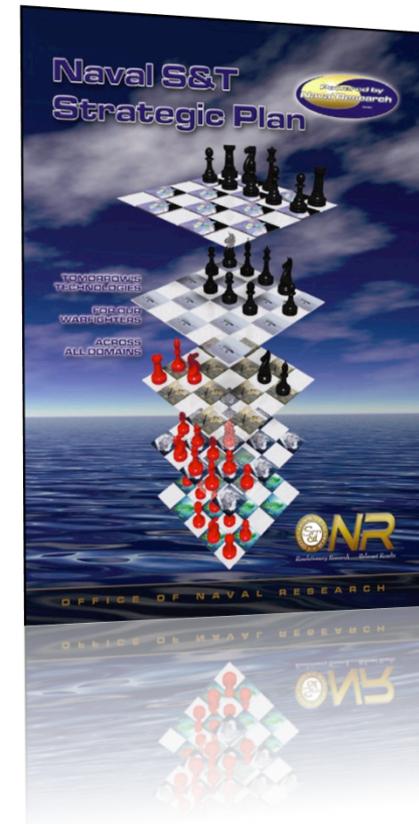
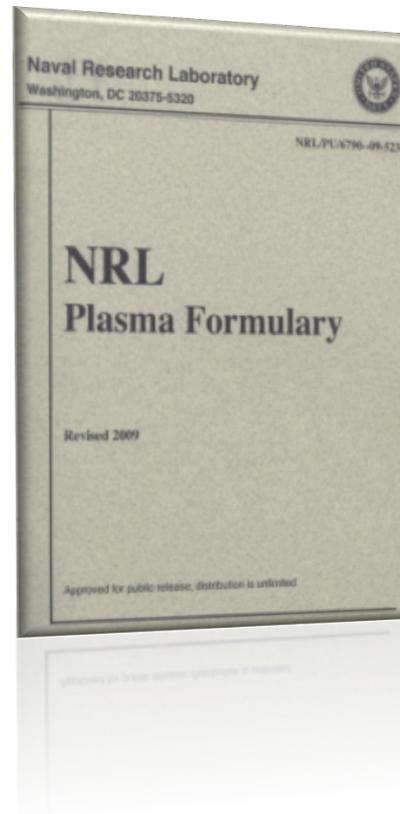
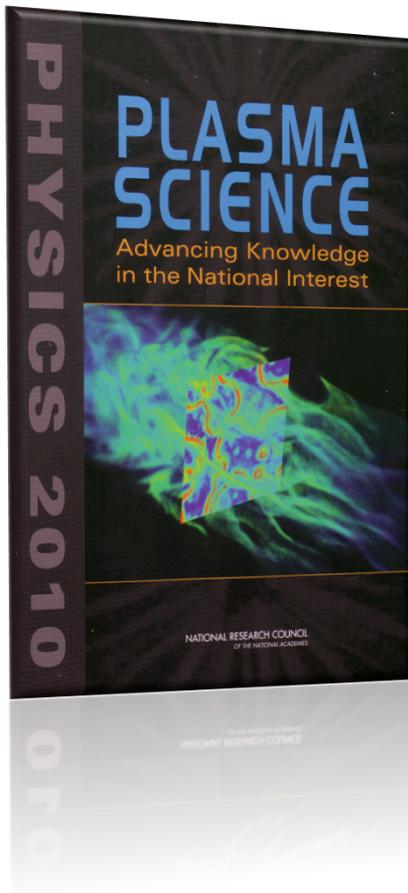
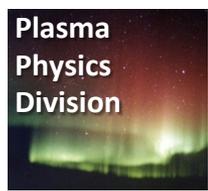
Ex-USS Shadwell, Mobile, AL





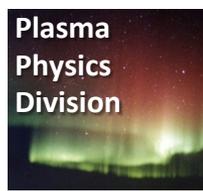
NRL has world-wide recognition in plasma physics & related technologies

Plasma
Physics
Division





Non-LTE and non-local phenomena underlie High Energy Density (HED) plasmas



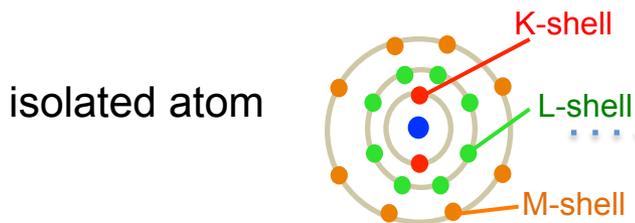
LTE

(Local Thermodynamic Equilibrium)

internal energy of a plasma
(thermal + excitation + ionization)
determined by local
density and temperature

blackbody radiation spectrum $\dots \dots \lambda_{\gamma, mfp} > \frac{\rho}{\nabla \rho} \dots \dots$

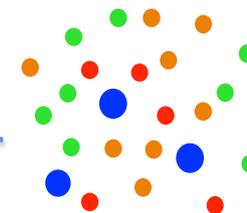
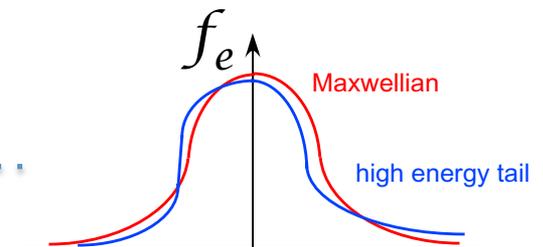
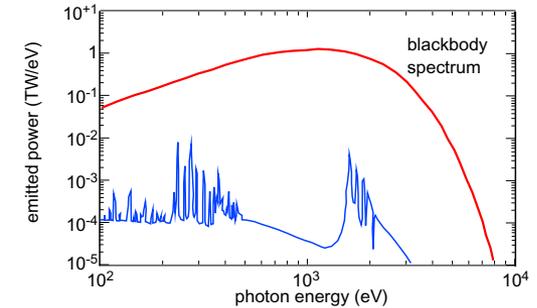
heat conduction = $\kappa \nabla T$ $\dots \dots \lambda_{e, mfp} > \frac{T}{\nabla T} \dots \dots$



$\mathcal{E}_{laser} = \nabla \phi > \frac{e}{a_B^2} \dots \dots$

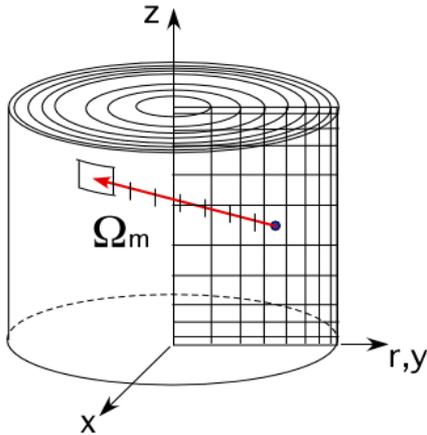
non-LTE

internal energy of a plasma
also depends on gradients
and thereby non-local

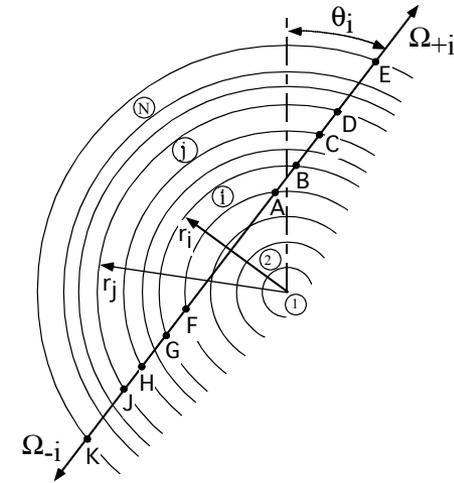
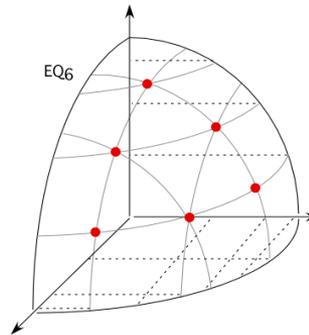


Non-local means spatial dependence, requiring some form of transport model

Raytracing



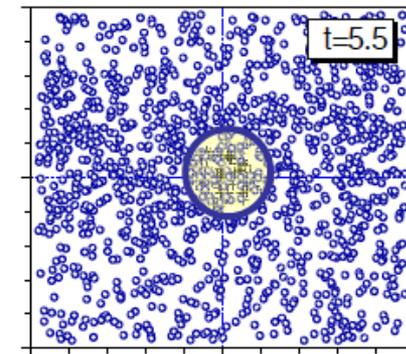
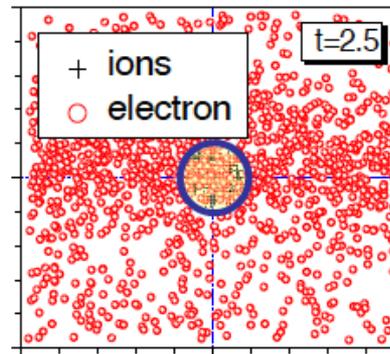
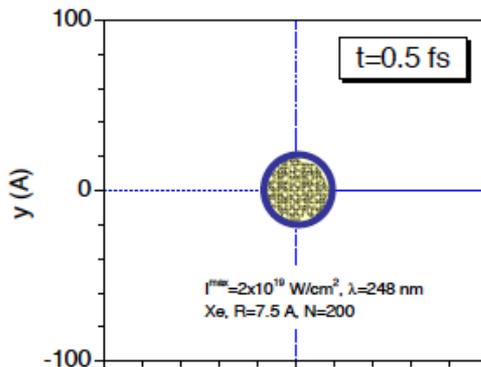
Discrete Ordinates



Vlasov model

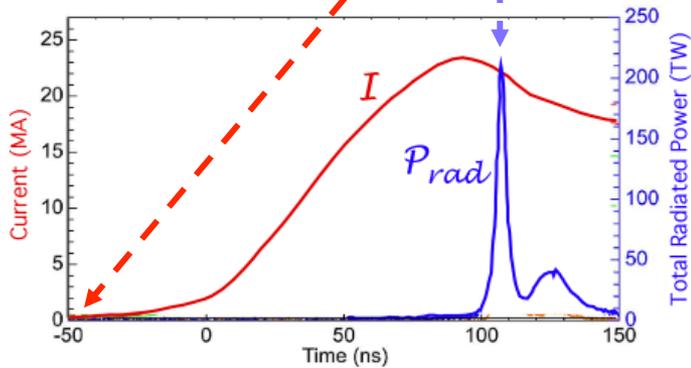
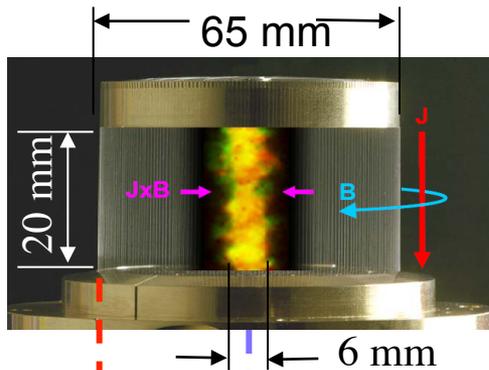
$$V \cdot \nabla f - \frac{eE}{m} \cdot \nabla_V f_m = -v_e(V)(f - f_m) + \frac{v_i(V)}{2} \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] f$$

Molecular Dynamics

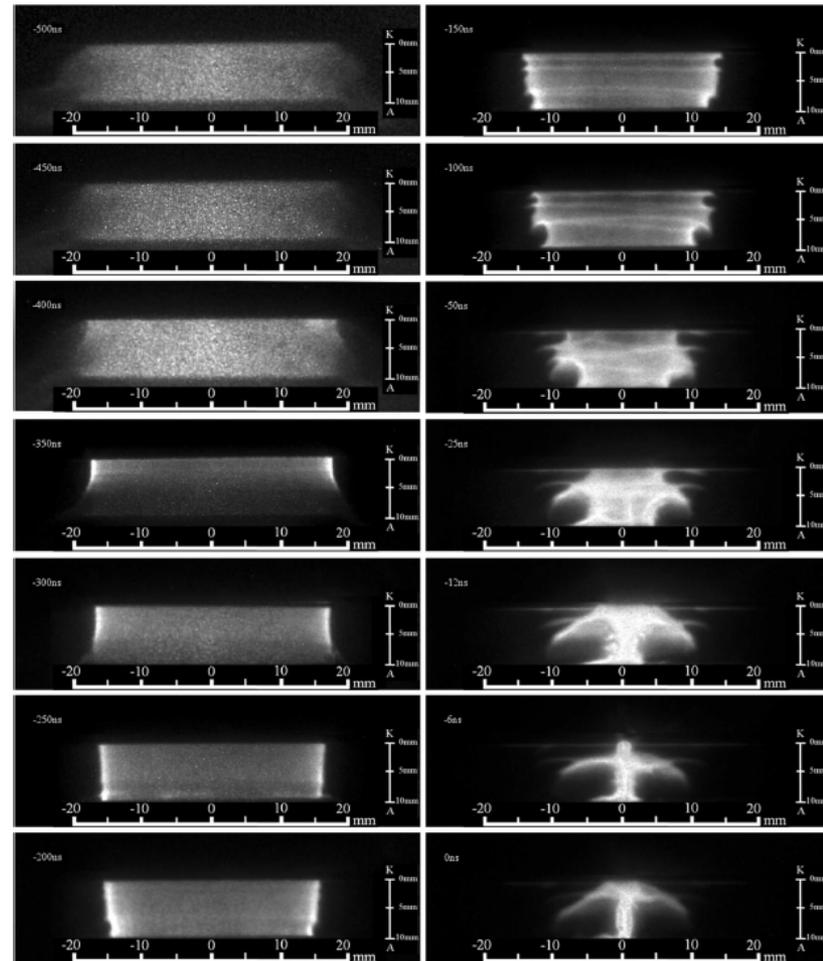


Z pinches: magnetically imploded plasma producing intense radiation

wire array

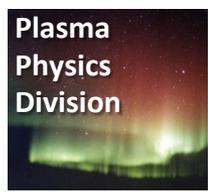


gas puff

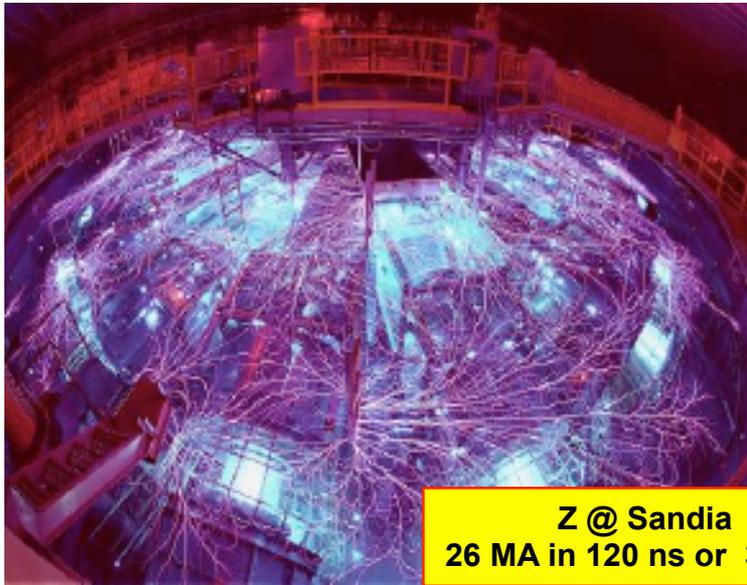




Z-pinch research in MHD and radiation production in is internationally active



34 m



Z @ Sandia
26 MA in 120 ns or 300 ns

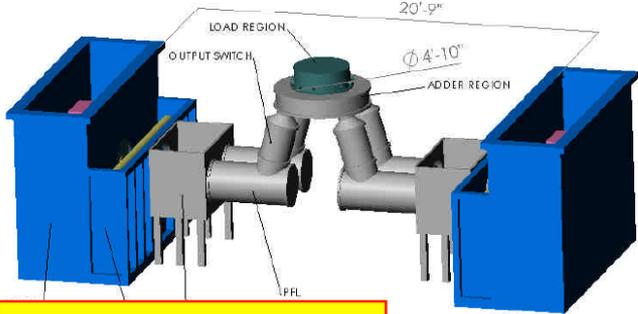
ZEBRA @ NTF, UNR
~1.6 MA in 80 ns



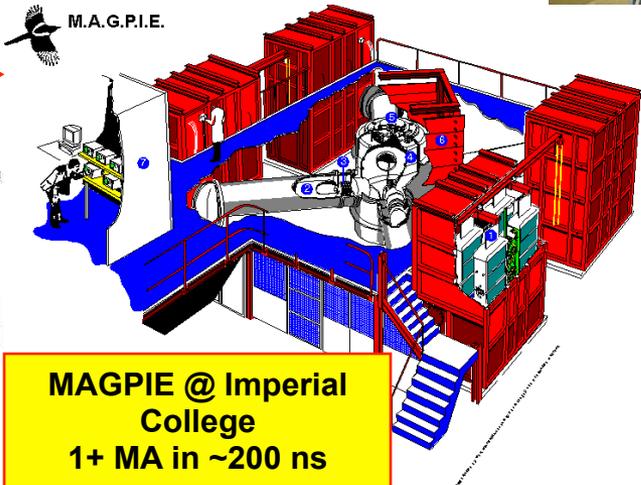
MAIZE @ U Michigan
1 MA LTD



7 m



COBRA @ Cornell
~1 MA in 100 or 200 ns



MAGPIE @ Imperial College
1+ MA in ~200 ns

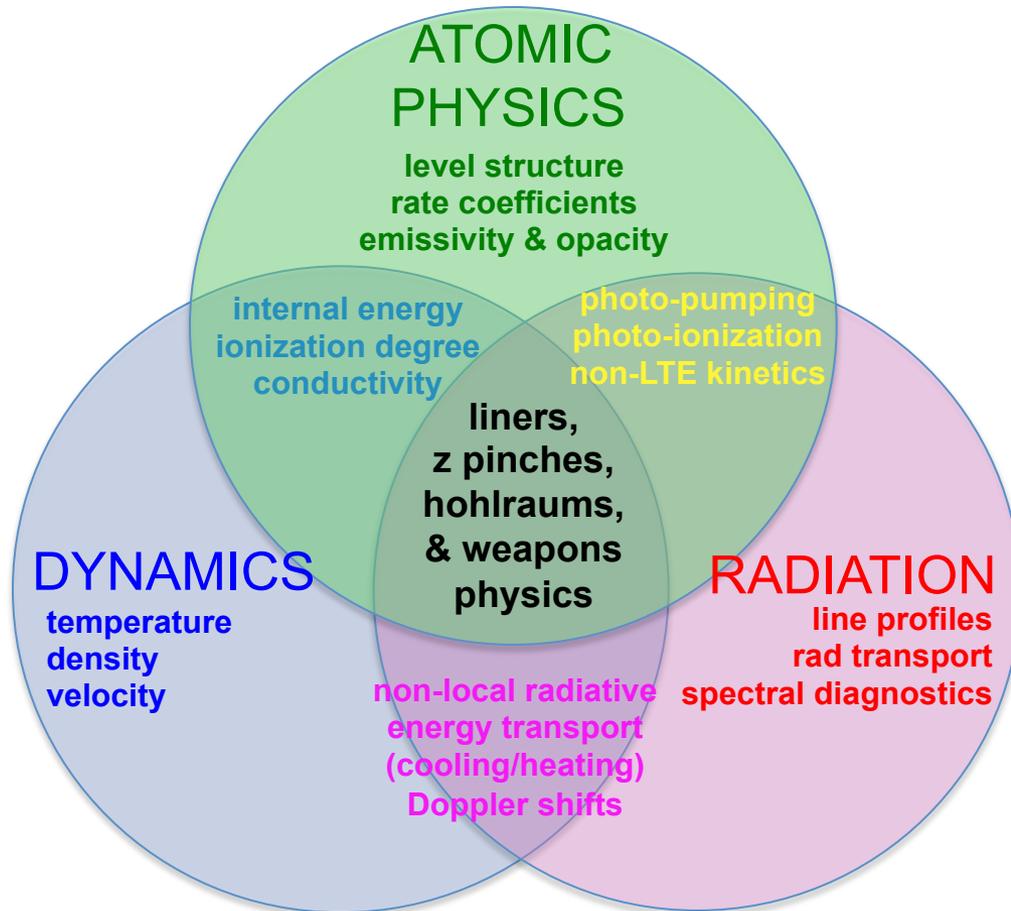
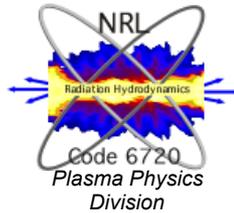
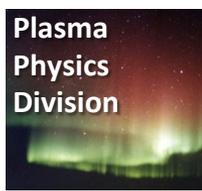
2 m



WIS @ Israel
~0.5 MA in 500 ns



Advanced simulations of Z-pinch loads require an integrated physics approach

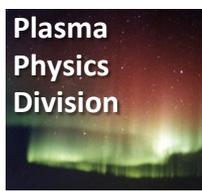


products:

- Verification tests for non-LTE radiation & MHD codes.
- Validation of simulations through yields & synthetic spectra.
- Interpretation of plasma conditions from spectral & imaging diagnostics.
- Predictions for next generation pulse power machines.



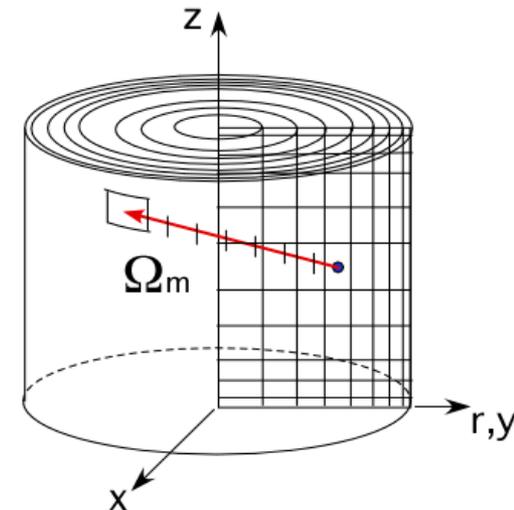
Non-LTE/non-local physics is important in radiation-dominated Z-pinch plasmas



Radiation transport: The collection of processes in which radiation is emitted within a medium, and is subsequently absorbed elsewhere within the medium, or else escapes without further interaction

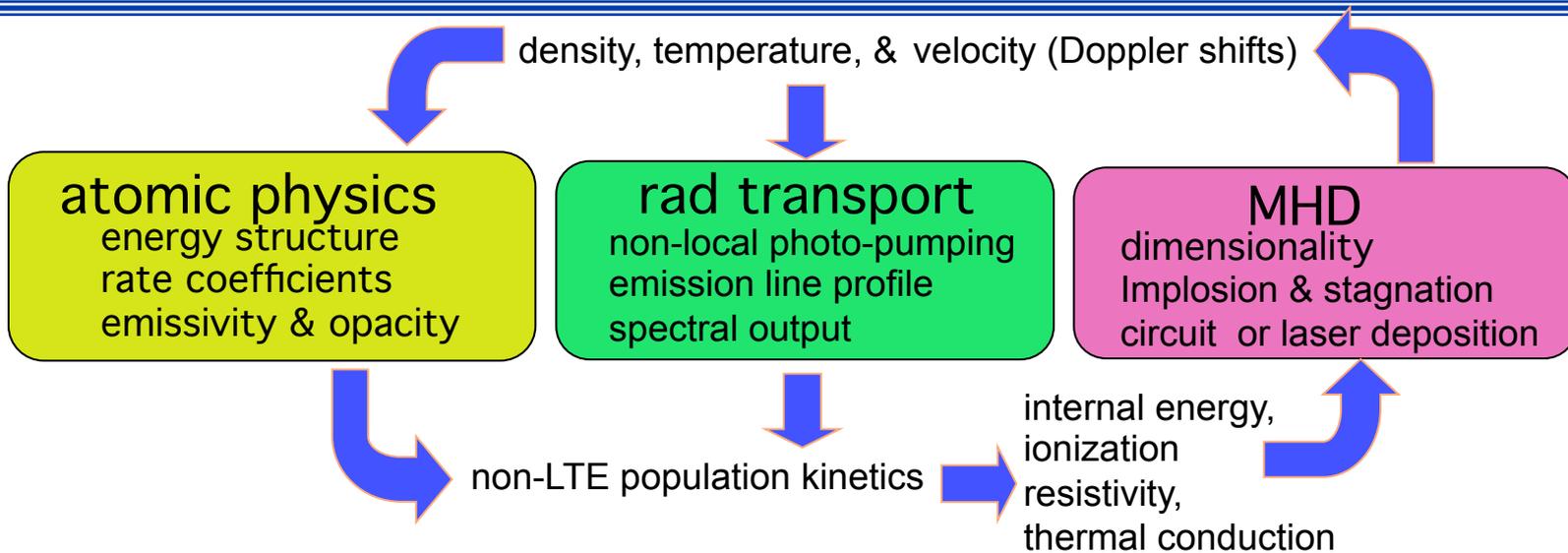
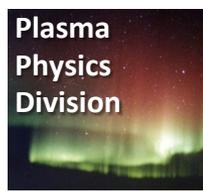
Effects:

- Emitted radiative power from an optically thick medium is reduced by reabsorption
- Energy is redistributed within the medium, resulting in localized heating or cooling
- Photoexcitation and/or photoionization results in enhancement of the medium's degree of excitation and ionization
- Boundary effects of the radiation field create gradients in ionization and excitation even if temperature and density are uniform
- Spectral line or continuum features of varying optical depth can provide valuable diagnostics of , e.g., temperatures, densities, and their gradients





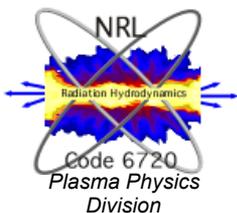
In non-LTE radiation couples non-locally to populations & energy, affecting MHD



Bound-bound emission $\epsilon_{b-b}(\omega) = \frac{h\nu}{4\pi} L(\omega) A_{UL}^{z,a} N_L^{z,a}$

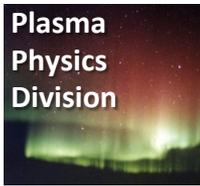
Bound-free emission $\epsilon_{f-b} \approx \text{const} \left(\frac{E_H}{kT} \right)^{3/2} g_{f-b} e^{-\frac{h\nu}{kT}} N_e \sum_{n,z,a} \frac{z^4}{n^3} e^{\frac{z^2 E_H}{n^2 kT}} N_a^z$

Free-free emission $\epsilon_{f-f}(\omega) \approx \text{const} \left(\frac{E_H}{kT} \right)^{1/2} g_{f-f} e^{-\frac{h\nu}{kT}} N_e \sum_{z,a} z^2 N_a^z$

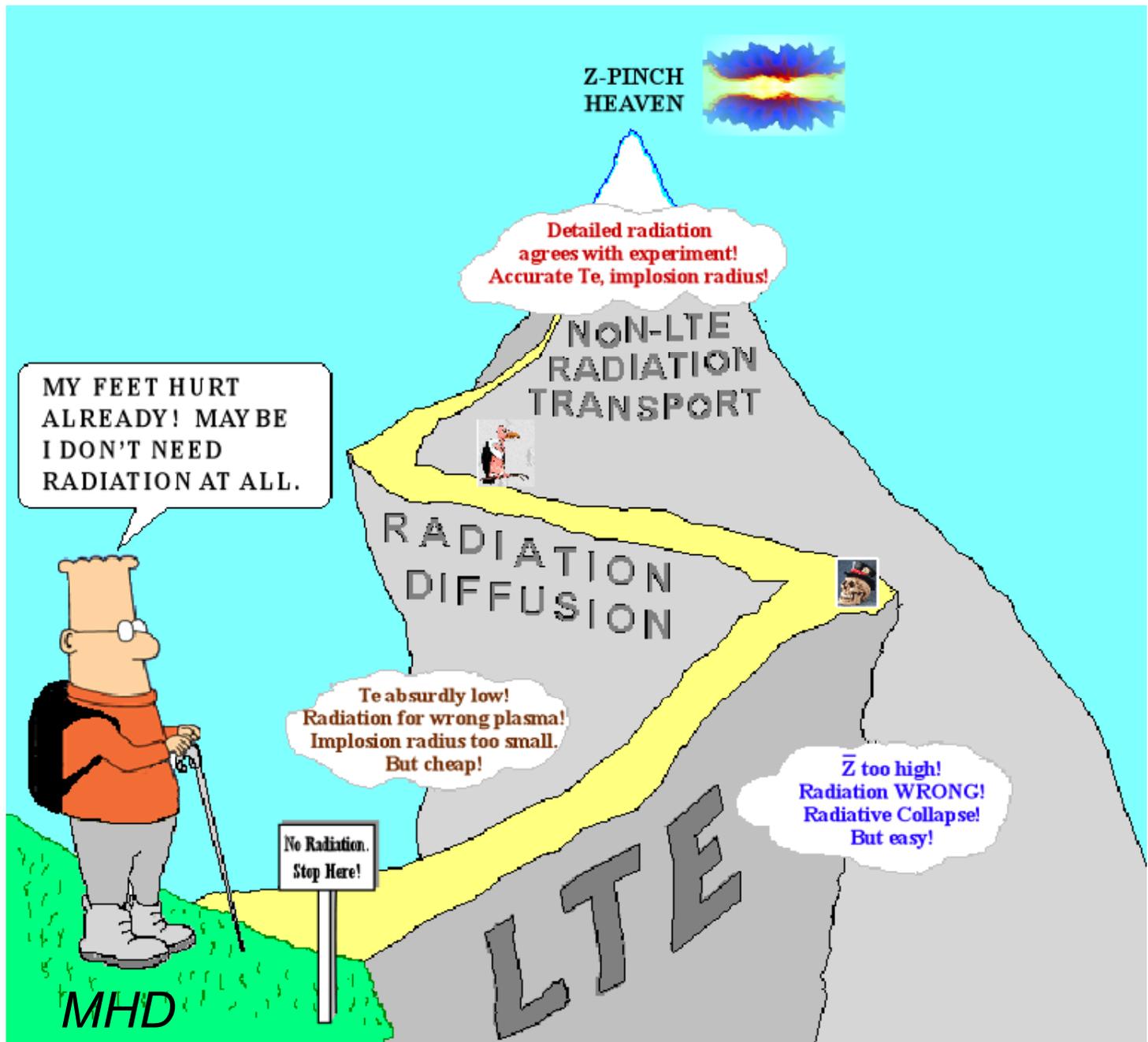




In LTE ion populations are independent of radiation, which is not necessarily Planckian,

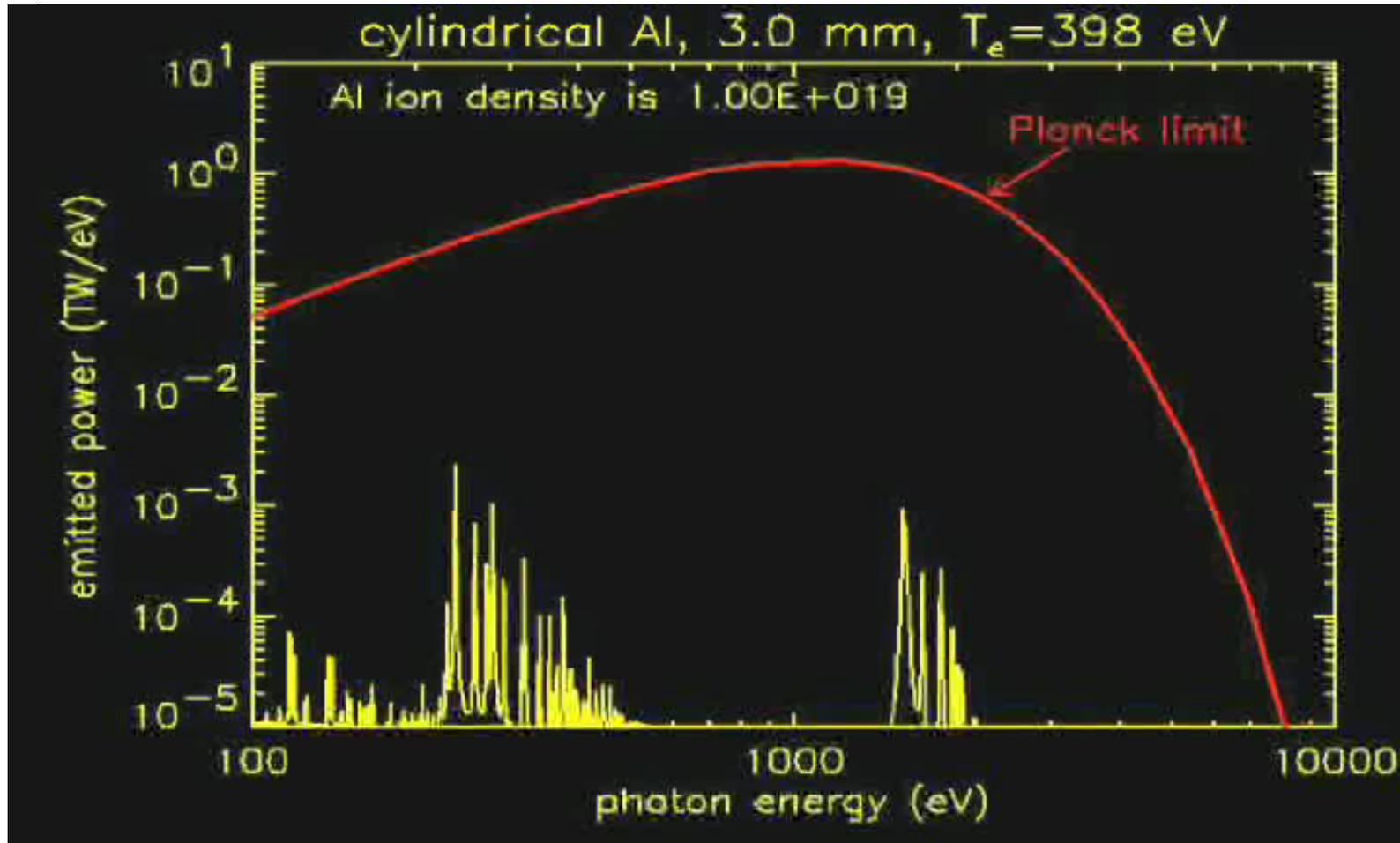
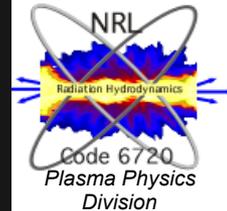
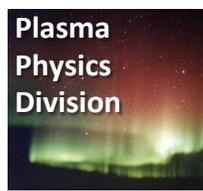


- Local Thermodynamic Equilibrium (LTE) means that the ionization state distribution and bound state populations are given by the Saha and Boltzmann equations, respectively, evaluated at the local temperature and density.
 - The particles which dominate the population kinetics must have a Maxwellian velocity distribution, *and*
 - The population kinetics must be dominated by collisional processes, or the medium must be effectively thick
- In HED plasmas radiation is an important energy term:
 - Simple emission model can be used if radiation is Planckian
 - *else* frequency-dependent emission model required (e.g. multi-group diffusion, S_n , or IMC)





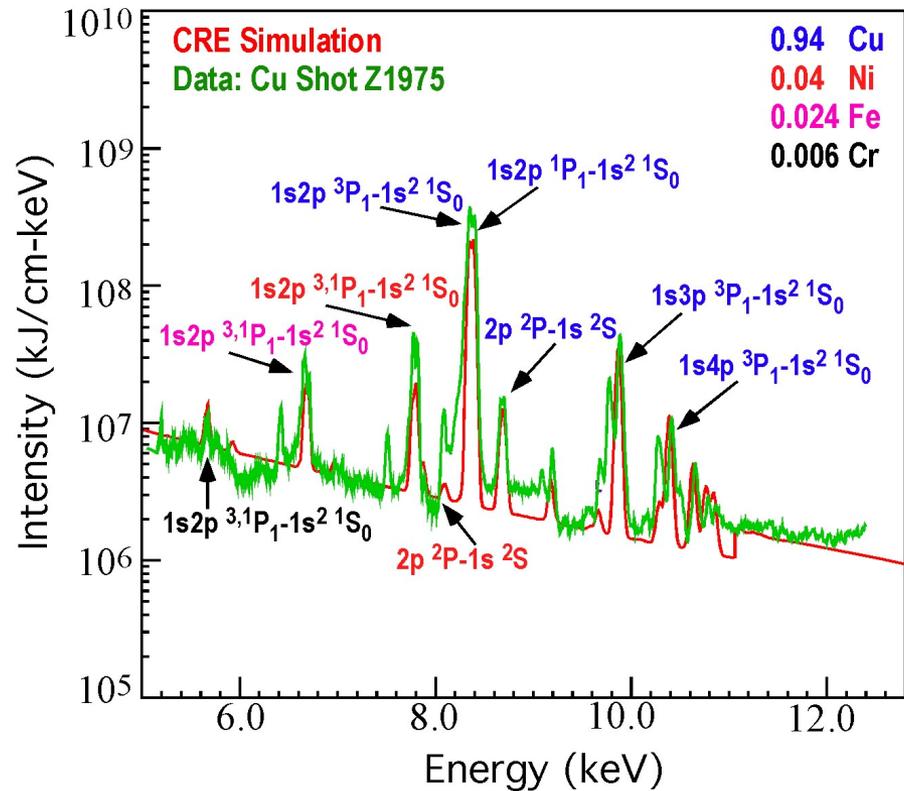
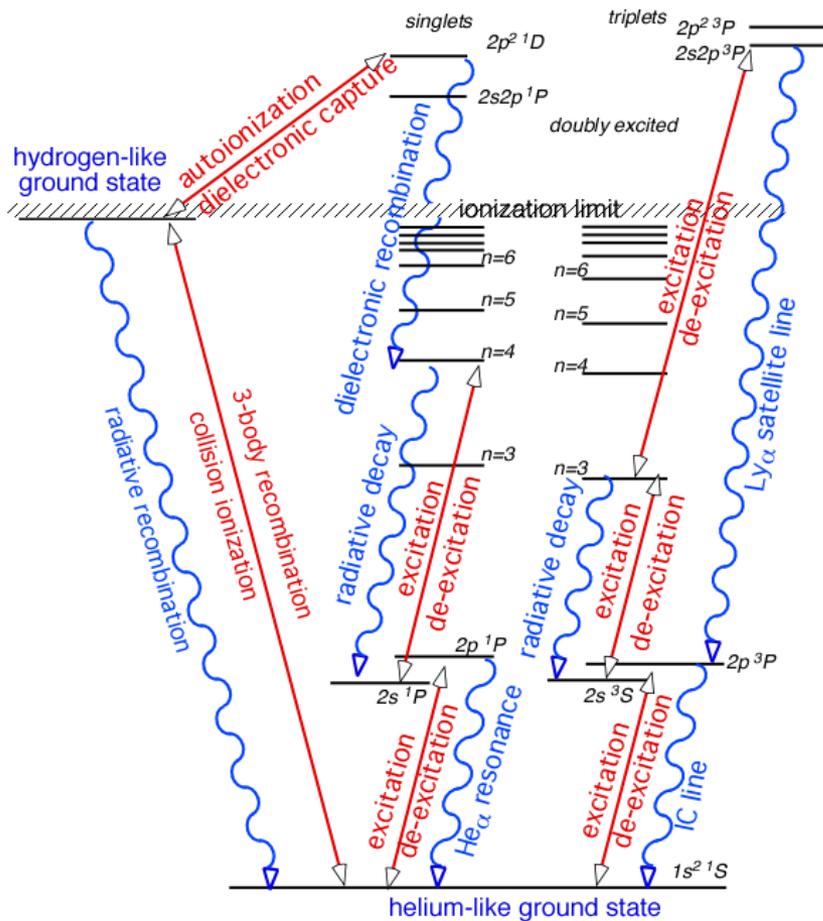
Animation to show the transition between an LTE & non-LTE plasma



For a plasma of fixed temperature and size the LTE radiation is given by the blackbody spectrum. For a non-LTE plasma the radiation increases with the density until collisions dominate the kinetics, eventually going to the LTE limit.

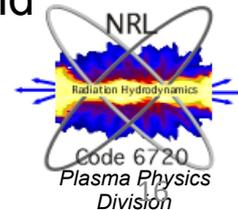


Detailed atomic structure + kinetic rates are fundamental data to non-LTE plasma models



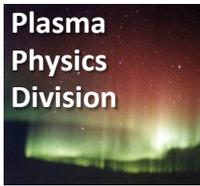
The simulated and experimental K-shell spectra reveal plasma conditions in the emitting region are $T_e \sim 3.5$ keV and $n_e \sim 3 \times 10^{22}$ cm⁻³.

Dasgupta, R. W. Clark, et al., *AIP* #1161, **207** (2009)
 Dasgupta, J. G. Giuliani, et al., *IEEE TPS*, **38**, 598 (2010)





Radiative transfer equation and its' formal solution



$$\frac{dI_\nu}{ds} = j_\nu - k_\nu I_\nu \left(-\frac{1}{c} \frac{\partial I_\nu}{\partial t} \right)$$

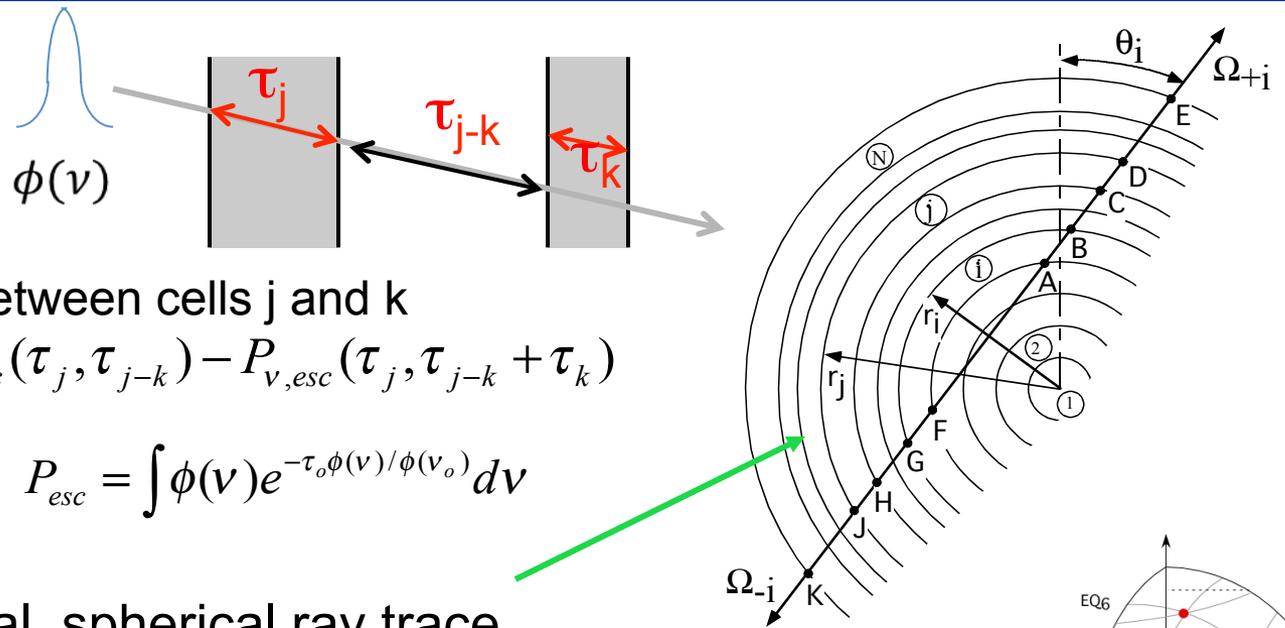
$$I_\nu(s_0) = I_\nu(0)e^{-\tau_\nu(0)} + \int_0^{s_0} j_\nu(s)e^{-\tau_\nu(s)} ds \quad \tau_\nu(s_0) = \int_s^{s_0} k_\nu(x) dx$$

emission coefficient, j_ν , is the radiative power emitted per unit volume, per unit frequency interval, per unit solid angle.

absorption coefficient, k_ν , is the product of the absorption cross section at frequency ν and the local density of absorbers

Optical depth τ_ν , is the line integral of the absorption coefficient along the path

Non-local radiation transport requires ray tracing between zones



multi-frequency:

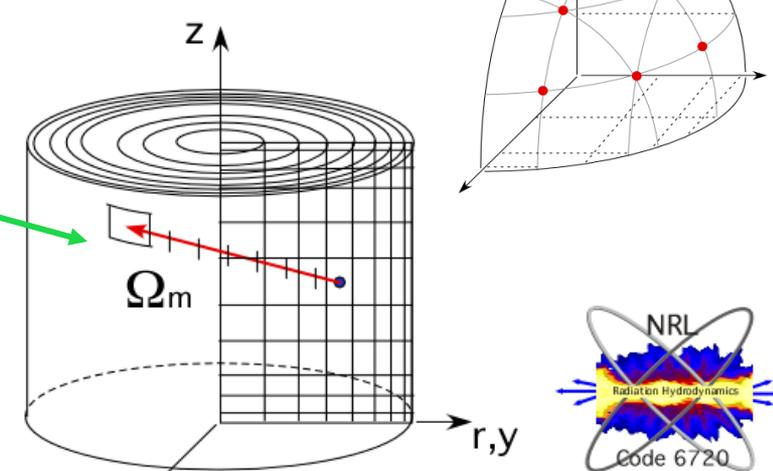
coupling coefficient between cells j and k

$$P_{v,esc}(\tau_j, \tau_{j-k}) - P_{v,esc}(\tau_j, \tau_{j-k} + \tau_k)$$

by frequency average $P_{esc} = \int \phi(v) e^{-\tau_o \phi(v)/\phi(v_o)} dv$

1D planar, cylindrical, spherical ray trace
by angle average with a unique ray per cell

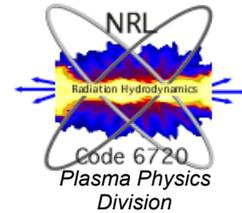
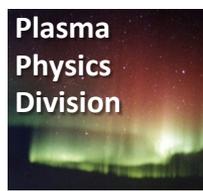
But higher dimensional problems,
even 2D R-Z, require transport in 3D.



Apruzese, *JQSRT*, **34**, 447 (1985)
Apruzese, Giuliani, *JSQRT*, **111**, 134 (2010)



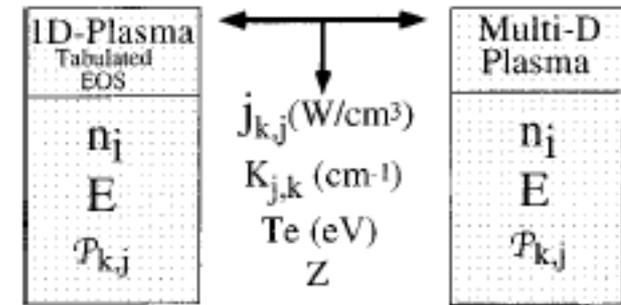
In multi-dimensional simulations advanced approaches to non-LTE are required



LTE tables the plasma ionization & radiation depend only on the local density and temperature.

In non-LTE the plasma ionization & radiation also depend upon the optical depth of each emission line and the photo-pumping from distant regions.

The Tabular Collisional-Radiative Equilibrium (TCRE) model incorporates these features using a three parameter look-up: density, internal energy (E), and probability-of-escape ($P_{k,j}$).



Properties determined from exact solutions of a uniform plasma.

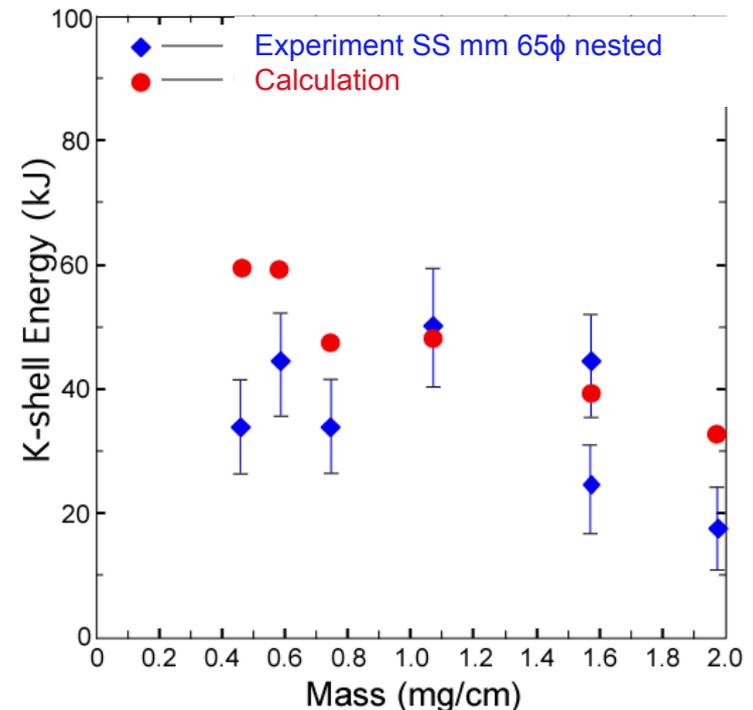
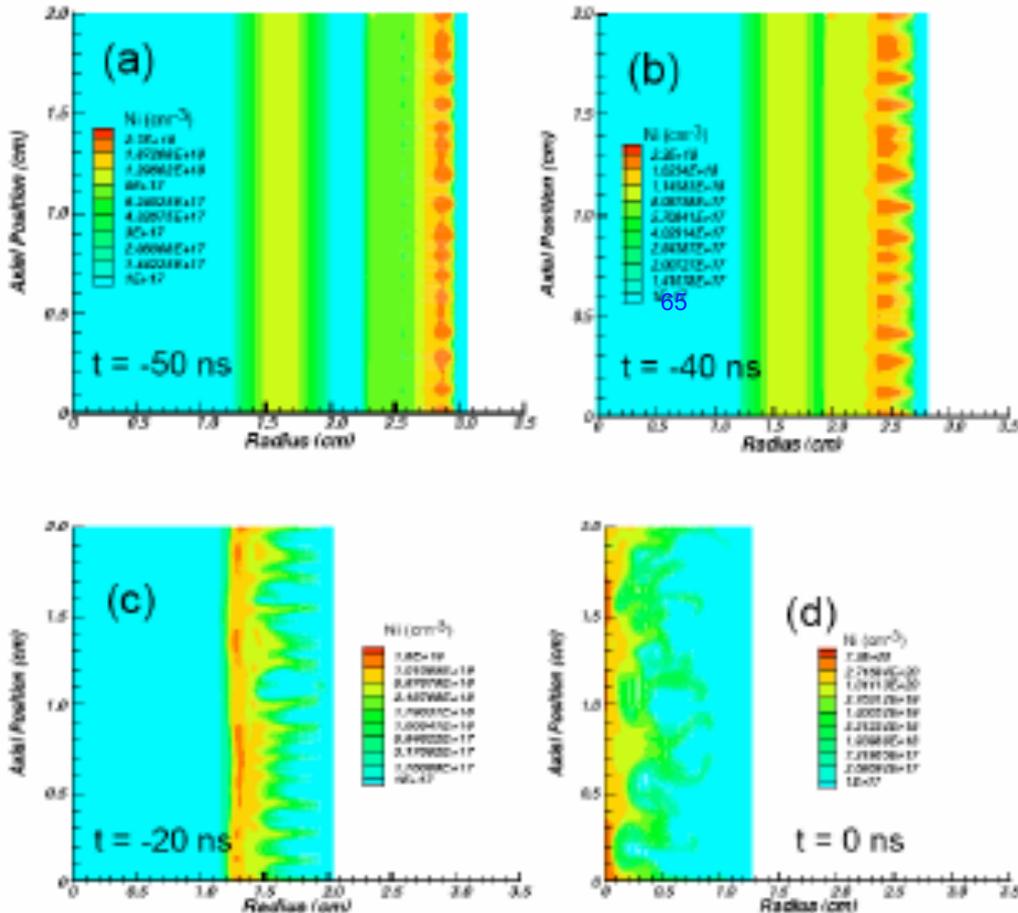
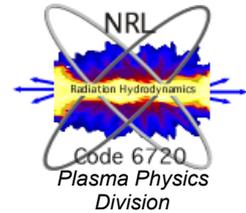
Thornhill, Apruzese, et al., *PoP*, 8, 3480 (2001)



Combine resistive MHD (MACH2) in R-Z with TCRE to match SS K-shell yields



Nested double SS wire array load ($M_{tot} = 2.5$ mg, $R = 55$ mm) on refurbished Z (Z1860/61)

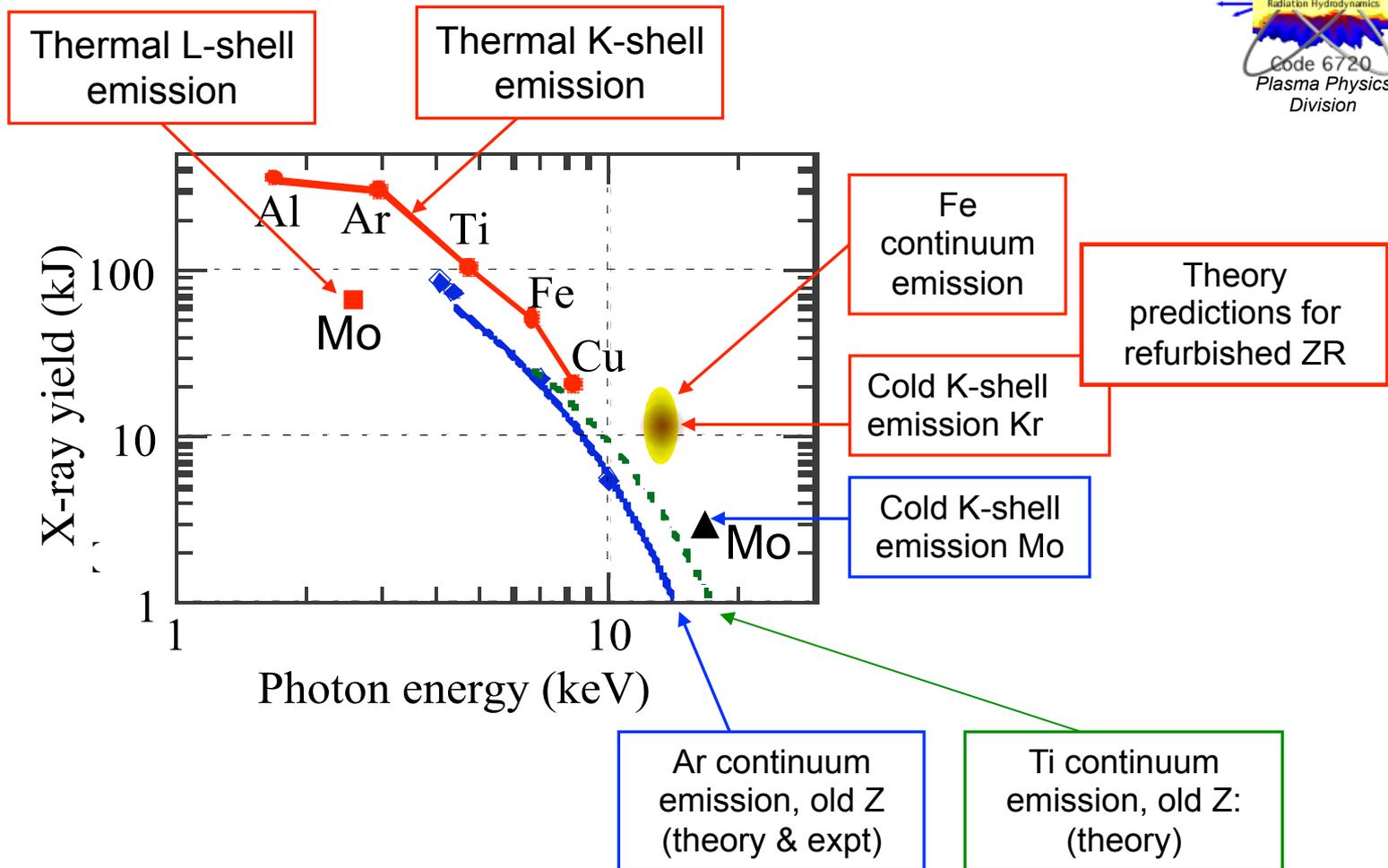
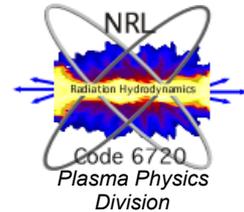


Thornhill, Giuliani, et al., *IEEE TPS*, **38**, 606 (2010)

Thornhill, Chong, et al., *PoP*, **14**, 063301 (2007)

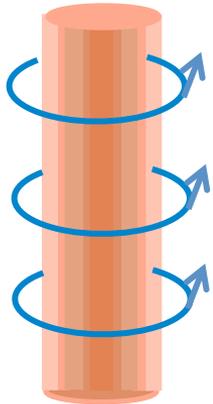


Advanced simulations also applied in a predictive mode seeking photons >10 keV



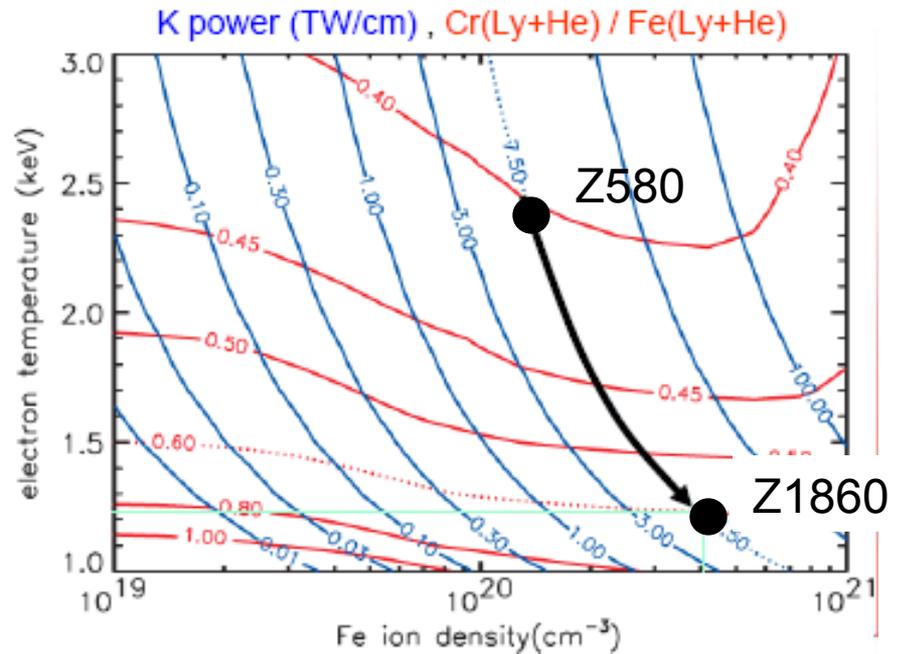
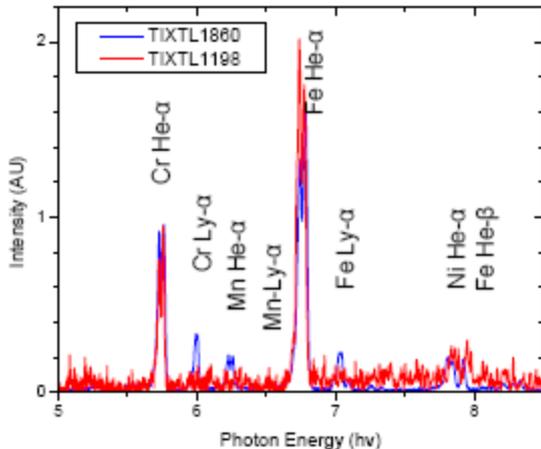
Velikovich, Apruzese, Davis, et al., *IEEE TPS*, **38**, 618 (2010).

Matching synthetic spectra to observed K-shell data provide averaged plasma conditions



Calculate synthetic spectra from a static cylindrical plasma. Use absolute power and line ratios to form a diagnostic plane.

calc powers and ratios from experimental spectra SS

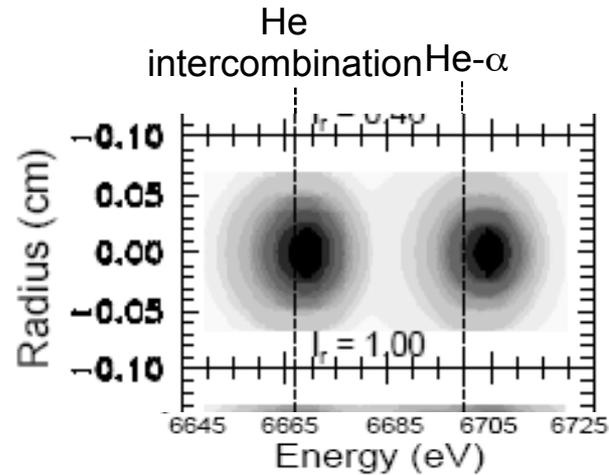
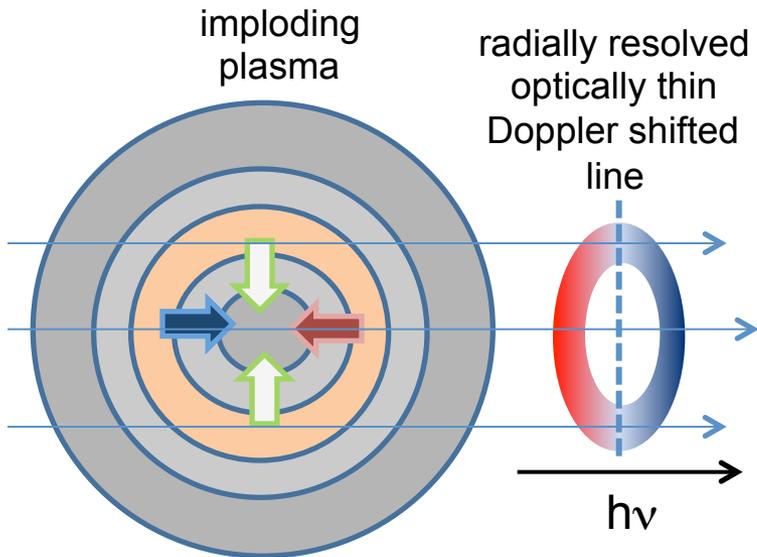


	Z580	Z1860
Pinch size	~1.2mm	0.9mm
Cr/Fe	~0.4	0.6
K-shell P	7.5TW/cm	7.5TW/cm
N_i (cm ⁻³)	1.2×10^{20}	4×10^{20}
T_e (keV)	2.6	1.25

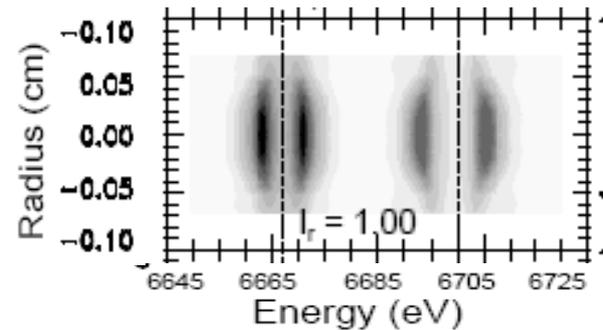
Deeney, Apruzese, Coverdale, et al., *PRL*, **93**, 155001 (2004).



Line opacity and Doppler shifts due to motion interact to give spectral features



Opacity interplays with Doppler shift to offset the lines.

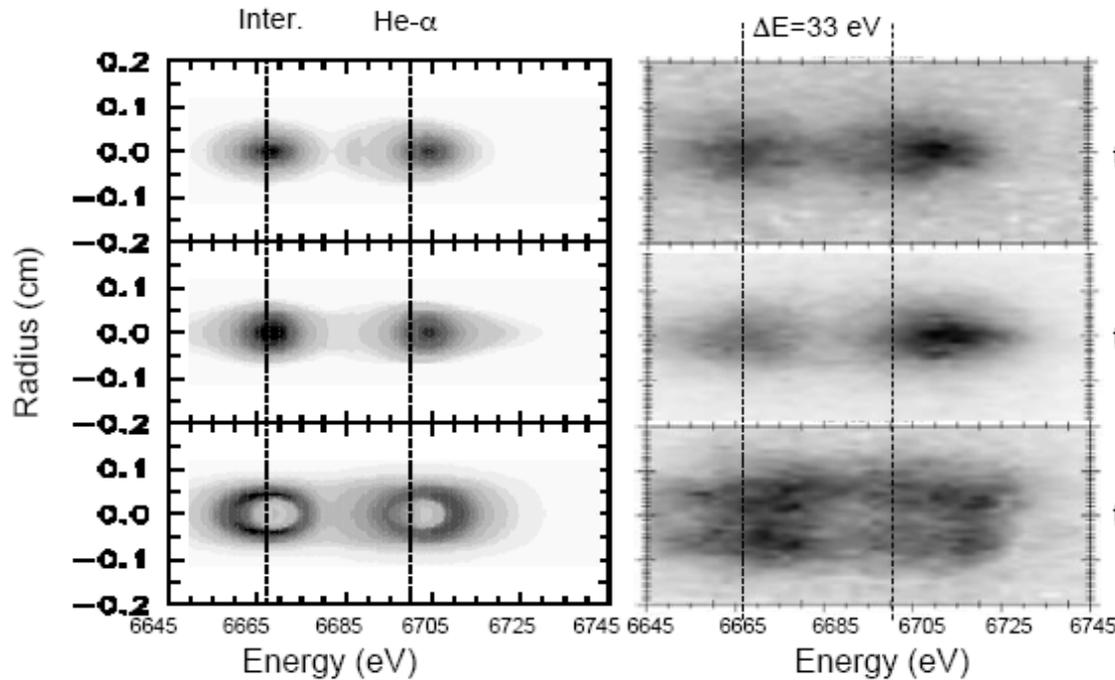


“self-reversal” at line center due to absorption

Comparison of radial and temporal resolved synthetic spectra with data

synthetic from TCRE-MACH2 simulation with Doppler

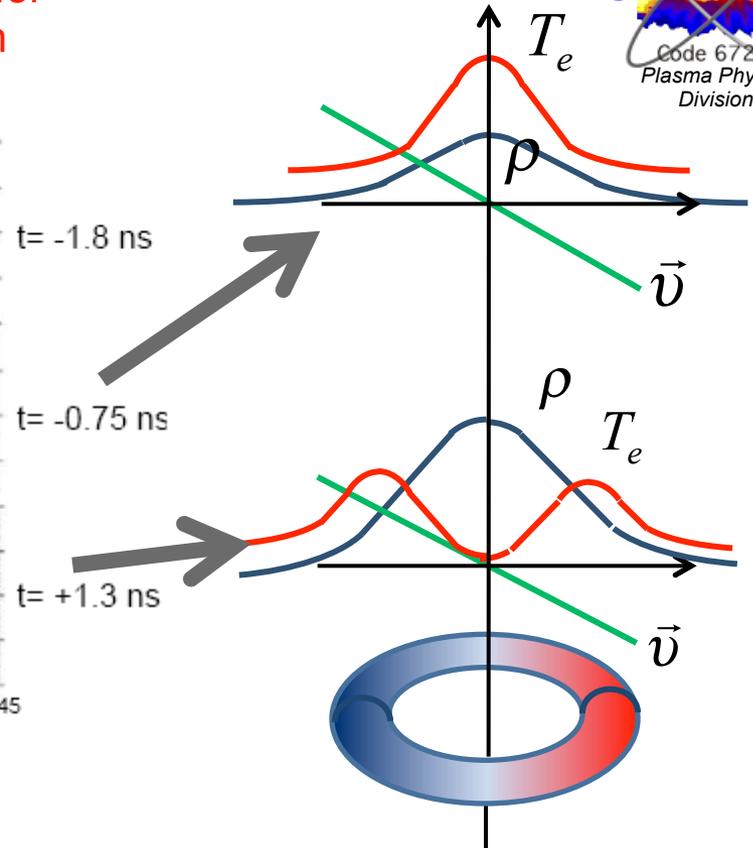
observed Fe spectra for Z1861 at stagnation



$t=0$ corresponds to the peak K-shell power.



(Absolute energy dispersion on spectra to be finalized by B. Jones)



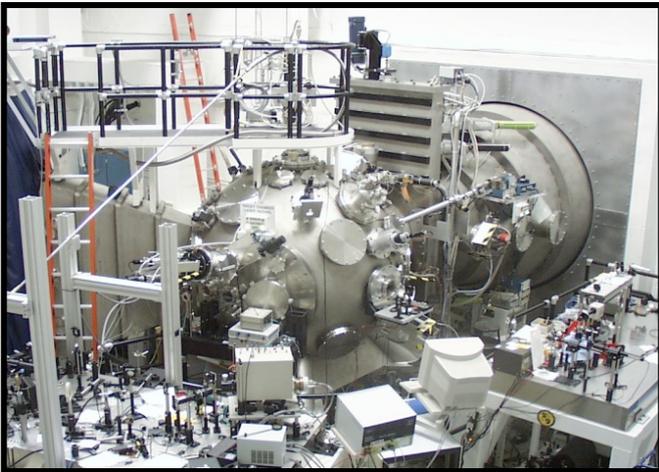
rapid radiative cooling in center produces a torus of He-like plasma



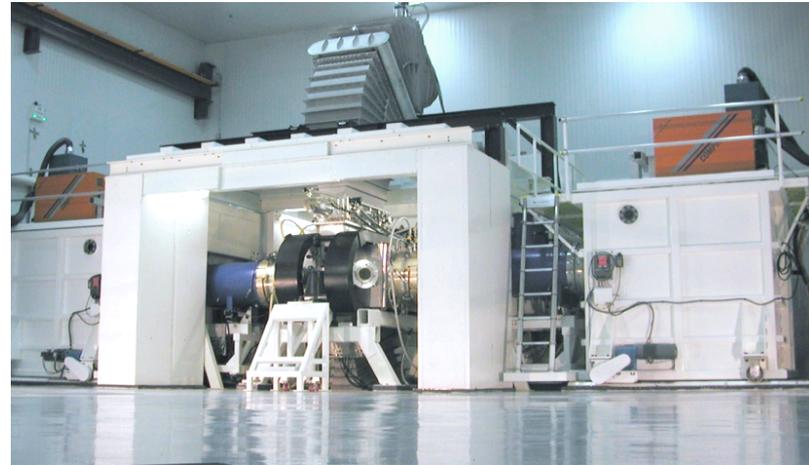
NRL is the world leader in direct drive inertial confinement fusion with KrF lasers



Nike Laser Target Chamber

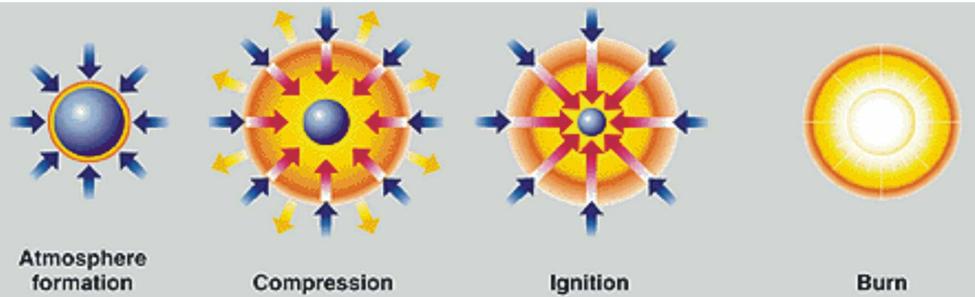


Electra 5 Hz electron-beam-pumped KrF laser

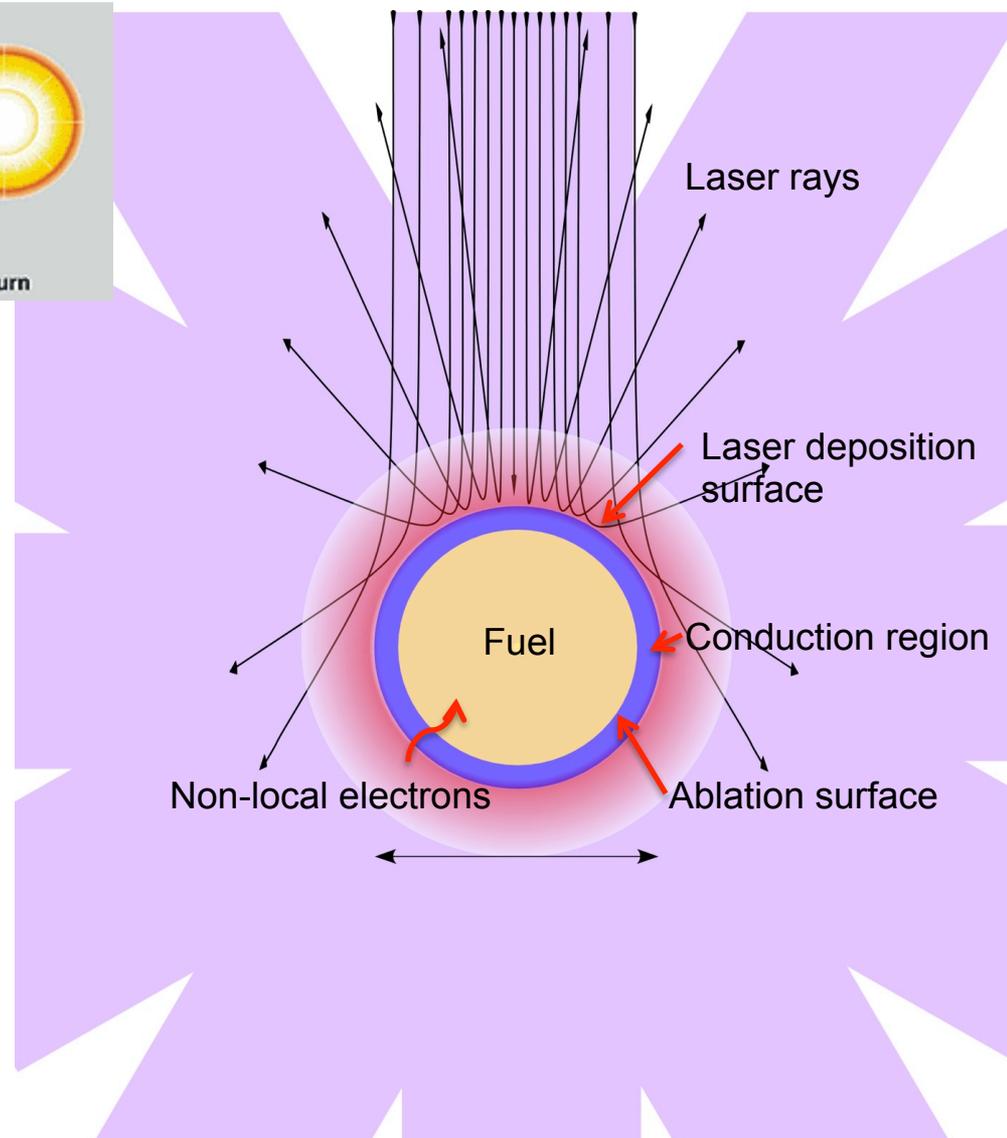


- **Laser facilities**
 - NIKE: 3 kJ KrF laser (0.25 μm , 4 ns) **S. Obenschain**
 - Electra KrF laser development facility (700 J, 5 Hz) **J. Sethian**
- **Research activities:**
 - ICF Target physics – Laser plasma interactions, RT instabilities, shock ignition
 - Laser Science – High power KrF, repetitive KrF and solid-state pulsed power
- **Vision:**
 - Contribute to future US Inertial Fusion Energy program

Non-local electron transport is important for direct-drive ICF targets

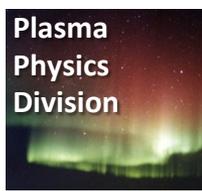


- Laser energy deposited at critical surface (Inverse Bremsstrahlung)
- Electron thermal conduction transports energy to ablation surface
- Normal diffusion ($q = -\kappa \nabla T$) invalid when thermal gradients between hot corona and cold fuel become too large
- Insufficient electrons to carry heat flux – transport becomes “flux limited”
- Generation of high-energy electrons with low collisionality can lead to energy deposition into fuel (preheat) – “non-local transport”

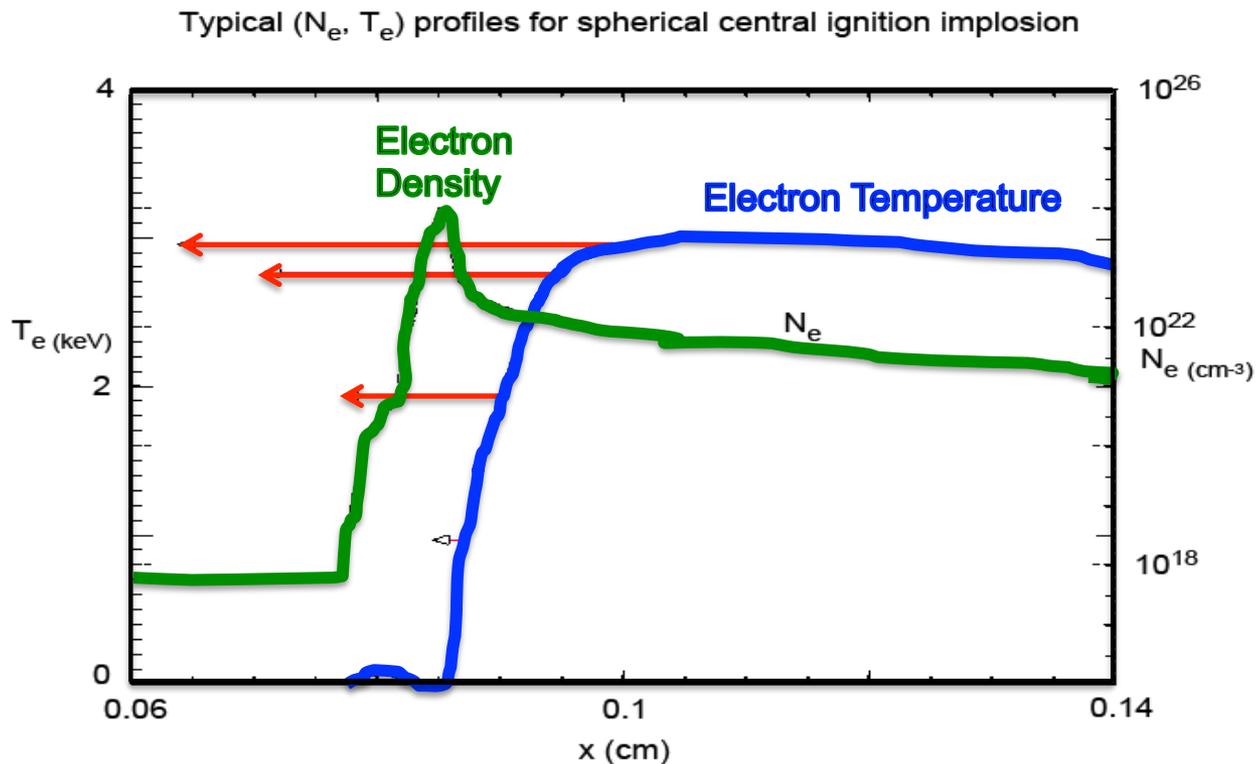




Question: Why is there a problem with classical transport?



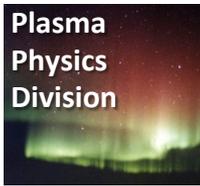
Answer: Because classical transport assumes mean free path of energy carrying electrons is small compared to gradient scale length.



Red arrows are electron mean free path for energy = $10T_e$



Why do we care about electron transport in ICF?



Direct Drive:

- Shock timing depends on electron transport
- Preheat from hot electrons increases adiabat & decreases compression (stabilizes RT?)

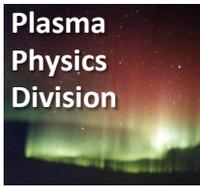
Indirect Drive:

- High flux model with $f=0.15$ gives cooler plasma in NIF hohlraum – changes laser-plasma growth rates
- “Hohlraum energy balance, as measured by x-ray power escaping the LEH, is quantitatively consistent with revised estimates of backscatter and incident laser energy combined with a more rigorous non-local-thermodynamic-equilibrium atomic physics model with greater emissivity than the simpler average-atom model used in the original design of NIF targets”*

*Town, R. P. J., M. D. Rosen, et al. (2011). "Analysis of the National Ignition Facility ignition hohlraum energetics experiments." Physics of Plasmas **18**(5): 056302-056308.



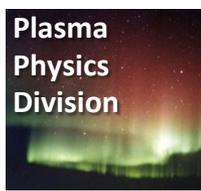
Many hydrocode models use a flux limiter on electron thermal conduction



- Don't expect the flux to be greater than nmv_e^3 , so many codes have a model to limit it to $q < fnmv_e^3$
- $f_e = \min(k_e dT/dx; f_L nvT)$ or smoother harmonic mean
- A properly chosen flux limit in a fluid simulation can almost always reproduce a single experimental result.



High Flux Model (HFM) gives better agreement with NIC hohlraum data

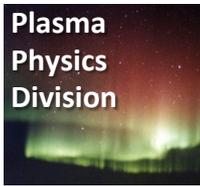


- “The HFM contains two principal changes from the standard model:
 - 1) It uses a detailed configuration accounting (DCA) atomic physics non-local-thermodynamic-equilibrium (NLTE) model, and
 - 2) It uses a generous electron thermal flux limiter, $f = 0.15$, that is consistent with a non-local electron transport model.
- Both elements make important contributions to the HFM’s prediction of a hohlraum plasma that is cooler than that predicted by the standard model, which uses an NLTE average atom approach, and a value of $f = 0.05$ for the flux limiter. This cooler plasma is key in eliminating most of the discrepancies between the NIC data and revised expectations based on this new simulation model.”

Rosen, M. D., H. A. Scott, et al. (2011). "The role of a detailed configuration accounting (DCA) atomic physics package in explaining the energy balance in ignition-scale hohlraums." High Energy Density Physics 7(3): 180-190.



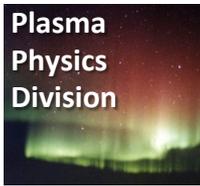
But there are many problems with a using a simple flux limiter



- $mfp > \text{scale length}$, so energy advances ahead of front:
 - $q < f n m v_e^3$ means $T > [q/f]^{2/3} m^{1/3}$
- Too low a flux limit gives too high a temperature (e.g. NIF hohlraum & impact on SRS threshold)
- It certainly cannot predict preheat, as this is absent from a flux limit formulation.
- Can one pick a flux limit to agree with more than one measurement?
- How do you pick f anyway?



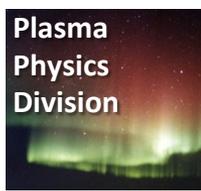
Beyond diffusion – the NRL velocity-dependent Krook (VDK) model



- Collision term in Vlasov Equation:

$$V \cdot \nabla f - \frac{eE}{m} \cdot \nabla_V f_m = -\nu_e(V)(f - f_m) + \frac{\nu_i(V)}{2} \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] f$$

Can solve analytically for q , it describes BOTH flux limitation and preheat.



VDK Solution for energy flux

Classical like flux but with reduced coefficient (flux limitation)

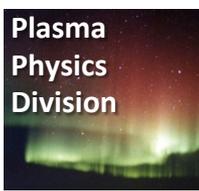
$$q = - \int_0^{\Xi_{cr}} d\Xi \alpha(\Xi) \frac{\partial T}{\partial x} \left(\equiv K \frac{\partial T}{\partial x}, K < K_{sp} \right) - \underbrace{\int_{-\infty}^{\infty} dx' \int_{\Xi_{cr}}^{\infty} d\Xi \frac{\alpha(x', \Xi)}{2\lambda(x', \Xi)} \frac{\partial T}{\partial x'} \exp - \left| \int_{x'}^x \frac{dx''}{\lambda(x'', \Xi)} \right|}_{\text{nonlocal effect (preheat)}}$$

(Ξ is a particle energy)

Flux limitation and preheat are two sides of the same coin.



1-D VDK results in good agreement with Fokker-Planck, flux limiter under predicts T_e @ front



FP: Matte, Ref 10

$$L / \lambda = 20, T_1 / T_2 = 4$$

$$t = 240 \tau$$

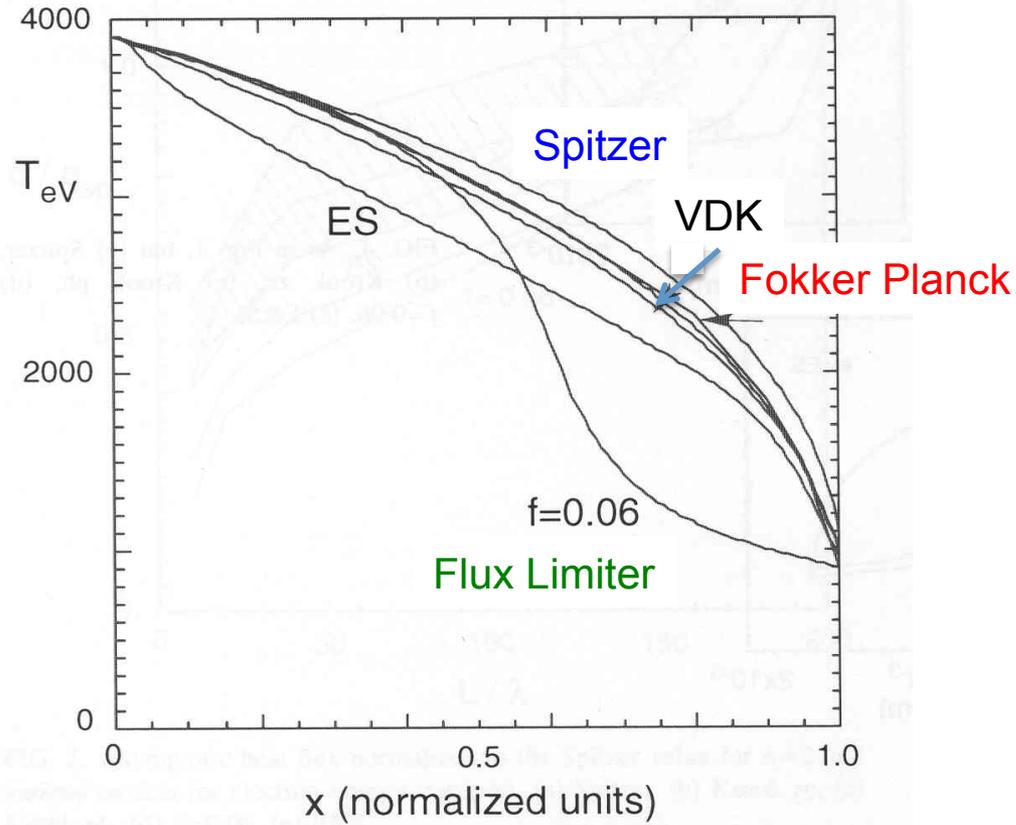
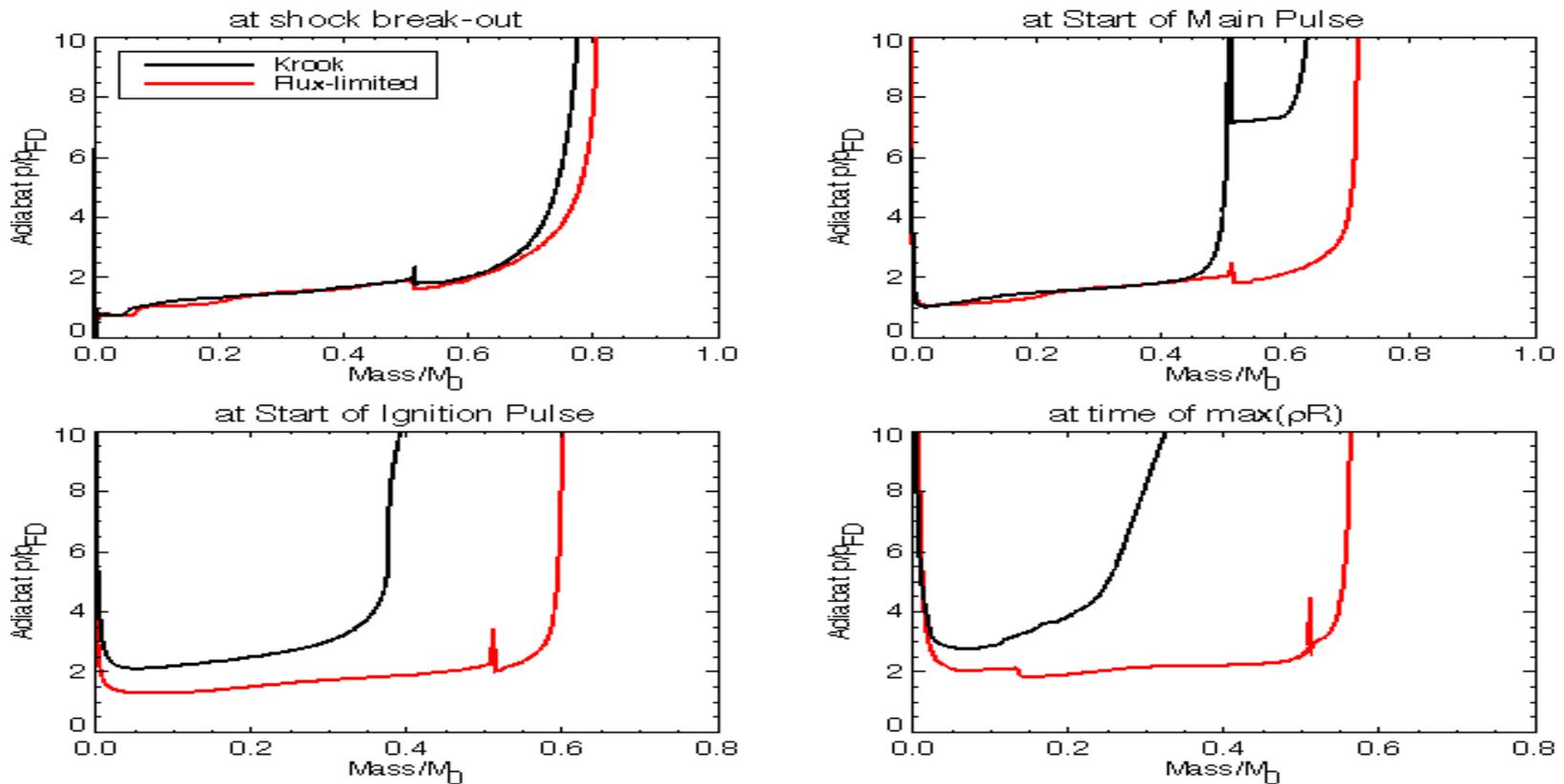
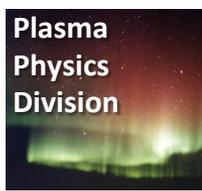


FIG. 6. As in Fig. 5(a), but at $t=240\tau$.



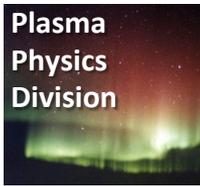
Application of Krook model to KrF shock ignition target implosion



- Comparison of shock ignition target calculations for VDK and $f=0.075$.
- Absorption increased from 85% to 90%, but gain drops from 140 to 100 due to preheat. (Ref 6)
- Increased alpha might in outer part of fuel might give rise to further RT stability.



Applying the Krook theory in two-dimensions is more challenging



Approach presently implemented and in testing:

- Assume single collision frequency and solve first order equation. Solution same in 1-, 2-, or 3-D, but have to sum over angles to get q .
- Let 1-D Legendre solution guide how to select collision frequency.
- If there is a dominant direction (i.e. r for spherical, z for foil acceleration), the result reduces to decoupled non-local diffusion in each direction.
- The result can be implemented densely (i.e. at every point in each direction) or sparsely, (i.e. at a subset of point with interpolation).

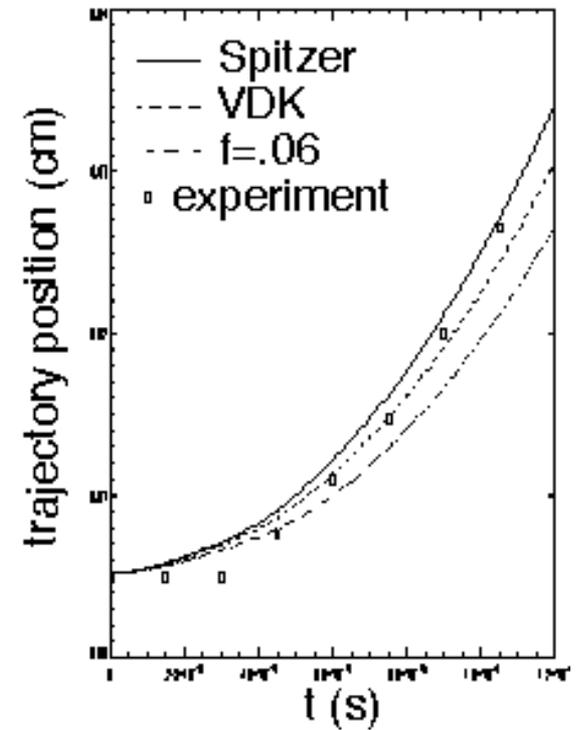
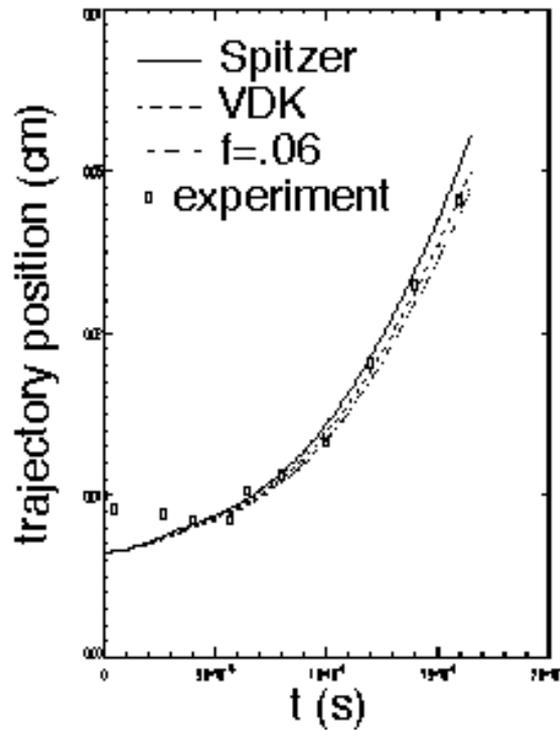
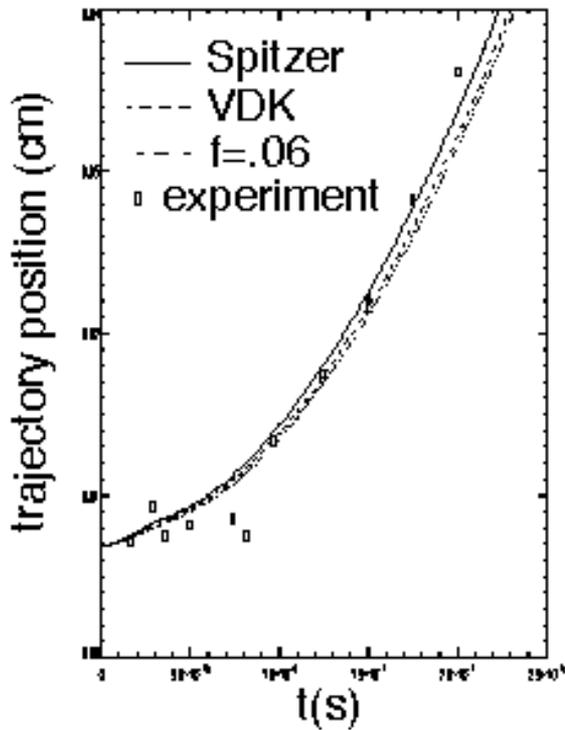
Note: Fokker Planck not numerically tractable – 1) too many orders of magnitude to resolve, 2) only valid for large Λ , but Λ is small in many regions of a laser plasma

Comparison of 2-D theory and experiment at the three irradiances on Omega @UR-LLE

$2 \cdot 10^{14} \text{ W/cm}^2$

$6 \cdot 10^{14} \text{ W/cm}^2$

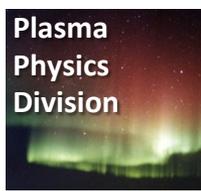
$9 \cdot 10^{14} \text{ W/cm}^2$



Impact of non-local transport greater with increasing laser irradiance



Velocity Dependent Krook best compromise between physics and numerical practicality



- Treats both flux limitation and preheat.
- Has proper treatment of both high and low velocity electrons.
- Shows a significant effect on laser pellet design, but certainly is not a show stopper.
 - So far we found redesigned pellet has reduced gain, but not by much ($\sim 10-25\%$).
- There may also be stabilizing effect on RT which we are examining now.



References

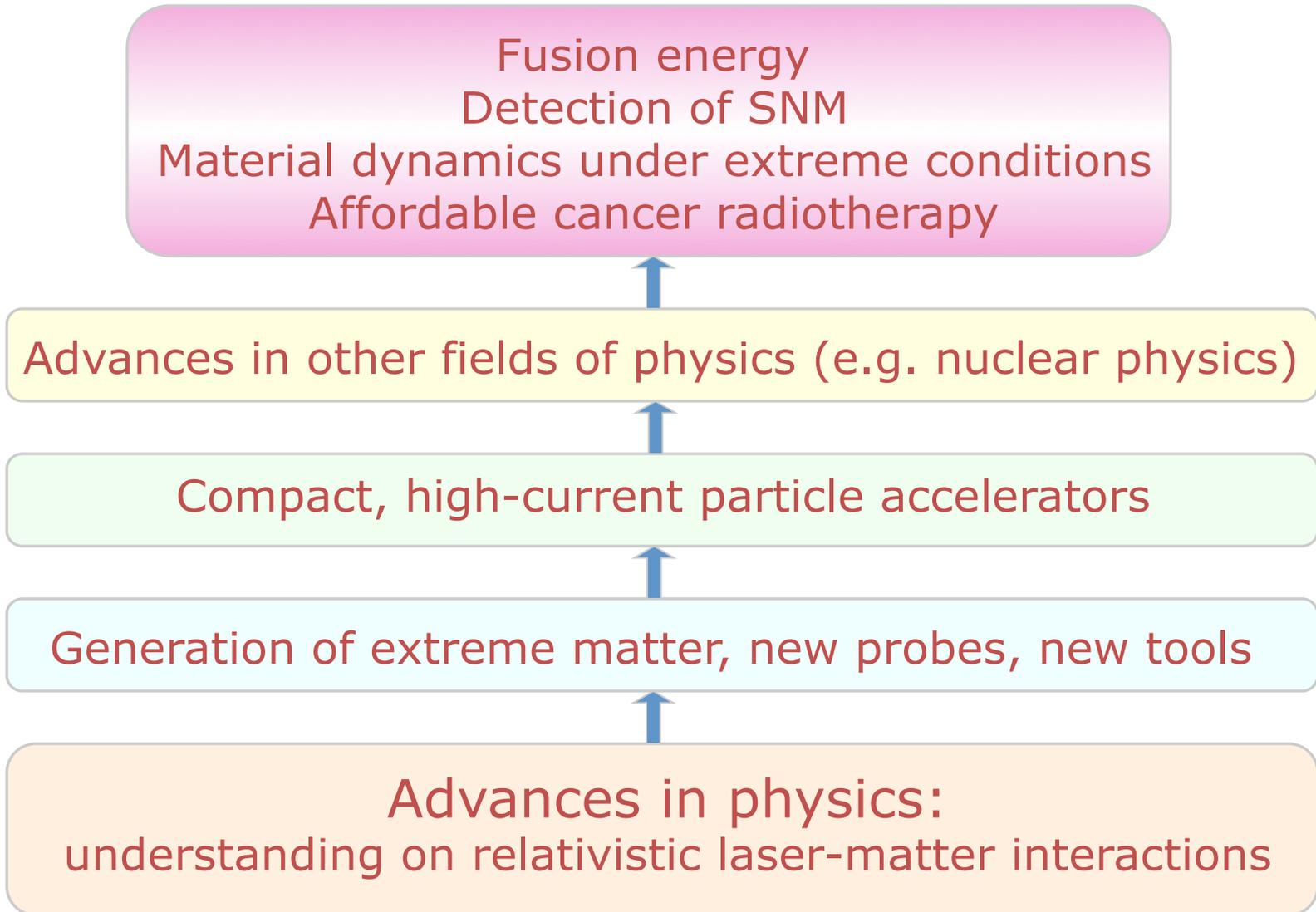
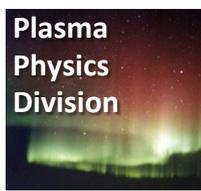
1. W. Manheimer, D. Colombant and V. Goncharov, Phys. Plasmas, **15**, 083103, 2008
2. D. Colombant and W. Manheimer, Phys. Plasmas, **15**, 083104, 2008
3. D. Colombant and W. Manheimer, Phys. Plasmas, **16**, 0627051, 2009
4. D. Colombant and W. Manheimer, J. Comp. Phys 229, 4369, (2010)
5. D. Colombant and W. Manheimer, Phys Plasmas, 17, 112706, (2010)
6. W. Manheimer, D. Colombant, and A Schmitt, submitted to Phys. Plasmas
7. V. Goncharov, et al, Phys. Plasmas, **13**, 012702, 2006
8. V. Goncharov, et al, Phys. Plasmas, **15**, 056310, 2008
9. G. Schurtz, P. Nicolai, and M. Busquet, Phys. Plasmas 7, 4238, 2000
10. J. Matte and J. Virmont, Phys Rev Let 49, 1936 (1982)

Reference on Fokker Planck:

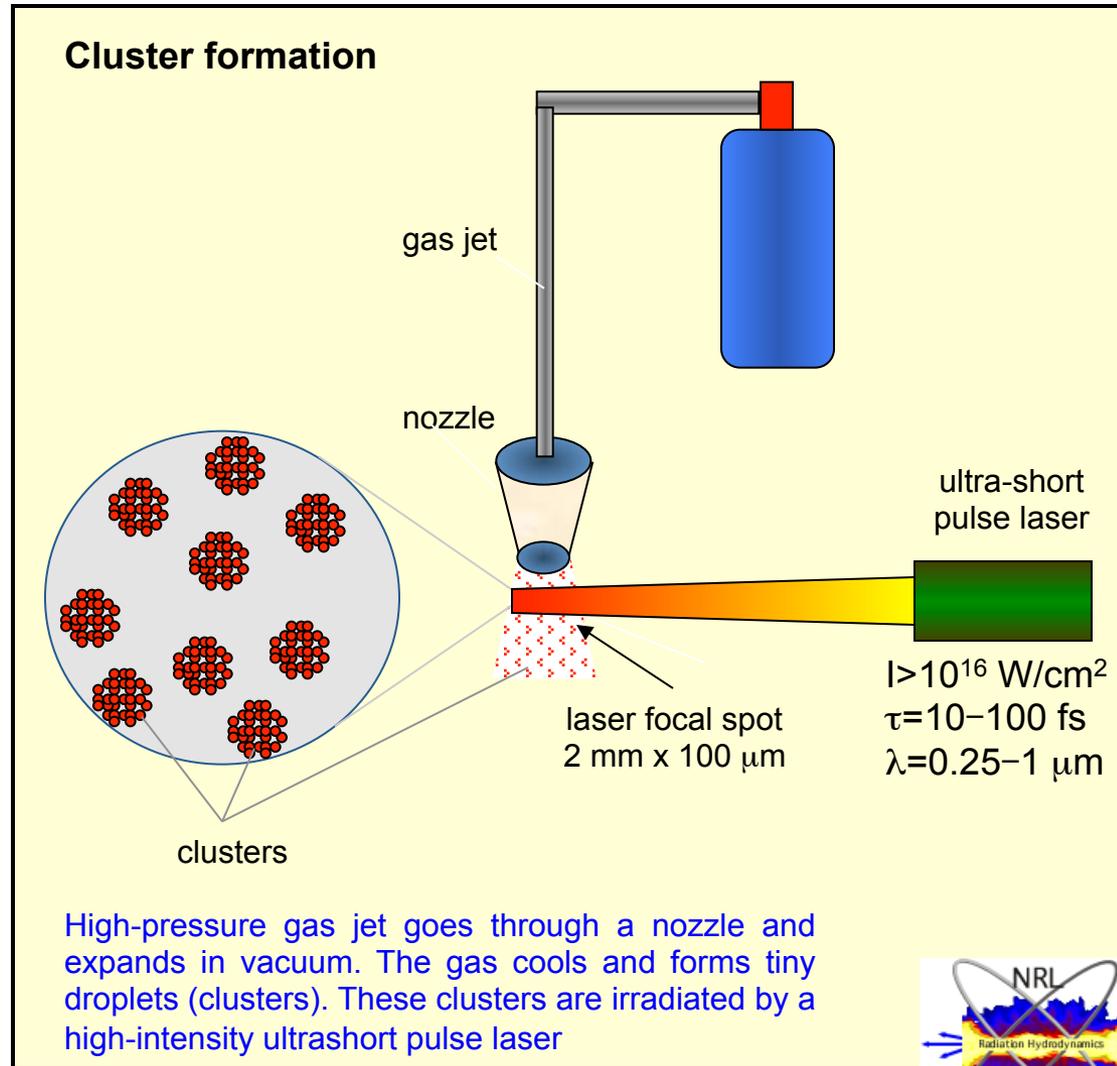
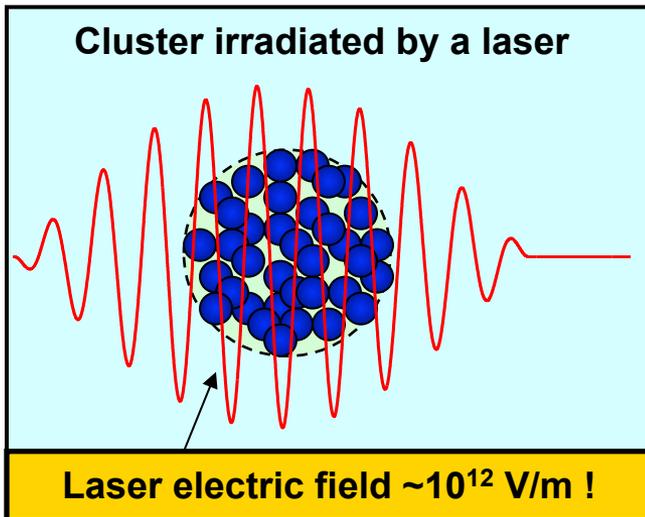
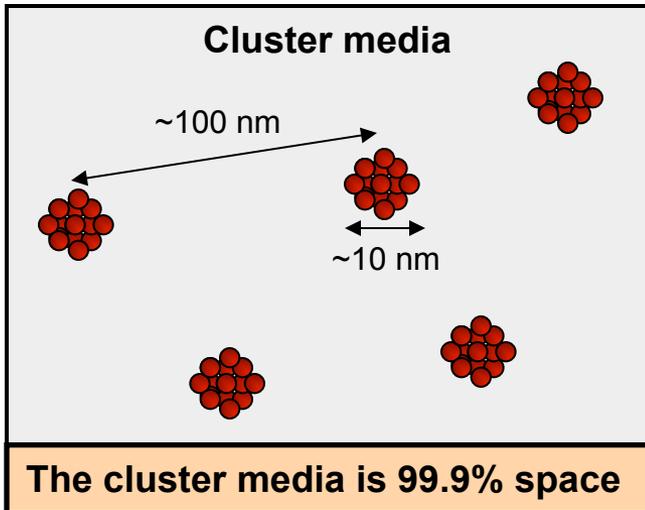
- Mehlhorn, T. A. and J. J. Duderstadt (1980). "A discrete ordinates solution of the Fokker-Planck equation characterizing charged particle transport." Journal of Computational Physics **38**(1): 86-106.



Ultra-Short Pulsed Lasers (USPL) – from physics to applications

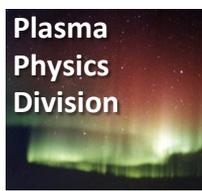


Laser cluster interactions: creation of hot dense plasma





Laser cluster interactions: creation of extreme state of matter



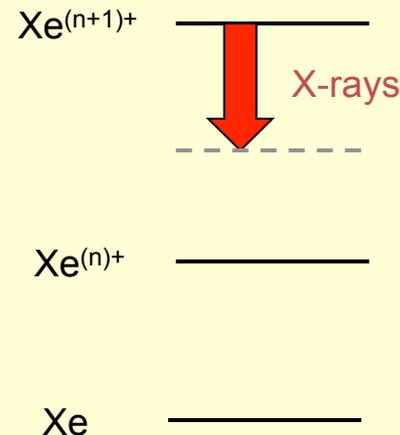
Typical cluster parameters

Atom density	$\sim 5 \times 10^{22} \text{ cm}^{-3}$ (solid density)
Cluster size	$\sim 10 \text{ nm}$
Cluster volume	$\sim 10^{-18} \text{ cm}^3$
Absorbed energy	$\sim 0.1 \text{ nJ}$
Absorbed energy density	$\sim 10^8 \text{ J/cm}^3$
Interaction time	$\sim 100 \text{ fs}$
State of matter	fully ionized, highly charged
Radiation emission	X-rays (1-100 Å)

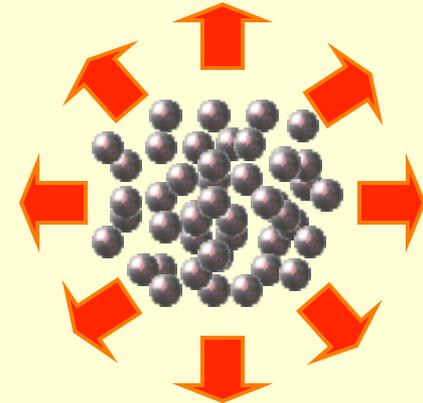
Absorbed energy density $\sim 10^8 \text{ J/cm}^3$

Cluster dynamics

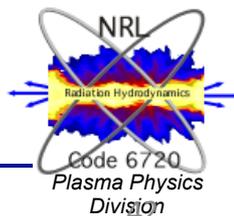
Formation of highly charged ions and X-ray generation



Cluster explosion & generation of high-energy particles



- Laser-cluster interactions create extreme conditions and lead to high-energy density laboratory plasma.
- The cluster dynamics is highly non-local and non-equilibrium due to the impact of the enormous electromagnetic fields of the laser (electric field $> 10^{12} \text{ V/m}$).
- Enhanced energy absorption leads to highly charged ions and X-ray generation



ATOMIC PHYSICS

$$V_{\text{Coul}} \gg V_{\text{Laser}}$$

Electric Field Strength E Increase

$$V_{\text{Laser}} \gg V_{\text{Coul}}$$

Perturbation

Conventional Schrödinger Equation
 Ψ, E

LTE

Saha Equation
Maxwellian EEDF

Non-LTE

Atomic Interactions
Non-Maxwellian EDF
Rate Equations

**PRESERVE EXISTING
CAPABILITIES**

USPL

Non-Linear Schrödinger Equation
 Φ, E

LTE

Strong Coupling
Saha Equation
Maxwellian EEDF

Non-LTE

Dressed Particles
Atomic Processes
AC Stark Shift
Multiphoton Ionization

**NEW PHYSICS
NEW TECHNOLOGIES**



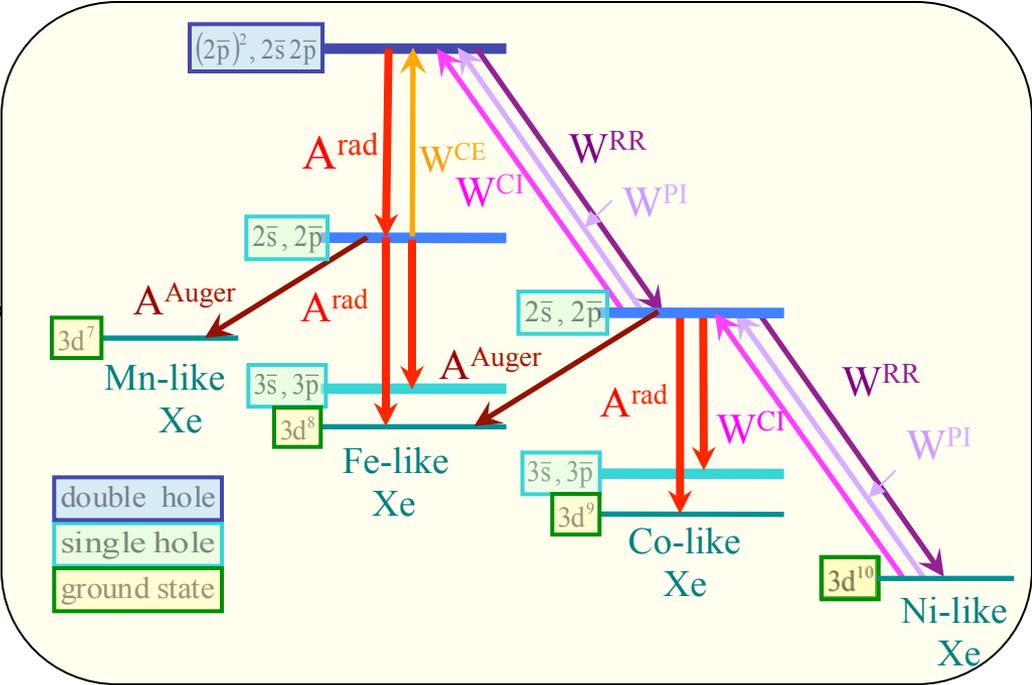
Simulating laser cluster interactions: synergy of particle simulations & atomic physics



Molecular Dynamics of Xe Clusters:
 Particle Equations
 Tunneling Ionization
 Collisional Ionization

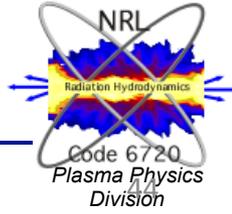
- Energy Absorption
- Cluster Expansion
- Electron & Ion Densities
- Electron & Ion Temperatures

Atomic Physics (FAC):
 Energy Levels
 Transition Probabilities
 Photoionization Cross Sec
 Auger Rates



Ionization Dynamics:
 Rate Equations
 Population Level Dynamics

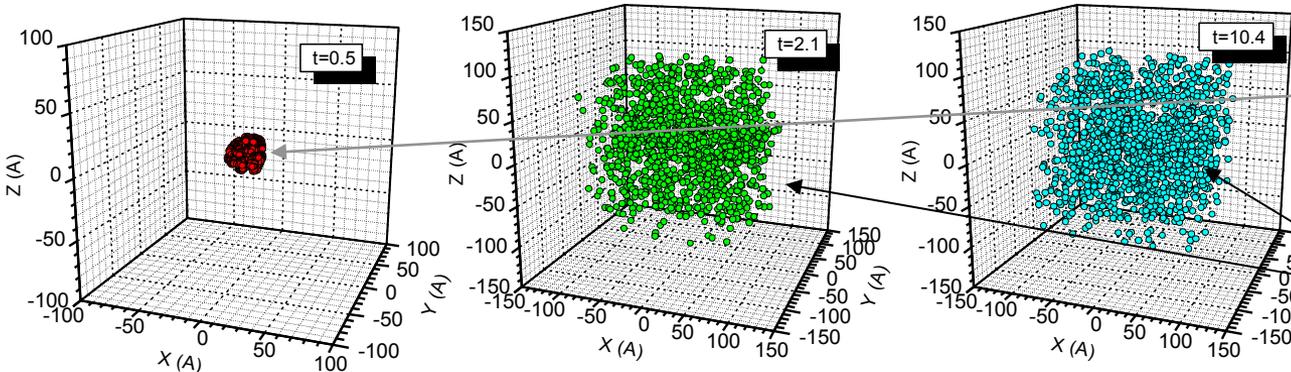
- X-ray radiation and spectra
- X-ray gain



Coupling of particle simulations to atomic physics

❑ Molecular dynamics simulation of small Xe clusters

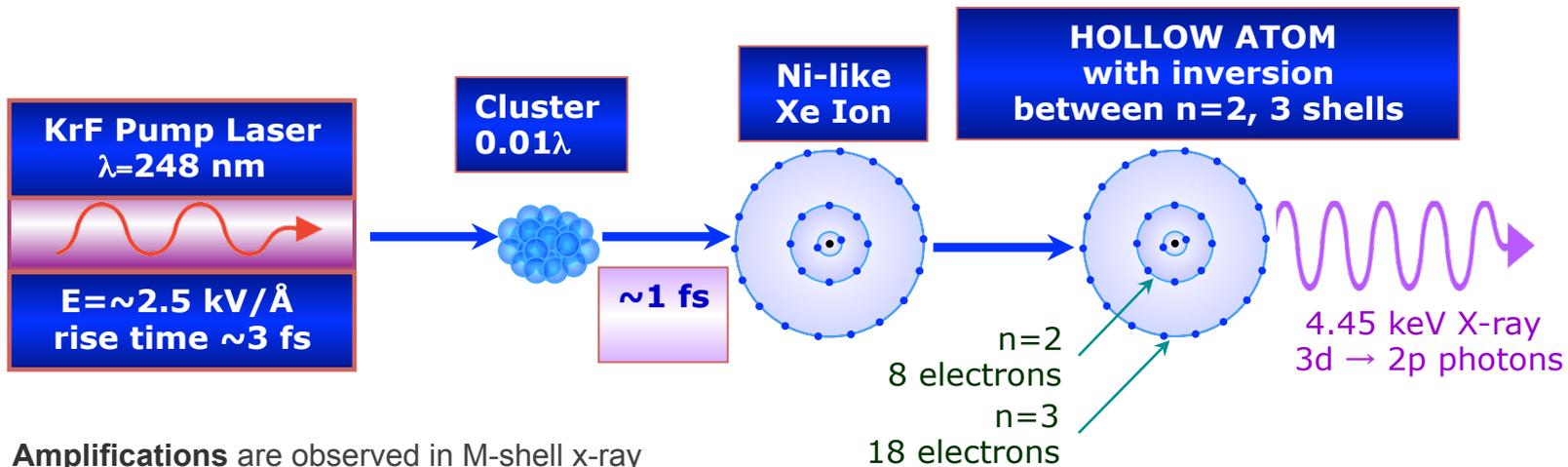
$N = 20$ atoms/cluster, $I_{\text{laser}}^{\text{max}} = 2 \times 10^{19}$ W/cm², $t = 8$ fs



enormous fields (> 10¹² V/m).

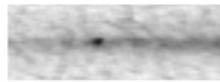
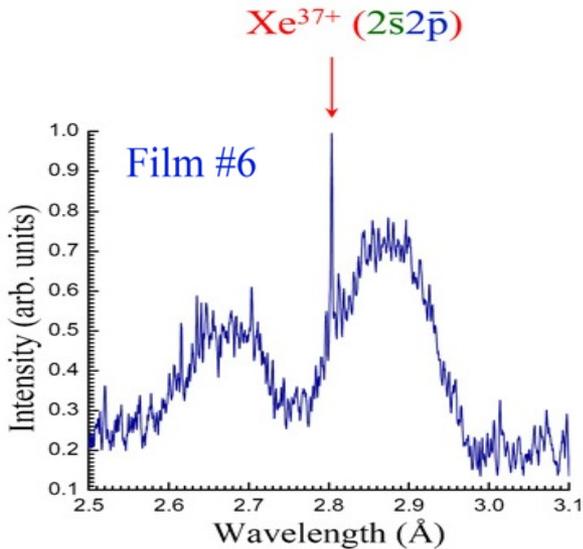
Highly non-local non-equilibrium dynamics

❑ Atomic physics of small Xe clusters



Amplifications are observed in M-shell x-ray emissions with short wavelengths (~2.5-3 Å).

Measured and simulated spectra from highly charged Xe



$\lambda = 2.804 \text{ \AA}$

Xe³⁷⁺ (2s̄2p̄) Double-Hole Line Amplification

Xe³⁷⁺ (2s̄2p̄) 2s2p⁶3s²3p⁶ ← 2s2p⁵3s²3p⁶3d

Ref: A. B. Borisov, J. Phys. B, **38** 3935–3944 (2005)

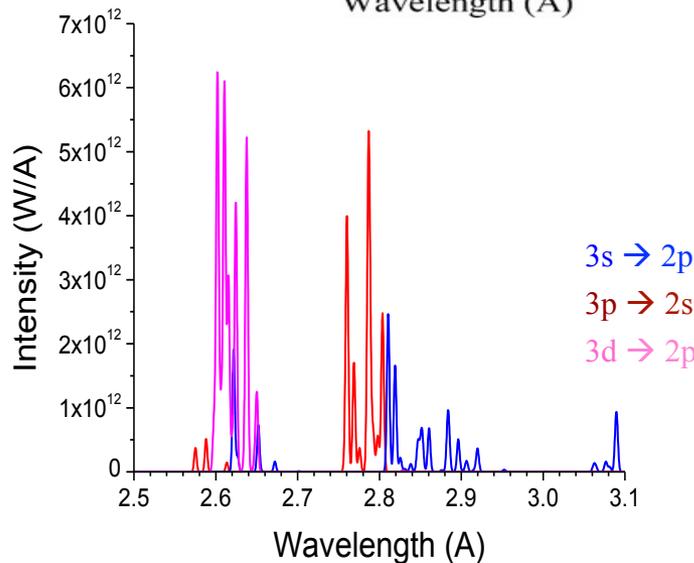
Recorded time-integrated spectrum from a plasma channel with a mica equipped von Hamos spectrograph demonstrating amplification on the (2s2p) Xe³⁷⁺ double-vacancy array at $\lambda=2.804 \text{ \AA}$. The magnitude of the amplification represented by the narrow line at $\lambda= 2.804 \text{ \AA}$ is estimated to be $\sim 10^6$.

Calculated oxygen-like xenon snapshot spectrum from small Xe clusters. Simulation parameters:

Ion density: $2 \times 10^{20} \text{ cm}^{-3}$

Ion temperature: 4 keV

Electron temperature: 40 keV





Non-LTE and non-local phenomena underlie High Energy Density (HED) plasmas



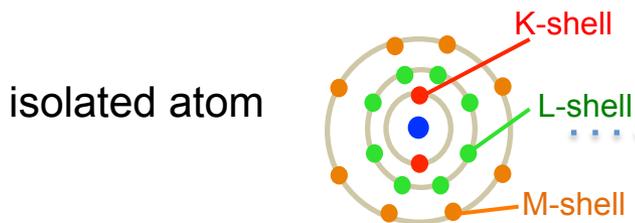
LTE

(Local Thermodynamic Equilibrium)

internal energy of a plasma
(thermal + excitation + ionization)
determined by local
density and temperature

blackbody radiation spectrum $\dots \dots \lambda_{\gamma, mfp} > \frac{\rho}{\nabla \rho} \dots \dots$

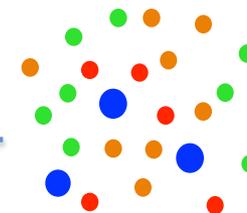
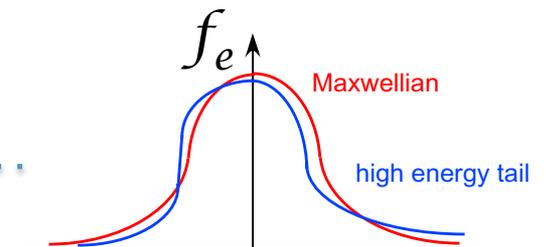
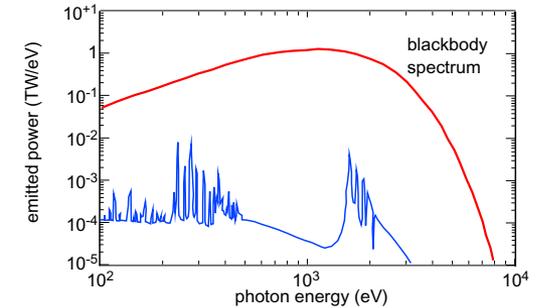
heat conduction = $\kappa \nabla T$ $\dots \dots \lambda_{e, mfp} > \frac{T}{\nabla T} \dots \dots$

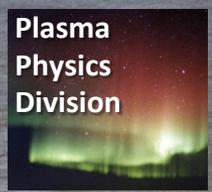


$\mathcal{E}_{laser} = \nabla \phi > \frac{e}{a_B^2} \dots \dots$

non-LTE

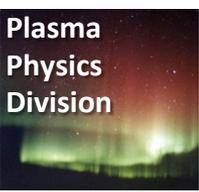
internal energy of a plasma
also depends on gradients
and thereby non-local





Thank you for your attention
Are there any questions?



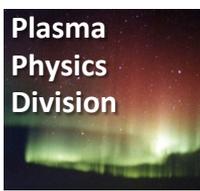


Workshop Goals

- Scientific Overview
- The physics of hot, dense plasmas is a field rich with physics and mathematics, spanning many different length and time scales. To accurately simulate hot, dense plasmas requires resolving the physics of hydrodynamics, radiation and electron transport, atomic physics, burn physics, wave-wave interactions, wave-particle interactions and particle-particle interactions, to name a few processes.
- To perform such a calculation that resolves such physics at all these length and time scales remains computationally unfeasible even with an exascale capability. Thus, it is important to differentiate between the physics that must be fully resolved, and the physics that can be included with a reduced model description in a fully integrated simulation. These fully integrated simulations including reduced model descriptions can then be validated through experiment.
- The goals of this workshop are:
 - to identify key physics components in integrated simulations of hot, dense plasmas
 - to identify critical computation issues at the different length and time scales
 - to propose reduced model descriptions that can be experimentally validated
 - to define experiments critical to an integrated simulation of hot, dense plasmas
 - to promote new collaborations
 - to engage young scientists
- It is the goal of this workshop to bring together mathematicians, computer scientists, and physicists, who work in the area of hot dense plasmas. We expect this workshop will to attract junior as well as senior participants.
- This workshop will include a poster session; a request for posters will be sent to registered participants in advance of the workshop.



The Role of Non-Local and Non-Equilibrium Physics in High Energy Density Plasmas



There is a large class of problems in high energy density plasmas where the approximations of locality and equilibrium are invalid. In this talk I will consider three different systems: 1) K-shell Z-pinch radiation sources are not in LTE (local thermal dynamic equilibrium) and where non-local line radiation transport affects the plasma dynamics; 2) in laser generated plasmas, the mean free path of the heat conducting electrons can be greater than the temperature gradient scale length and the classical, local model can be invalid; and 3) when atomic clusters are irradiated by high-intensity ultrashort laser pulses the electric field of the laser is orders of magnitude greater than the Bohr electric field associated with the atoms, the ionization kinetics is time dependent (non-equilibrium), and all the tools and methodologies used in the isolated atom regime are negated. Simulating HED plasmas in LTE and where local transport is valid can be challenging to algorithms, databases, and computational hardware. Including these non-local and non-equilibrium effects is even more formidable, requiring trade-offs to be made between physics fidelity and computationally practicality. The choice of computational algorithm (e.g. hydrodynamics, particle-in-cell, or molecular dynamics; or diffusion, Krook, or Fokker Planck) is highly dependent upon the specific problem and degree of non-locality. This talk will provide an overview of each of these systems and their applications, the role of non-local and non-equilibrium physics, the computational physics challenge of including these effects, and a roadmap for future improvements.

References:

- J.W. Thornhill, J.L. Giuliani, A. Dasgupta, et al., IEEE Trans. Plasma Sci., 38, 606 (2010).
G.M Petrov, J. Davis, Phys. Plasmas 15, 056705 (2008)
W. Mannheimer: APS DPP 2011: <http://meetings.aps.org/link/BAPS.2011.DPP.YI3.3>

In collaboration with A Dasgupta, J Davis, J Giuliani, W Mannheimer, and G Petrov, L Petrova, W Thornhill