Atomic Physics and Radiation Transport in Inertial Confinement Fusion Simulations

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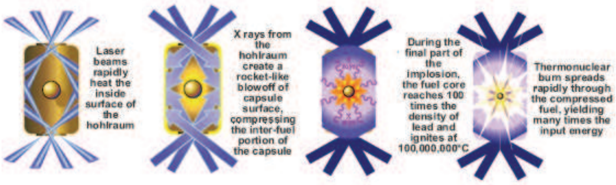
Outline

- ICF basics
  - Examples of radiation transport effects
- Radiation transport basics
- Solution methods
  - Requirements
  - Examples

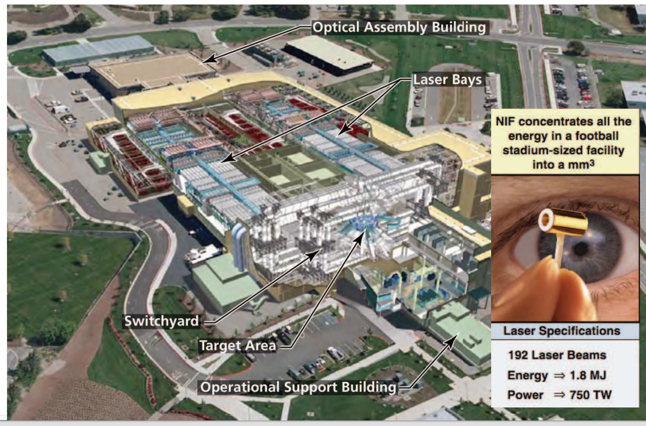
Indirect-drive Inertial Confinement Fusion (ICF) at the National Ignition Facility (NIF)



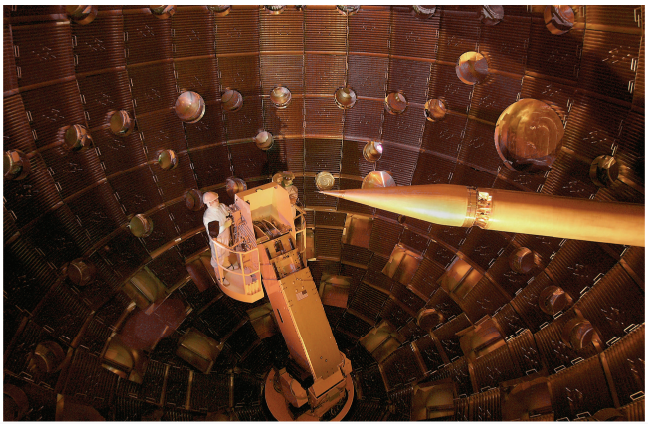
- NIF uses 192 laser beams to deliver 1-2 MJ of energy over several ns
- ~75% of the energy is converted to X-rays in the hohlraum
- Radiation field inside the hohlraum is ~thermal at T_r ~ 300 eV

NIF also provides a platform for High Energy Density (HED) experiments

National Ignition Facility (NIF) overview



NIF target chamber + positioner



Hohlraums and radiation are central to indirect-drive ICF

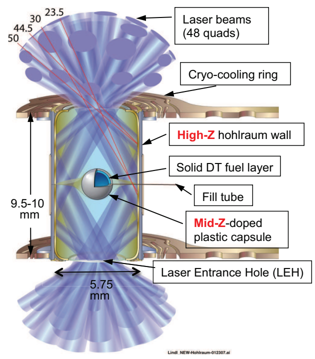
Radiation effects:

Wall
- Energy balance
- Provides smooth X-ray drive on capsule

Ablated material in hohlraum
- Hohlraum energy balance
- M-band radiation (preheats fuel)

Capsule shell
- Absorption ➔ ablative drive

Fuel impurities
- Emission provides diagnostic information



Radiation transport is a critical part of simulations

Representative parameters

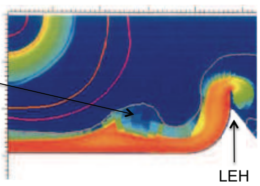
Wall
- T ~ 0-300 eV, ρ ~ 0.1-20 g/cm^3
- Z = 79, hν ~ 1 keV

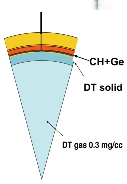
Ablated plasma (bubble)
- T ~ 1-3 keV, n_e ~ $10^{21\text{-}22}$ cm^{-3}
- Z = 79, hν ~ 1-3 keV

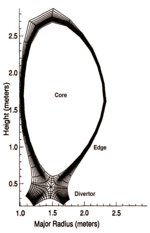
Capsule
- T ~ 100-300 eV, ρ ~ 1-200 g/cm^3
- Z = [6,32], hν ~ 1-3 keV, 10 keV

Fuel Impurities
- T ~ 1-3 keV, n_e ~ $10^{24\text{-}26}$ cm^{-3}
- Z = 32, hν ~ 10 keV

Edge plasma
- T ~ 1 eV, n_e ~ 10^{14} cm^{-3}
- Z = 1, hν ~ 10 eV



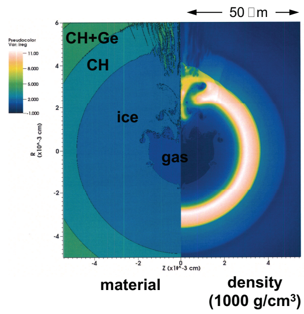


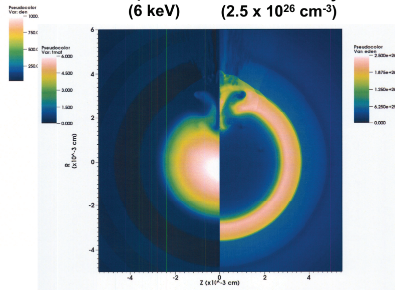


Perturbation growth brings Ge dopant into the hot spot

- 2D high-resolution HYDRA simulation
- Perturbation due to fill tube
- ~4 ps before peak compression

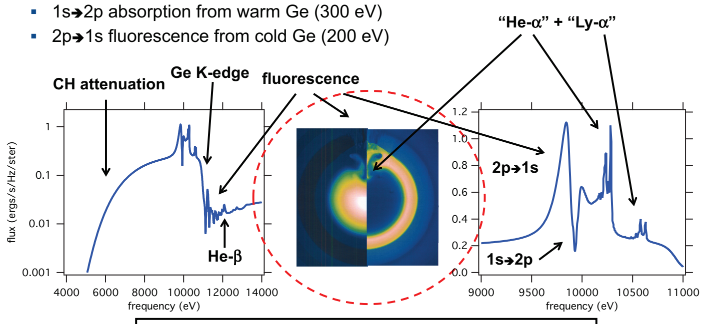
B. A. Hammel, et al, Phys. Plasmas **18**, 056310 (2011)





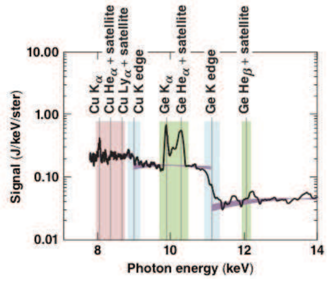
The spectrum reflects emission over a wide range of conditions and the effects of radiation transport

- K-shell emission from hot Ge (>2 keV)
- 1s→2p absorption from warm Ge (300 eV)
- 2p→1s fluorescence from cold Ge (200 eV)



"K-shell" features provide information on mix

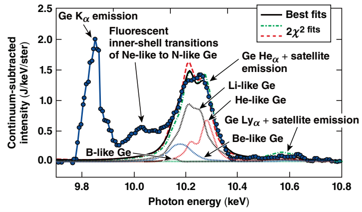
Experimental spectra show optically thick features similar to simulations



S. P. Regan, et al, Phys. Rev. Lett. **111**, 045001 (2013)

- Capsule doped with Si, Ge, and Cu
- Best fit uniform conditions:
  - $T_e \approx 3$ keV
  - $n_e \approx 10^{25}$ cm^{-3}
  - $(\rho R)_{Ge} \approx 0.3$ mg/cm^2

→ $\tau_{\text{He-}\alpha} \approx 10$



Radiation transport basics

- Radiation transport equation:

$$\frac{1}{c}\frac{\partial I_\nu}{\partial t} + \vec{\Omega}\bullet\nabla I_\nu = -(\alpha_\nu I_\nu - \eta_\nu)$$

$I_\nu =$ specific intensity
$\alpha_\nu =$ absorption coefficient
$\eta_\nu =$ emissivity

- Equivalent to a Boltzmann equation for the photon distribution function, f

$$\frac{1}{c}\frac{\partial f}{\partial t} + \vec{\Omega}\bullet\nabla f = \left.\frac{\partial f}{\partial t}\right|_{collisions} \qquad I_\nu = \frac{2h\nu^3}{c^2} f(\vec{r},\nu,\vec{\Omega})$$

- The LHS describes the flow of radiation in phase space
  - Conserves photon number
- The RHS describes absorption and emission
  - Absorption & emission coefficients depend on atomic physics
  - Photon # is not conserved (except for scattering)
- Photon mean free path $\lambda_\nu = 1/\alpha_\nu$

Formal solution along characteristics:

Define the source function S_ν and optical depth τ_ν:

$S_\nu = \eta_\nu/\alpha_\nu$ ($= B_\nu$ in LTE) $\qquad d\tau_\nu = \alpha_\nu\, ds$

Along a characteristic, the radiation transport equation becomes

$$\frac{dI_\nu}{d\tau_\nu} = -I_\nu + S_\nu \;\Rightarrow\; I_\nu(\tau_\nu) = I_\nu(0)e^{-\tau_\nu} + \int_0^{\tau_\nu} e^{-(\tau_\nu - \tau_\nu')} S_\nu(\tau_\nu')\,d\tau_\nu'$$

This solution is useful when material properties are fixed, e.g. postprocessing for diagnostics

Important features:

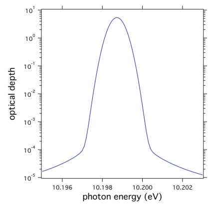
- Explicit non-local relationship between I_ν and S_ν
- Escaping radiation comes from depth $\tau_\nu \sim 1$
- Implicit $S_\nu(I_\nu)$ dependence comes from radiation / material coupling

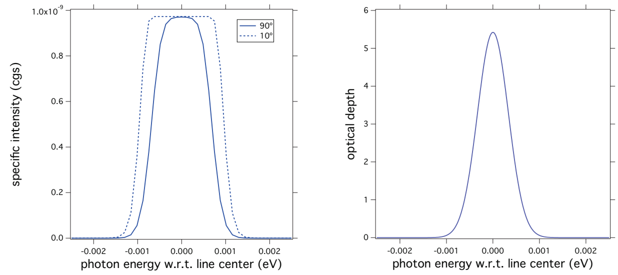
Self-consistently determining S_ν and I_ν is the hard part of radiation transport

Example – Hydrogen Ly-α

Ly-α emission from a uniform plasma

- T_e = 1 eV, $n_e = 10^{14}$ cm^{-3}
- Moderate optical depth $\tau \sim 5$
- Viewing angles 90° and 10° show optical depth broadening

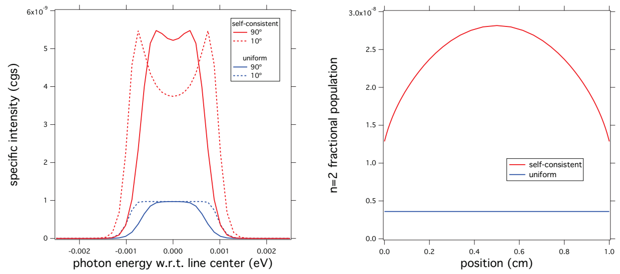




Example – Hydrogen Ly-α

Ly-α emission from a uniform plasma

- T_e = 1 eV, $n_e = 10^{14}$ cm^{-3}
- Self-consistent solution displays effects of
  - Radiation trapping / pumping
  - Non-uniformity due to boundaries



Absorption / emission coefficients

Macroscopic description – energy changes

- Energy removed from radiation passing through material of area dA, depth ds, over time dt

$$dE = -\alpha_\nu I_\nu\, dA\, ds\, d\Omega\, d\nu\, dt$$

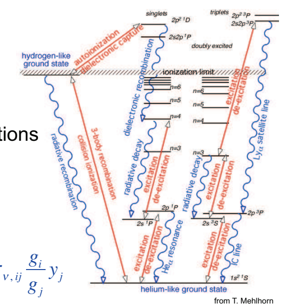
- Energy emitted by material

$$dE = \eta_\nu I_\nu\, dA\, ds\, d\Omega\, d\nu\, dt$$

Microscopic description – radiative transitions

- Absorption and emission coefficients are constructed from atomic populations y_i and cross sections σ_{ij}:

$$\alpha_\nu = \sum_{i<j}\sigma_{\nu,ij}\left(y_i - \frac{g_i}{g_j}y_j\right),\quad \eta_\nu = \frac{2h\nu^3}{c^2}\sum_{i<j}\sigma_{\nu,ij}\frac{g_i}{g_j}y_j$$



from T. Mehlhorn

Population distribution

LTE: Saha-Boltzmann equation

- Excited states follow a Boltzmann distribution $\frac{y_i}{y_j} = \frac{g_i}{g_j}e^{-(\varepsilon_i-\varepsilon_j)/T_e}$ $\quad \varepsilon_i =$ energy of state i, $T_e =$ electron temperature
- Ionization stages obey the Saha equation

$$\frac{N_q}{N_{q+1}} = \frac{1}{2}n_e\frac{U_q}{U_{q+1}}\left(\frac{h^2}{2\pi m_e T_e}\right)^{3/2} e^{-(\varepsilon_0^{q+1}-\varepsilon_0^q)/T_e}$$

$N_q = \sum_{i\in q} y_i e^{-(\varepsilon_i-\varepsilon_0^q)/T_e}$ number density of charge state q

$U_q = \sum_{i\in q} g_i e^{-(\varepsilon_i-\varepsilon_0^q)/T_e}$ partition function of charge state q

NLTE: Collisional-radiative model

- Calculate populations by integrating a rate equation

$$\frac{dy}{dt} = \mathbf{A}y \quad A_{ij} = C_{ij} + R_{ij} + (other)_{ij} \quad C_{ij} = n_e\int v\sigma_{ij}(v)f(v)\,dv$$

$$R_{ij} = \int\sigma_{ij}(\nu)J(\nu)\frac{d\nu}{h\nu},\quad R_{ji} = \int\sigma_{ij}(\nu)\left[J(\nu) + \frac{2h\nu^3}{c^2}\right]e^{-h\nu/kT}\frac{d\nu}{h\nu}$$

Timescales for strong atomic transitions

For T_e and ΔE in eV , n_e in 10^{20} cm^{-3} :

	collisional (C)	radiative (R)
De-excitation	$\sim 10^{14}\ \frac{n_e}{\Delta E_{ij} T_e^{1/2}}\ \mathrm{s}^{-1}$	$\sim 10^{8}\ (\Delta E_{ij})^2\ \mathrm{s}^{-1}$
Recombination	$\sim 10^{10}\ \frac{n_e^2}{\Delta E_{ij} T_e^2}\ \mathrm{s}^{-1}$	$\sim 10^{7}\ Z\ \frac{n_e (\Delta E)^{1/2}}{T_e^{1/2}}\ \mathrm{s}^{-1}$

Collisional rates increase with density ➔ thermal equilibrium
Radiative rates increase with Z, ΔE ➔ non-equilibrium

Examples

Wall: T ~ 100 eV, n_e ~ 10^{23} /cm^3, ΔE ~ 300 eV	C/R ~ 1	t_R ~ 10^{-13} s
Fuel Impurities: T ~ 2 keV, n_e ~ 10^{25} /cm^3, ΔE ~ 10 keV	C/R ~ 10^{-2}	t_R ~ 10^{-18} s
Edge plasma: T ~ 1 eV, n_e ~ 10^{14} /cm^3, ΔE ~ 10 eV	C/R ~ 10^{-2}	t_R ~ 10^{-12} s

Radiative timescales << hydrodynamic / transport timescales
➔ Requires implicit solution of radiation transport

Transport methods need to fulfill 2 requirements

1. Accurate formal transport solution which is
   - conservative,
   - non-negative
   - 2nd order (spatial) accuracy (diffusion limit as τ >> 1)
   - causal (+ efficient)

   Many options are available – each has advantages and disadvantages

2. Method to converge solution of coupled implicit equations
   - Multiple methods fall into a few classes
     - Full nonlinear system solution
     - Accelerated transport solution
     - Incorporate transport information into other physics
   - Optimized methods are available for specific regimes, but no single method works well across all regimes

Coupled equations

$$\frac{1}{c}\frac{\partial I_\nu}{\partial t} + \vec{\Omega}\bullet\nabla I_\nu = -\alpha_\nu (I_\nu - S_\nu)\ ,\quad J_\nu = \frac{1}{4\pi}\int I_\nu \, d\Omega$$

LTE :
- Coupled to energy balance

$$\frac{dE_m}{dt} = 4\pi \int \alpha_\nu (J_\nu - S_\nu)\, d\nu$$
$$\alpha_\nu = \alpha_\nu(T_e)\ ,\ S_\nu = B_\nu(T_e)$$

- Indirect radiation-material coupling through energy/temperature
- Collisions couple all frequencies locally, independent of J_ν
- Solution methods concentrate on non-local aspects

NLTE :
- Coupled to rate equations

$$\frac{dy}{dt} = \mathbf{A}\mathbf{y}\ ,\ \mathbf{A}_{ij} = \mathbf{A}_{ij}(T_e, n_e, J_\nu)$$
$$S_\nu = \tfrac{2h\nu^3}{c^2} S_{ij}\ ,\ S_{ij} \approx a + b\bar{J}_{ij}$$

- Direct coupling of radiation to material
- Collisions couple frequencies over narrow band (line profiles)
- Solution methods concentrate on local material-radiation coupling
- Non-local aspects are less critical

Solution method 1 – source iteration

1. Evaluate source function
2. Formal solution of radiation transport equation
3. Use intensities to evaluate temperature / populations

iterate to convergence

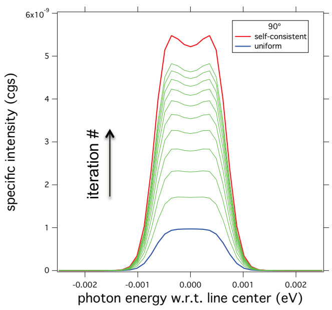
Advantages –
Simple to implement
Independent of transport method

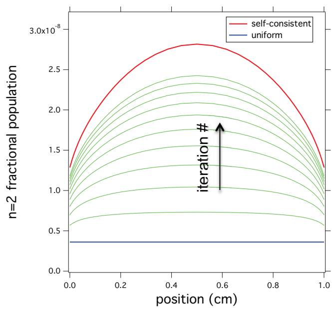
Disadvantages –
Can require many iterations: # iterations ~ τ
False convergence is a problem for τ >> 1

Hydrogen Ly-α revisited

- Source iteration (green curves) approaches self-consistent solution slowly
- Linearization achieves convergence in 1 iteration

$$S_{ij} = a + b\bar{J}_{ij}\ ,\ \bar{J}_{ij} = \int J_\nu \phi_\nu \, d\nu \quad \text{🡐 linear function of } J_\nu$$





Solution method 2 – Monte Carlo

Implicit Monte Carlo (IMC) for LTE systems [4] provides a semi-implicit solution to the radiation transport + energy balance equations

Parameter $\beta = {4aT^3}/{\rho C_v}$ characterizes linearized radiation/material coupling

➔ fraction β of absorptions treated as effective scatterings also reduces cost

Advantages –
Works well for complicated geometries
Not overly constrained by discretizations ➔ does details very well

Disadvantages –
Statistical noise improves slowly with # of particles
Expense increases with optical depth
Iterative evaluation of coupled system is not possible / advisable
Semi-implicit nature requires careful timestep control

Notes –
Equivalent procedures for NLTE systems have been used for strong lines
Symbolic IMC [5] provides a fully-implicit NLTE solution at the cost of a solving a single mesh-wide nonlinear equation

Solution method 3 – Discrete Ordinates (S_N)

Discretization in angle converts integro-differential equations into a set of coupled differential equations

Effective solution algorithms exist for both LTE and NLTE versions [6] –
e.g. LTE – synthetic grey transport (or diffusion)
NLTE – complete linearization, accelerated lambda iteration

Advantages –
Handles regions with τ<<1 and τ>>1 equally well
Modern spatial discretizations achieve the diffusion limit
Deterministic methods can be iterated to convergence

Disadvantages –
Ray effects due to preferred directions
angular profiles become inaccurate well before angular integrals
Required # of angles in 2D/3D can become enormous
Discretization in 7 dimensions requires large computational resources

This is our preferred method for NLTE systems
using detailed post-processing of rad-hydro simulations

Solution method 4 – Escape factors (NLTE)

Escape probability [7] averaged over line profile, p_e, is used to eliminate radiation field from net radiative rate

$$y_j R_{ji} - y_i R_{ij} = y_j A_{ji}\, p_e$$

Equivalent to incorporating a (partial) transport operator into the rate equations

Advantages –
Very fast – no transport equation solution required
Can be combined with other physics with no (or minimal) changes

Disadvantages –
Details of transport solution are absent
Escape factors depend on line profiles, system geometry
Iterative improvement is possible, but usually not worthwhile

Notes –
Evaluating p_e can be complicated by overlapping lines, Doppler shifts, etc.
Many variations and extensions exist in a large literature

Radiation transport effects with plasma transport [8]

- Plasma transport model explicitly treats ion and (ground state) neutral atoms
- Excited states are assumed to be in equilibrium on transport timescales:

$$n_x = f_x^g n_g + f_x^i n_i \ , \ f_x^{g,i} = f_x^{g,i}(n_e, T_e)$$

- Transport model uses effective ionization / recombination and energy loss coefficients which account for excited state distributions, e.g.

$$\frac{\partial n_i}{\partial t} + \nabla \cdot (n_i \mathbf{V}_i) = P_i n_n - P_r n_i \ , \ \frac{\partial n_n}{\partial t} + \nabla \cdot (n_n \mathbf{V}_n) = -P_i n_n + P_r n_i$$

- Tabulated coefficients are evaluated with a collisional-radiative code in the optically thin limit

Optically thin data depend only on n_e and T_e

Radiation effects are incorporated into the effective ionization and heating rates

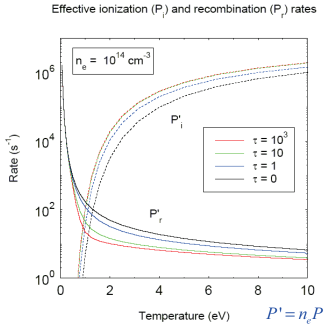
- Radiation introduces spatial dependence into the atomic rates through the radiation field
- Rates are parameterized by the (approximate) optical depth of Lyman α:

$$P(n_e, T_e) \to P(n_e, T_e, \tau),$$

$$\tau = \int_0^s 10^{14} n_n(s') ds'$$

- Tabulated values generated with escape factors for midpoint of uniform plasma of depth 2τ

Effective ionization (P_i) and recombination (P_r) rates

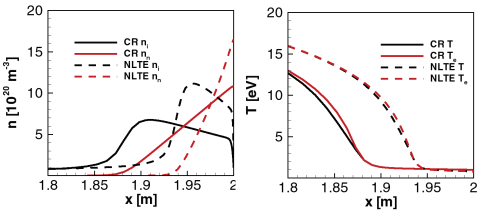


$P' = n_e P$

This generalizes the approach of Stotler, Post and Reiter
Bul. Am. Phys. Soc. **38** (1993) 1919

Detached divertor simulations exhibit large radiation effects

Specifications: $L=2$ m, $n=10^{20}$ m^{-3}, $q_{in}=10$ MW/m^2, $\beta=0.1$



Flux	Q_r	q_{out}
CR	-0.805	+0.195
NLTE	-0.555	+0.445
ESC	-0.537	+0.463

Q_r : radiative flux
q_{out} : particle flux

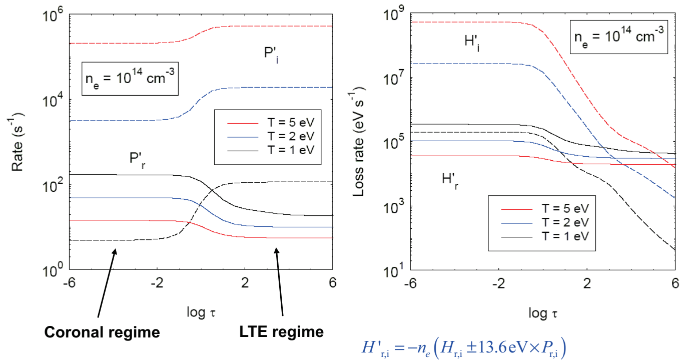
CR : collisional-radiative tables (optically-thin)
NLTE : collisional-radiative model w/ radiation transport
ESC : parameterized tables

Qualitative description of the detached divertor region remains unchanged, *Quantitative* details of the particle and power balance change dramatically.

Optical depth parameterization allows coverage from coronal to LTE regimes

Effective ionization / recombination rates

Effective energy loss rates



$$H'_{r,i} = -n_e \left(H_{r,i} \pm 13.6\mathrm{eV} \times P_{r,i} \right)$$

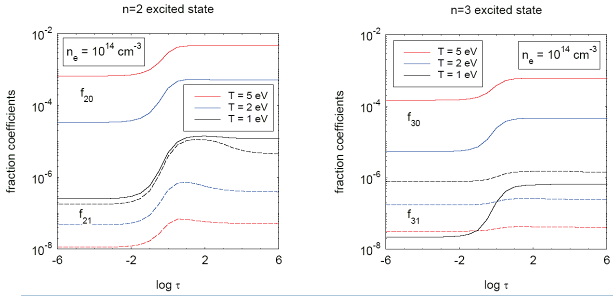
Excited state populations are critical for spectroscopic diagnostics

Determined from ground state and ion densities:

$n_2 = f_{20} n_i + f_{21} n_g$, $n_3 = f_{30} n_i + f_{31} n_g$

n=2 excited state

n=3 excited state



τ>>1 values can differ by orders of magnitude from τ<<1 values

Summary

- Radiation transport effects are important to
  - Energy balance
  - Ionization balance
  - Diagnostics
- Self-consistency is important for simulations when $\tau \geq 1$
- Acceleration methods can speed up convergence dramatically
- Details can usually come from post-processing
- Many numerical approaches are possible

References

1. J. Castor, *Radiation Hydrodynamics,* Cambridge Univ. Press, 2004.
2. E.E. Lewis and W.F. Miller, Jr., *Computational Methods of Neutron Transport*, American Nuclear Society, 1993.
3. D. Mihalas, *Stellar Atmospheres*, Freeman & Co., 1978.
4. J.A. Fleck, Jr. and J.D. Cummings, J. Comp. Phys. **8**, 313-342 (1971).
5. E.D. Brooks III, J. Comp. Phys. **83**, 433-446 (1989).
6. H.A. Scott, HEDP **1**, 31-41 (2005).
7. G.B. Rybicki, in *Methods in Radiative Transfer*, W. Kalkofen, ed., Cambridge University Press, 1984.
8. H.A. Scott and M.L. Adams, Contr. Plasma Phys. **44**, 51-56 (2004).