IAEA 60 Years
Atoms for Peace and Development

A generalized model of atomic processes in plasmas : FLYCHK

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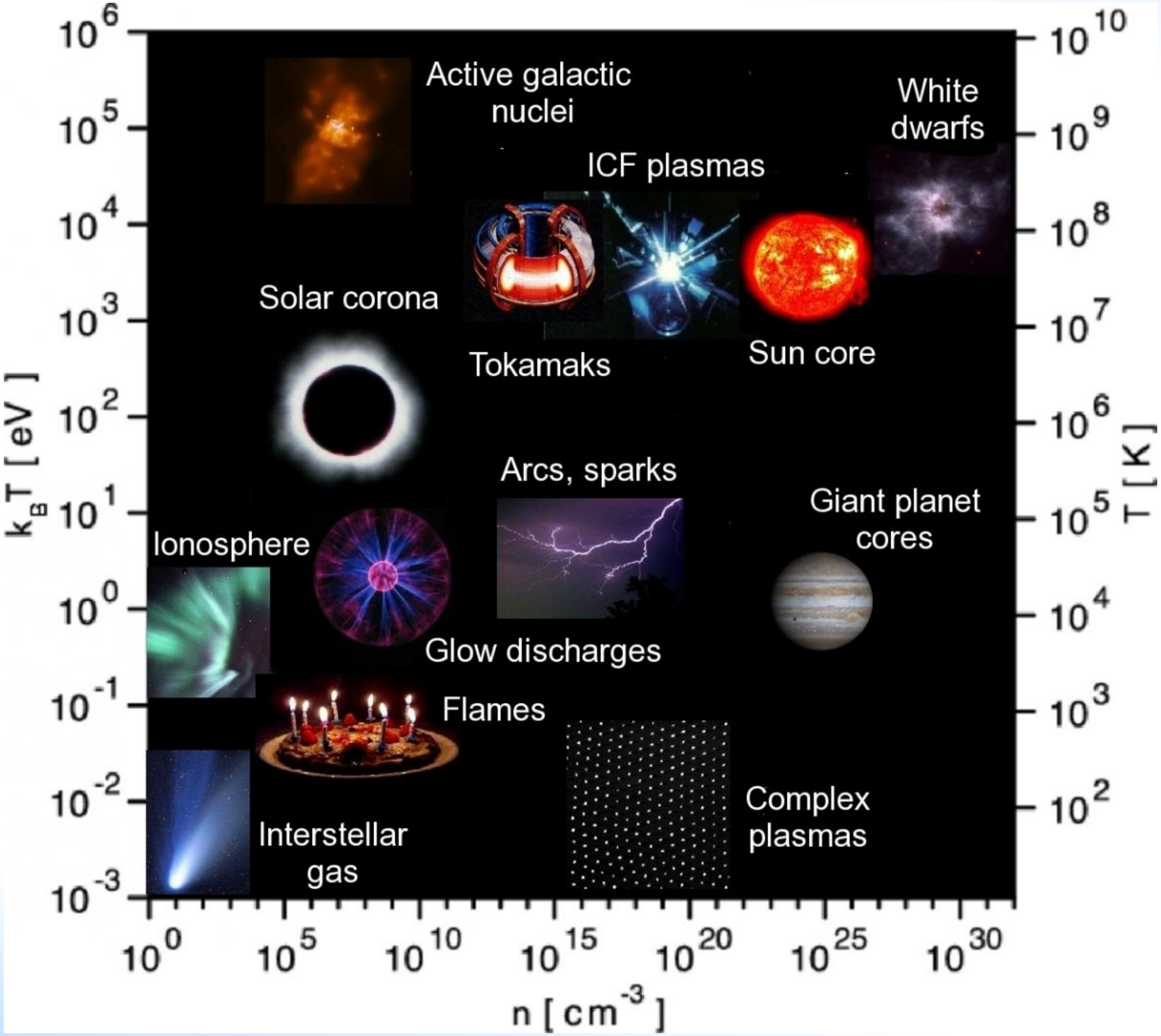
29-30 September 2016

Outline

- Motivation
- FLYCHK code
- Applications of FLYCHK results

MOTIVATION

Plasmas occur over a vast range of conditions in Universe



Temperature

10^{-6}K – 100 keV

Density

10^{5} – 10^{24} cm^{-3}

Advances in plasma generation access new regimes of matter

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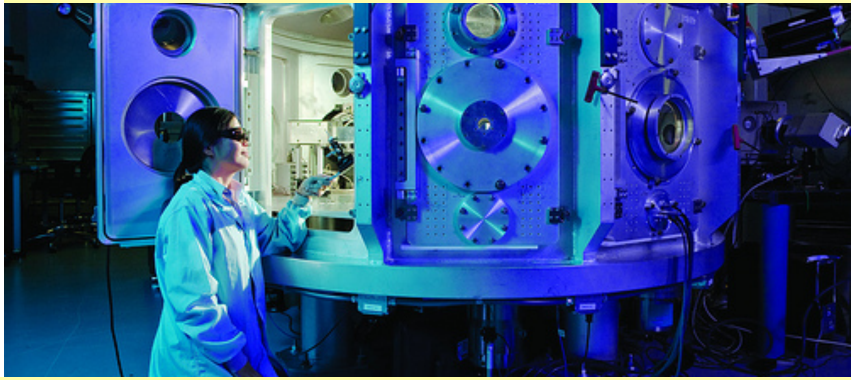
High Power Optical Lasers
(NIF, LMJ, Omega etc)

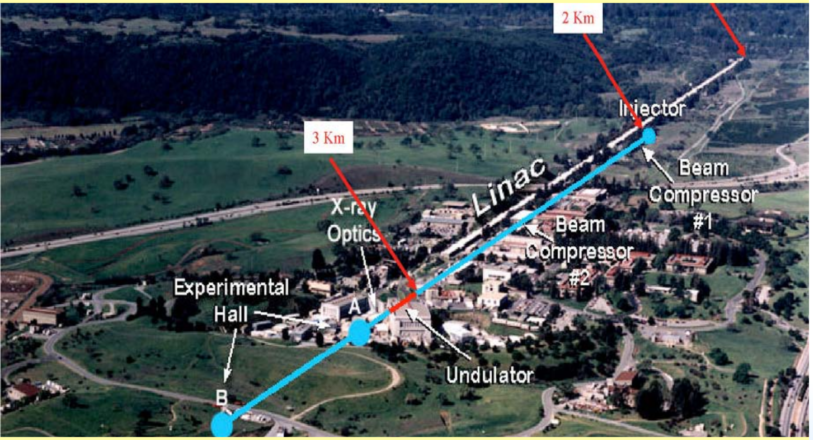
Hotter and denser matter

USP: Ultra Short Pulse Laser
(RAL, LULI, Gekko, Titan, Texas, etc)



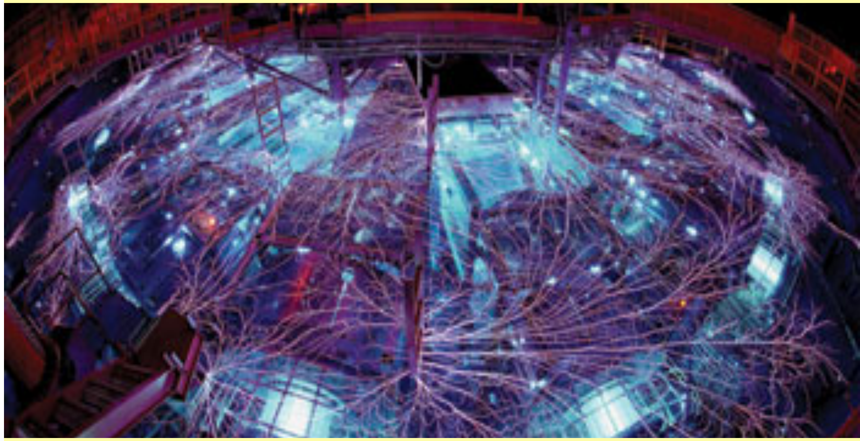
Transient states of matter

XFEL: X-ray Free Electron Lasers
(LCLS, SACLA, PAL-XFEL etc)



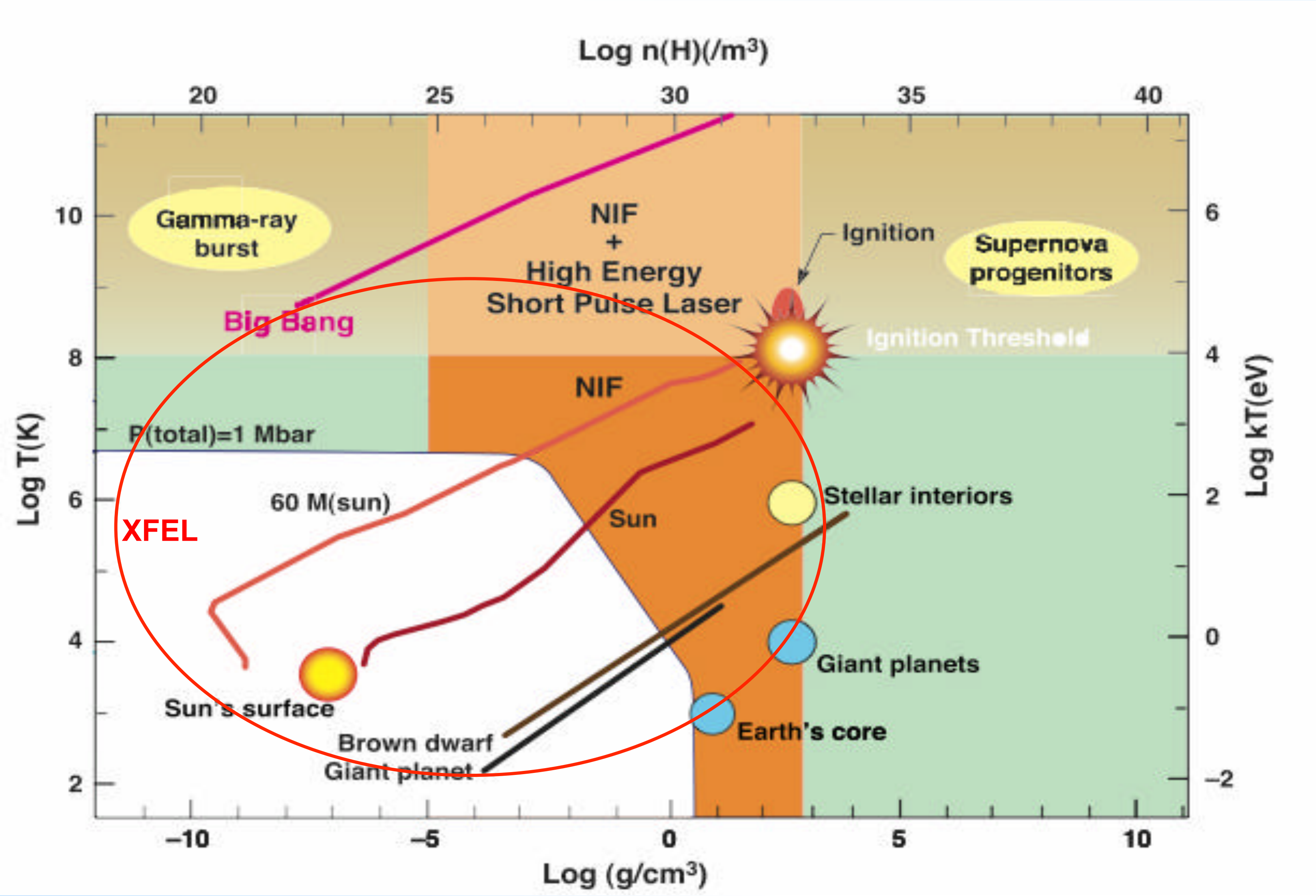
Warm dense matter

Pulse Power: X-Pinches, Z-Pinches...
(Sandia, Cornell, UNR)



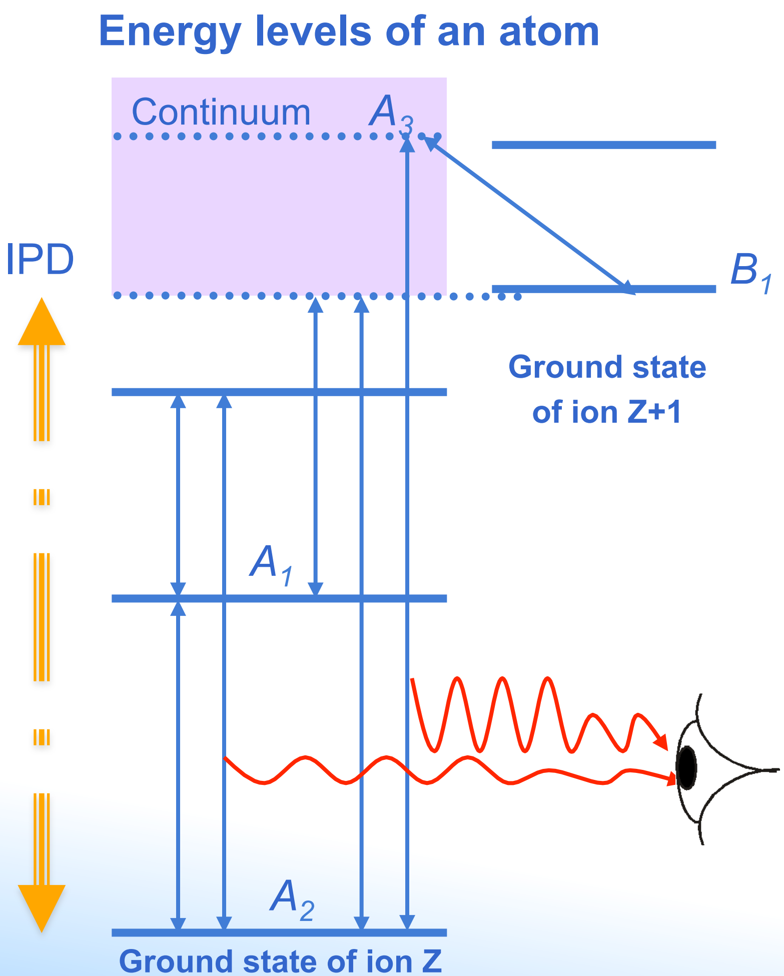
Astronomical X-ray applications

Laboratory plasmas can create extreme states of matter



General Description of Atomic Processes in plasmas are needed

Mean ionization states <Z>, Charge state distributions, Spectral intensity, Emissivity, Opacity, Equation of state, Electrical conductivity require population distributions of ions in the plasma.



BOUND-BOUND TRANSITIONS

$A_1 \rightarrow A_2 + h\nu_2$ Spontaneous emission

$A_1 + h\nu_1 \leftrightarrow A_2 + h\nu_1 + h\nu_2$ Photo-absorption or emission

$A_1 + e_1 \leftrightarrow A_2 + e_2$ Collisional excitation or deexcitation

BOUND-FREE TRANSITIONS

$B_1 + e \rightarrow A_2 + h\nu_3$ Radiative recombination

$B_1 + e \leftrightarrow A_2 + h\nu_3$ Photoionization / stimulated recombination

$B_1 + e_1 \leftrightarrow A_2 + e_2$ Collisional ionization / recombination

$B_1 + e_1 \leftrightarrow A_3 \leftrightarrow A_2 + h\nu_3$ Dielectronic recombination

(autoionization + electron capture)

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Generalized Population Kinetics Codes Applied to “Any Plasmas” in zeroth order approximation

FLYCHK CODE

Population Kinetics Models for Charge State Distributions

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Coronal plasmas (low N_e) ⇒ Rate formalism

Charge state distributions are determined by rates of *collisional ionization (CI) and excitation autoionization (EA)* & *radiative recombination (RR) and dielectronic recombination (DR), Rates originating from the ground states*

LTE plasmas (high N_e) ⇒ Statistical distributions

Collisional processes are dominant and population distribution is governed statistically by *Boltzmann relations and Saha equation*.

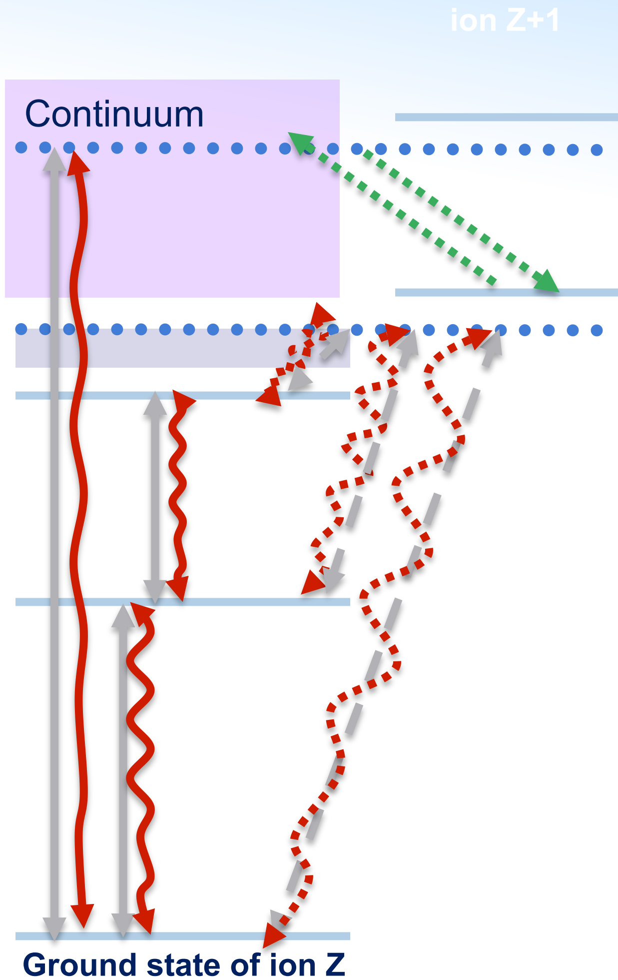
Collisional-radiative plasmas (intermediate N_e) ⇒ Rate equation model

At a given electron temperature and density, population distribution is determined by solving *Rate equations considering collisional and radiative processes*.

Collisional-Radiative results should converge to Coronal Limit or LTE Limit at low and high Ne limits, respectively.

Collisional-Radiative Model
(Non-Local Thermodynamic Equilibrium Model)

- Population distribution is obtained by rate equations considering collisional and radiative processes, along with plasma effects
- *Excited states* are substantially populated and *increase the total ionization* by step-wise ionization processes
- The 3-body recombination to *high-lying excited states* is proportional to n^4 and N_e^2 and excited states can significantly *enhance the total recombination*.
- *Plasma effects* such as non-local radiation transport, fast particle collisions and density effects should be included in the model.
- *Self-absorption (radiation pumping)* should be included for treating radiative processes involving optically thick lines.



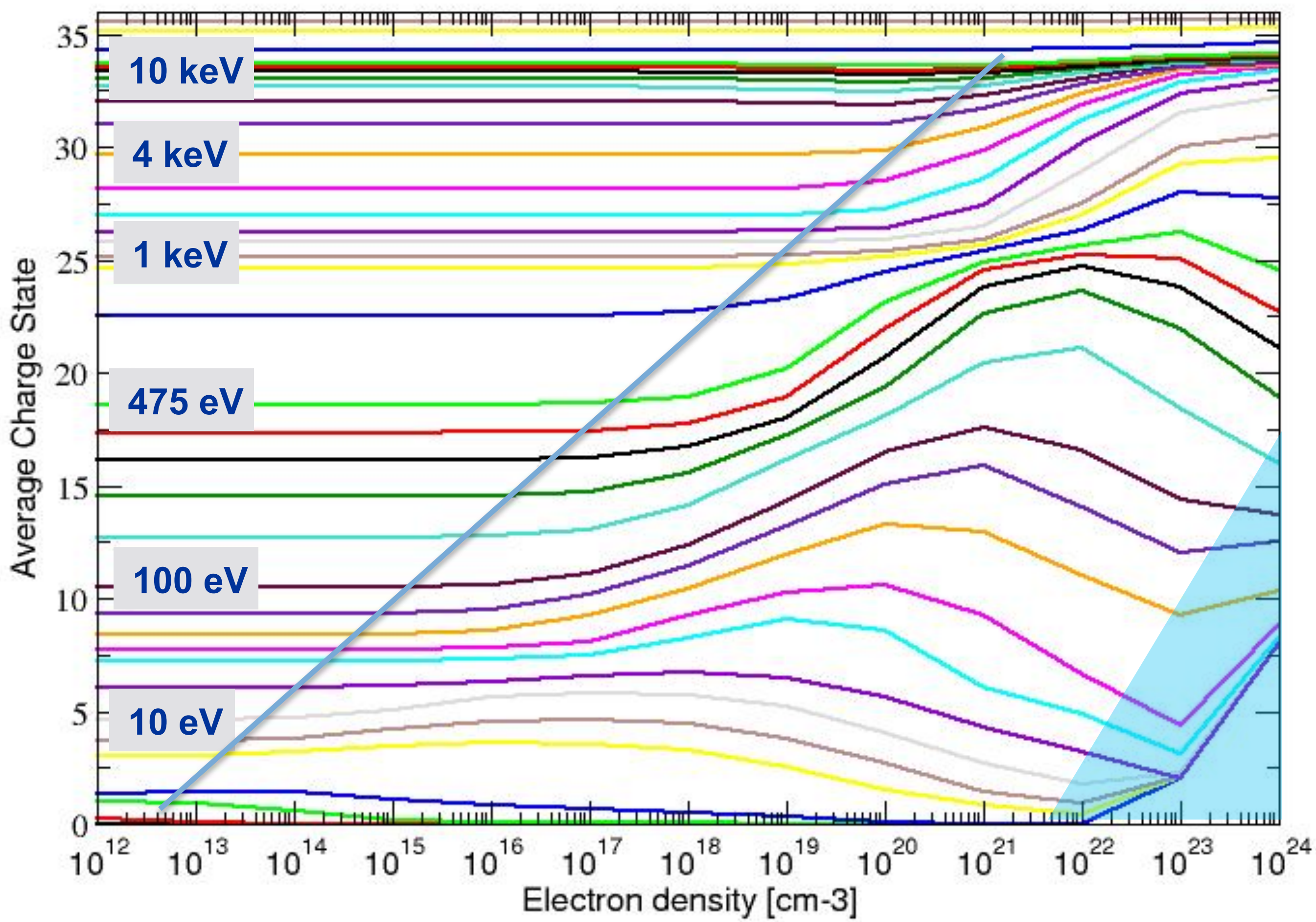
Collisional-Radiative Model

Average charge states as a function of electron density

Stepwise excitation via excited states → <Z> increase

3-body recombination via Rydberg states → <Z> decrease

Pressure ionization of excited states and ionization potential depression → <Z> increase



Krypton

FLYCHK

T_e=0.5 eV-100 keV

$N_e=10^{12}-10^{24}$ cm^{-3}

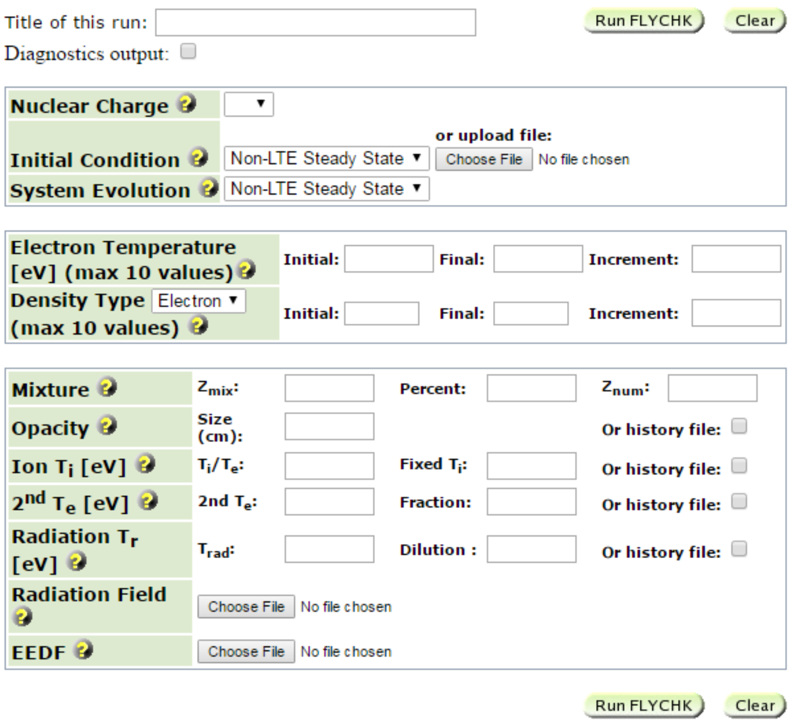
FLYCHK code:

http://nlte.nist.gov/FLY

- A *time-dependent* 0-d collisional-radiative (Non-LTE) model to provide charge state distributions and spectral intensities

- Available online at NIST

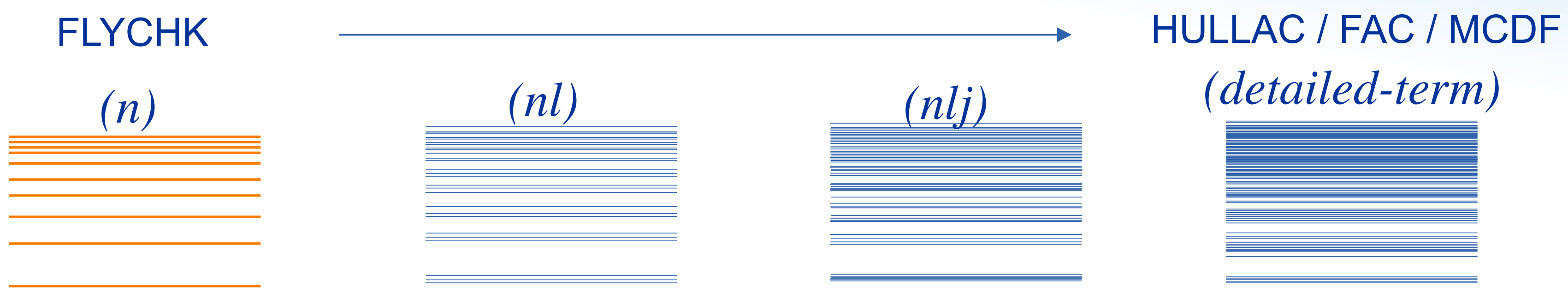
- Applications
  - Long-pulse laser produced plasmas
  - Short-pulse laser produced plasmas
  - XFEL laser produced plasmas
  - Electron beam produced plasmas
  - Time-dependent plasmas
  - Tokamak plasmas



- More than 750 registered users

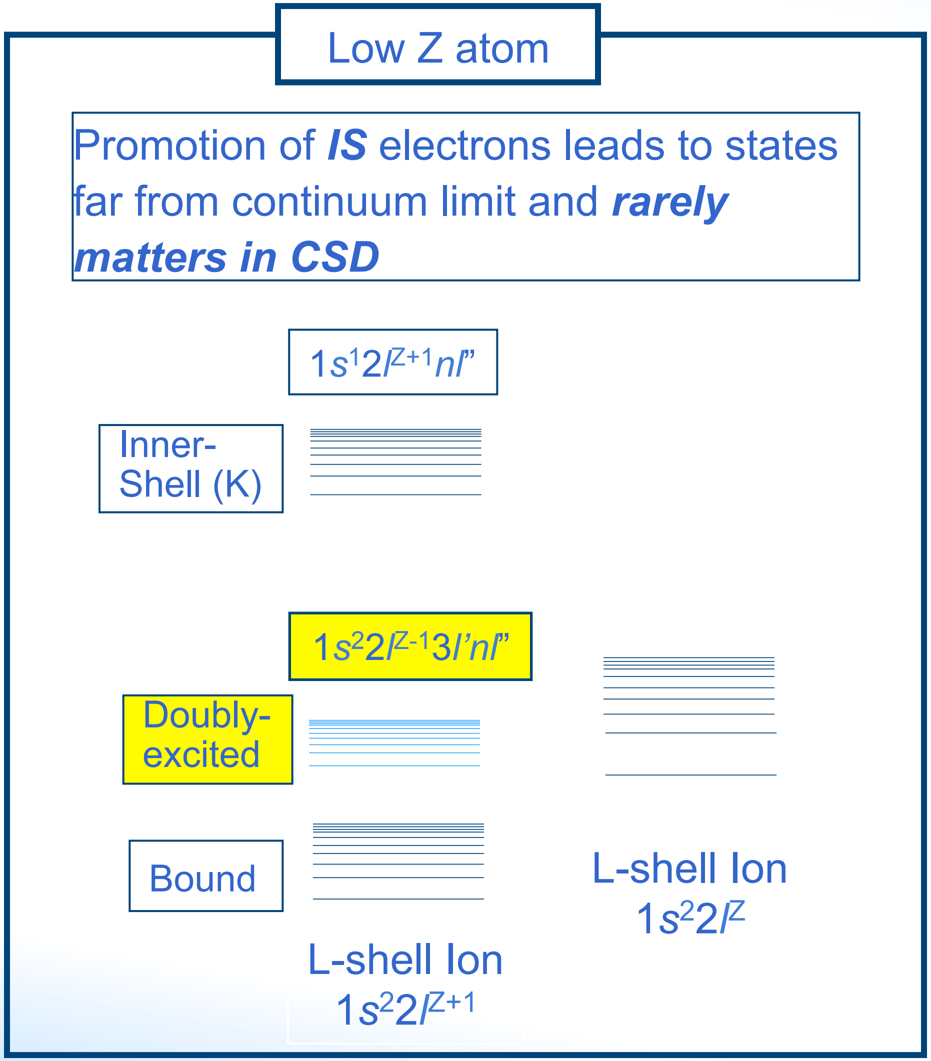
- High Energy Density Physics, v.1, p.3 (2005) cited by ~ 300 times since 2005

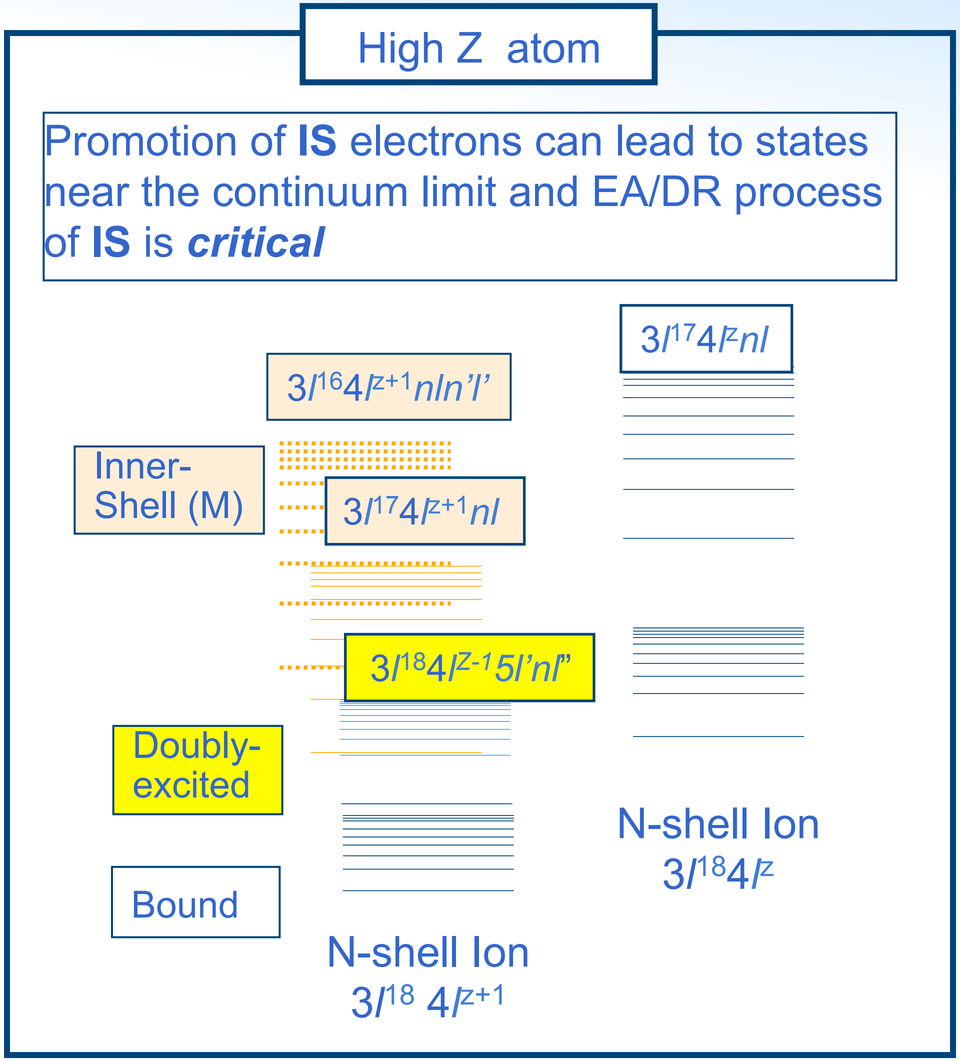
FLYCHK Model :
simple, but complete



- Screened hydrogenic energy levels with relativistic corrections
- Relativistic Hartree-Slater oscillator strengths and photoionization cross-sections (J. Scofield, M. Chen)
- Fitted collisional cross-section to PWB approximation
- Semi-empirical cross-sections for collisional ionization
- Detailed counting of autoionization and electron capture processes
- Continuum lowering (Stewart-Pyatt, Ecker-Kroll)

Dielectronic Recombination & Excitation Autoionization

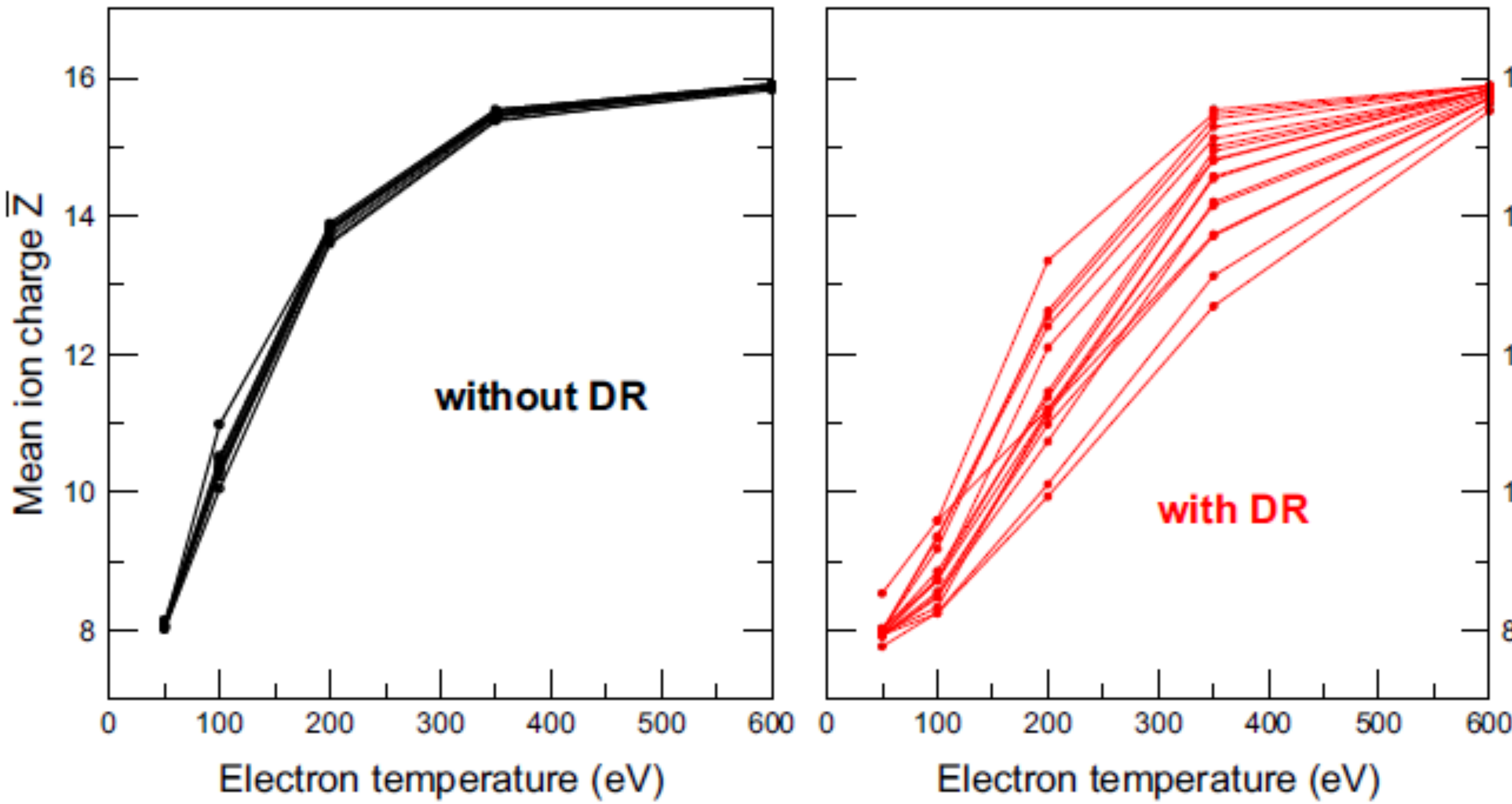




Excitation autoionization (EA) /Dielectronic recombinationa (DR) processes are modeled with doubly-excited and inner-shell (IS) excited states

NLTE Kinetics Model Issues: DR & EA

NLTE6 code comparison workshops (2011)
Mean ion charges for Ar case, $n_e = 10^{12}$ cm^{-3}



NLTE Workshops, Chung et al. HEDP 9, 645 (2013)

Total line emissivity and energy-dependent spectral intensity in the STA formalism

Total line emissivity: plots show approximate line emission spectra and provides information on energy range of dominant emission

$$S = n_u A_{ul} E_{ul} / N_e \quad \text{[eVcm}^3\text{/s/atom]}$$

Spectral emissivity is computed in the STA (Super Transition Array) formalism using configuration-average atomic data generated by the DHS (Dirac-Hartree-Slater) code (M.Chen)

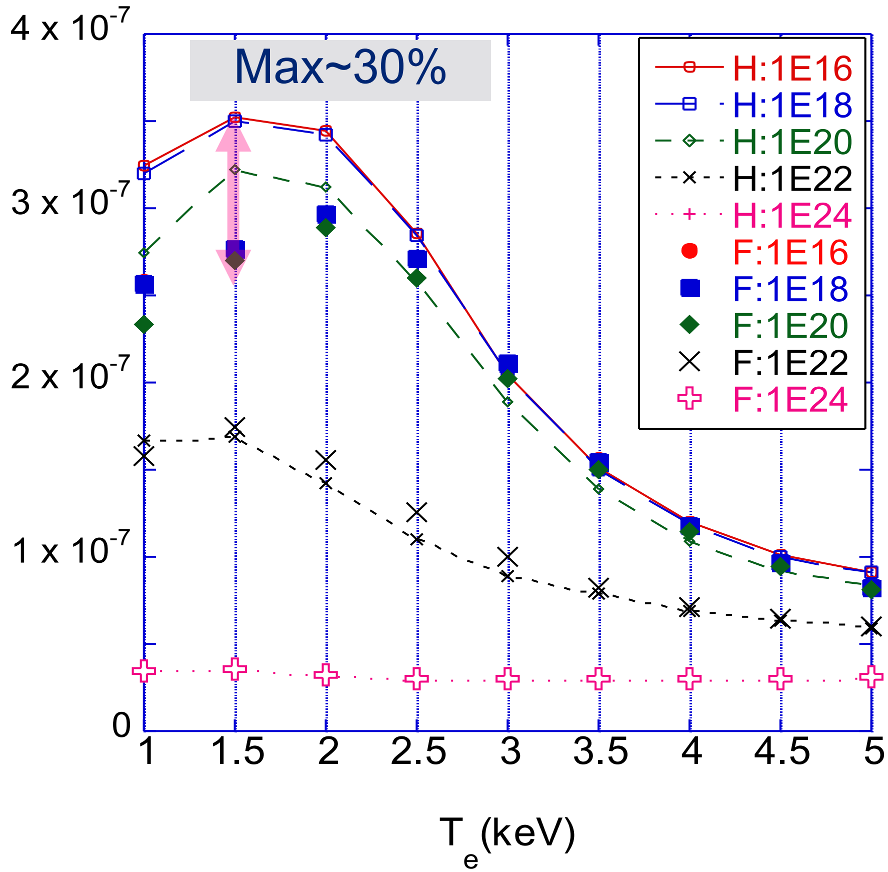
$$\eta(\nu) = n_A A_{AB} E_{AB} \phi(\nu) = \frac{n_A \sum_{i \in A: j \in B} g_i \exp(-E_i / kT_e) A_{ij} E_{ij} \phi(\nu)}{\sum_{i \in A: j \in B} g_i \exp(-E_i / kT_e)} \quad \text{[ergs/s/Hz/cm}^3\text{/ster]}$$

$$A_{AB} = \frac{\sum_{i \in A: j \in B} g_i \exp(-E_i / kT_e) A_{ij}}{\sum_{i \in A: j \in B} g_i \exp(-E_i / kT_e)} \qquad E_{AB} = \frac{\sum_{i \in A: j \in B} g_i \exp(-E_i / kT_e) A_{ij} E_{ij}}{\sum_{i \in A: j \in B} g_i \exp(-E_i / kT_e) A_{ij}} \qquad \mu_{AB}^2 = \left[\frac{\sum_{i \in A: j \in B} g_i \exp(-E_i / kT_e) A_{ij} E_{ij}^2}{\sum_{i \in A: j \in B} g_i \exp(-E_i / kT_e) A_{ij}} \right]^2 - E_{AB}^2$$

APPLICATIONS

FLYCHK radiative loss rates give quick estimates

Calculated Kr radiative cooling rates per N_e [eV/s/atom/cm^{-3}]



Better agreement for higher N_e

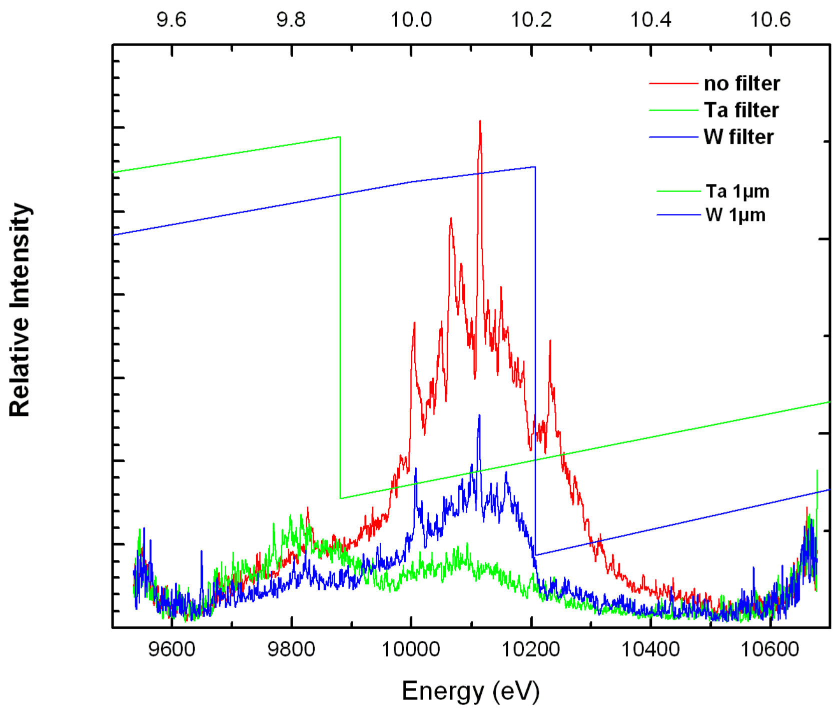
# of radiative transitions

Ion	HULLAC+DHS	FLYCHK
1	3049	45
2	27095	107
3	30078	89
4	404328	140
5	3058002	140
6	5882192	140
7	7808014	140
8	6202123	140
9	5544814	140
10	1050919	131
11	841094	122
sum	30,851,708	1334
Time	~2 days	~mins

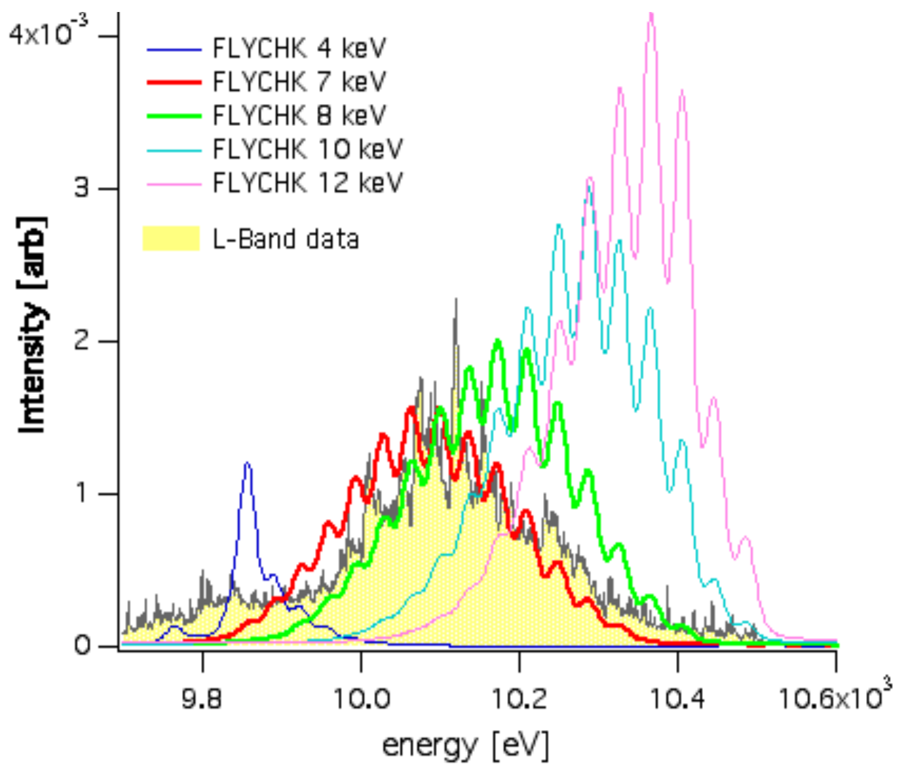
Gold ionization balance in high temperature hohlraum experiments

- High-T hohlraum reach temperatures: ~ 10 keV
- Spectrum from n_e ~ $4x10^{21}$ cm^{-3}, T_e ~ 7-10 keV measured for first time

L-shell gold spectra (K. Widmann)

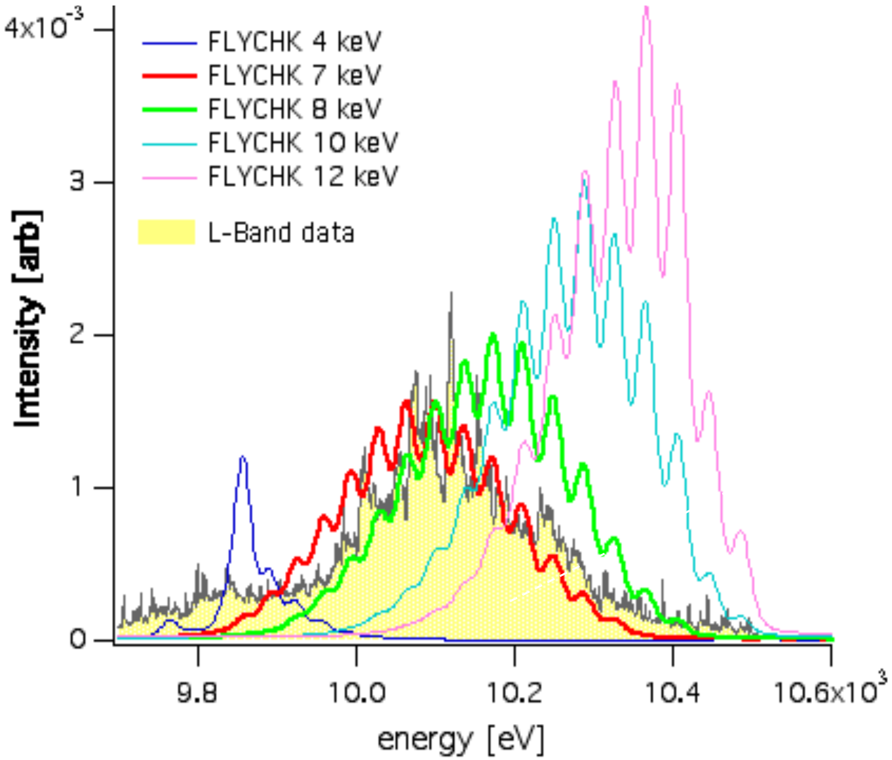


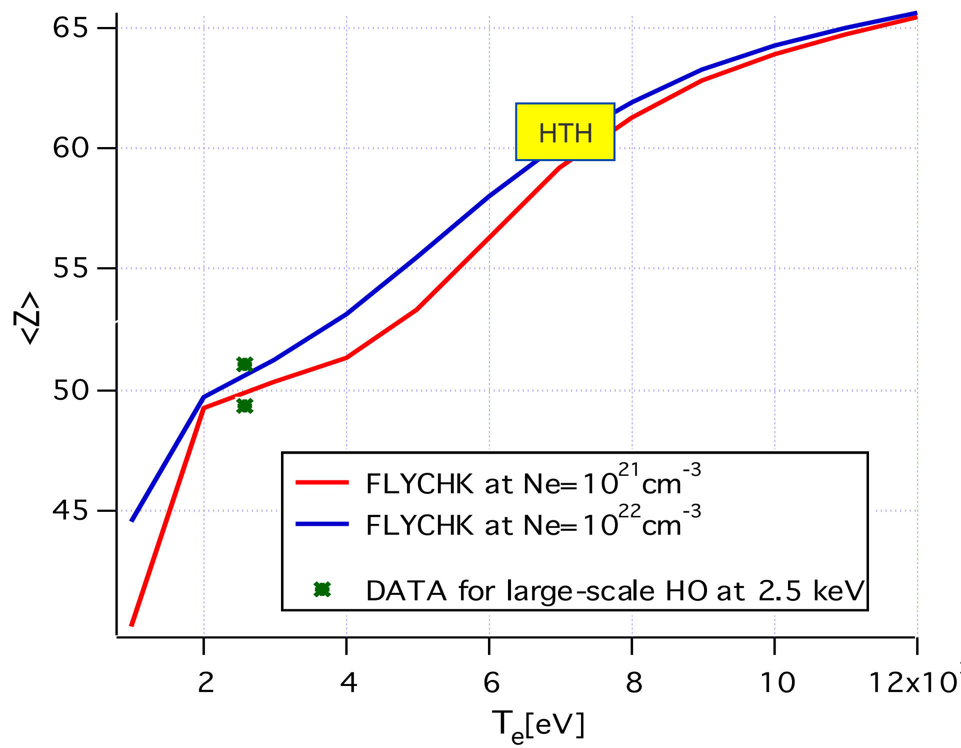
FLYCHK Spectra



Steady-State Spectra and <Z> over a wide range of conditions

FLYCHK Gold ionization balance



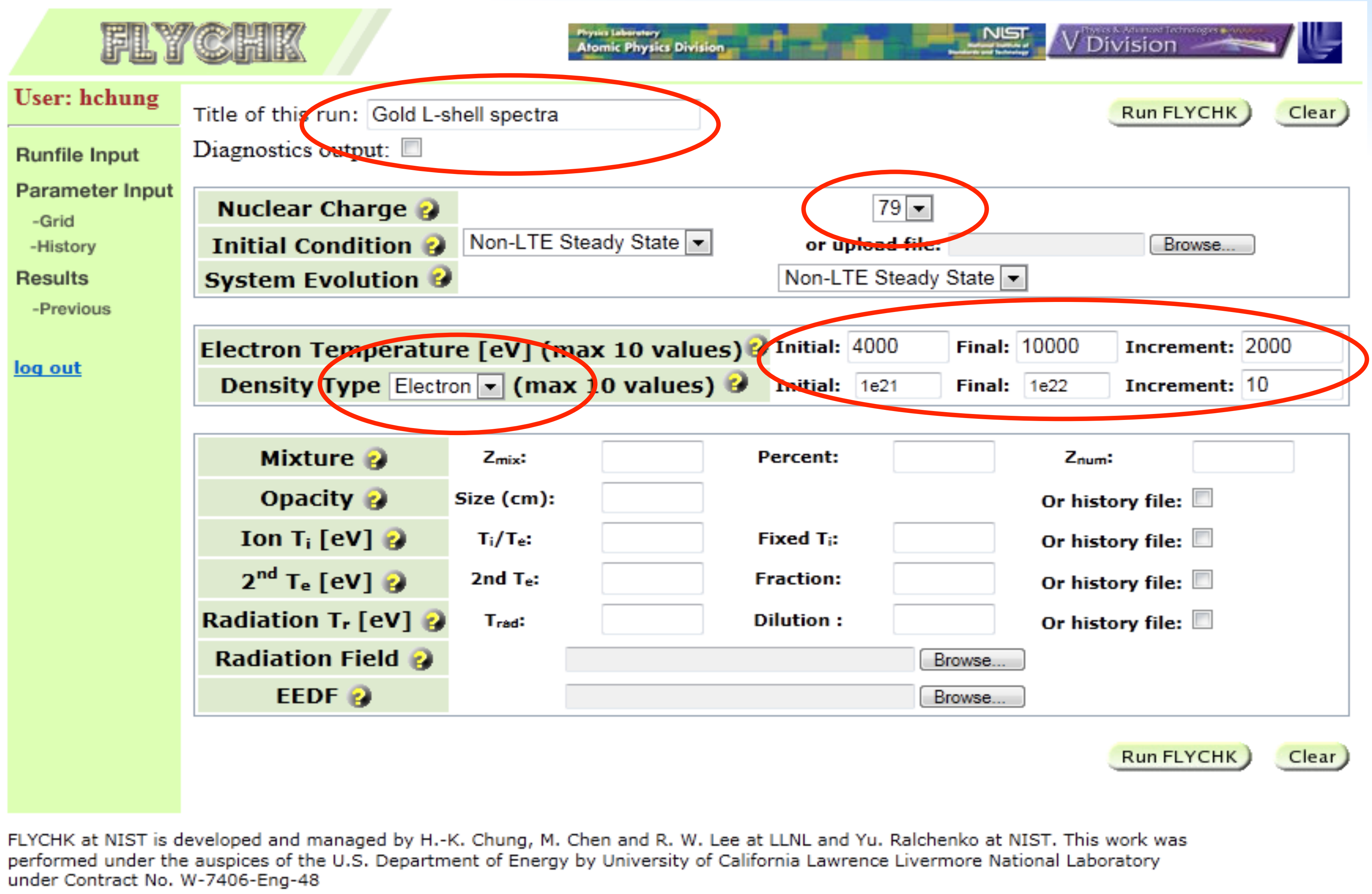


FLYCHK gives an estimate of Gold Charge state distributions and L-shell spectra

FLYCHK gives an estimate of <Z> for a wide range of plasma conditions, which is suitable for experimental design and analysis

HEDP 4, 78 (2008)

Long pulse laser plasmas: Gold L-shell spectroscopy



Long pulse laser plasmas: Gold L-shell spectroscopy

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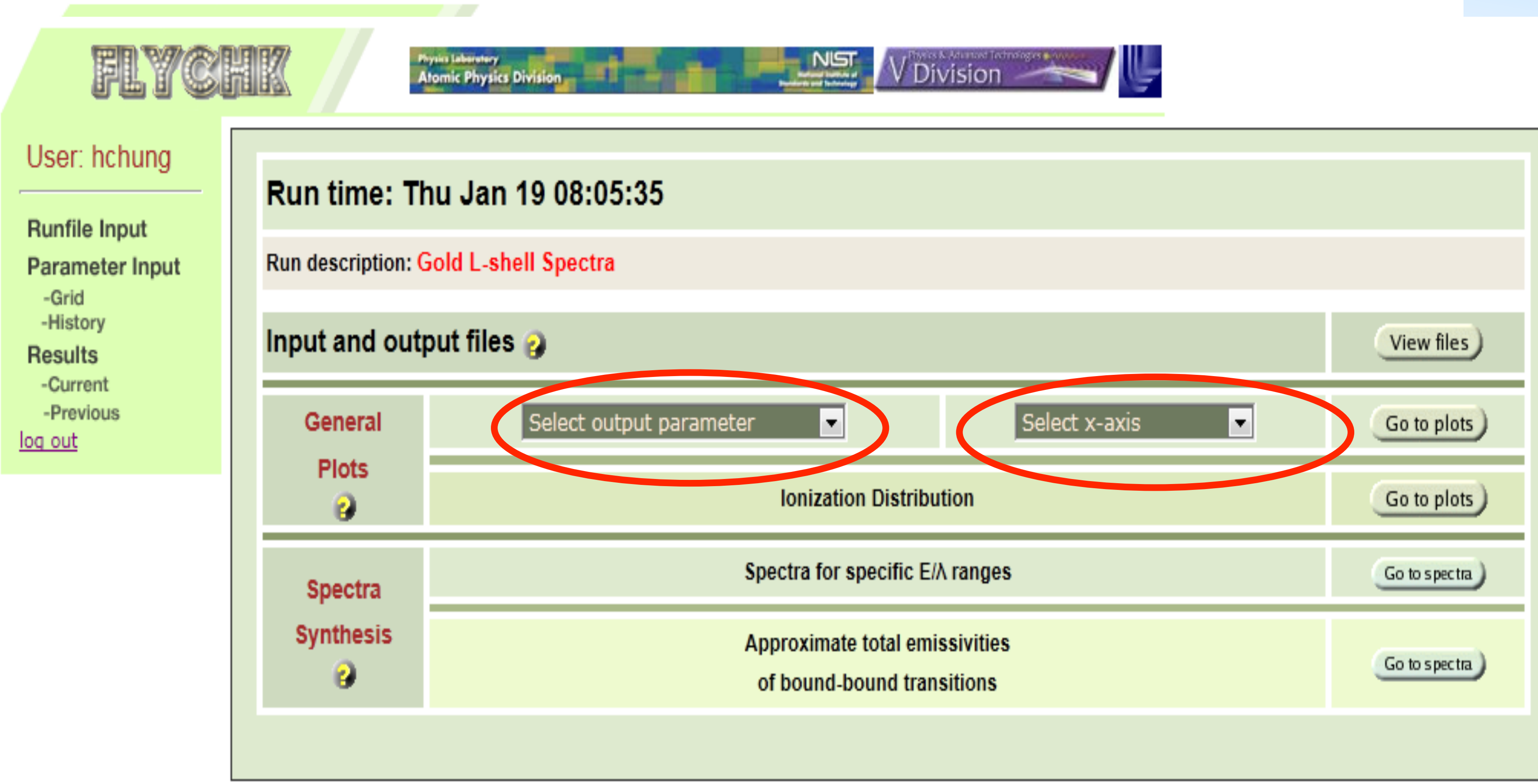

FLYCHK at NIST is developed and managed by H.-K. Chung, M. Chen and R. W. Lee at LLNL and Yu. Ralchenko at NIST. This work was performed under the auspices of the U.S. Department of Energy by University of California Lawrence Livermore National Laboratory under Contract No. W-7406-Eng-48 (H.-K.C., M.C., and R.W.L.) and the Office of Fusion Energy Sciences of the U.S. Department of Energy (Yu.R.).

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Long pulse laser plasmas: Gold L-shell spectroscopy

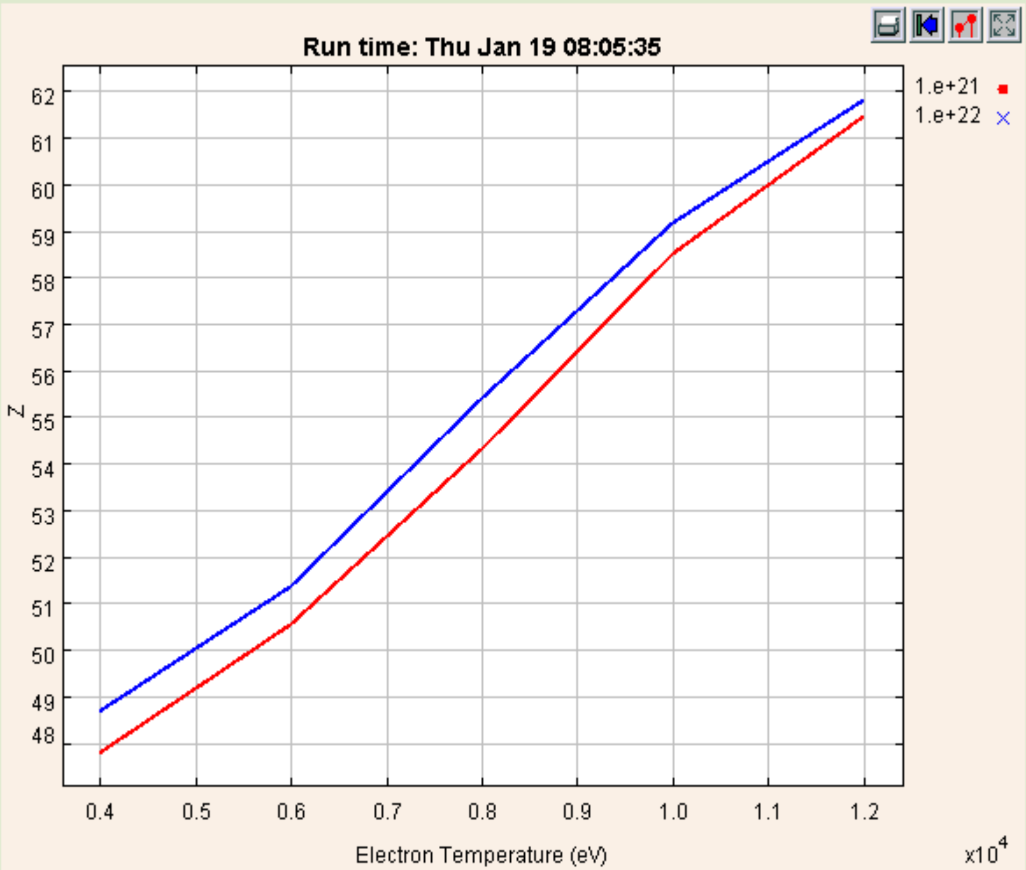
User: hchung

- Runfile Input
- Parameter Input
  - -Grid
  - -History
- Results
  - -Current
  - -Previous
- log out

Element: Au

Comments: Gold L-shell Spectra

The Java applet (PtPlot v.5.5) requires Java installed.



Static plots: PDF | PS

List of Selected Cases	
Dens	Data
1.e+21	file
1.e+22	file

http://nlte.nis...

nist.gov

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```
# Dens: 1.e+21
# Parameter: Z
4.0000E+03        4.7775E+01
6.0000E+03        5.0538E+01
8.0000E+03        5.4306E+01
1.0000E+04        5.8517E+01
1.2000E+04        6.1452E+01
```

100%

Long pulse laser plasmas: Gold L-shell spectroscopy

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FLYCHK

Physics Laboratory Atomic Physics Division NIST

Physics & Advanced Technologies V Division

User: hchung

- Runfile Input
- Parameter Input
  - -Grid
  - -History
- Results
  - -Current
  - -Previous
- log out

Plot | Clear

Run time: Thu Jan 19 08:05:35

Run description: Gold L-shell Spectra

Plot ionization distribution at given grid cases

Select density [Check all]

1.000e+21 ☑	1.000e+22 ☐

Select temperature [Uncheck all]

4000 ☑	6000 ☑	8000 ☑	10000 ☑	12000 ☑

Plot options

Log X ☐	X_{min}	X_{max}	Show data values on the plot ☐
Log Y ☐	Y_{min}	Y_{max}	Remove grid lines on the plot ☐

Plot | Clear

FLYCHK at NIST is developed and managed by H.-K. Chung, M. Chen and R. W. Lee at LLNL and Yu. Ralchenko at NIST. This work was performed under the auspices of the U.S. Department of Energy by University of California Lawrence Livermore National Laboratory under Contract No. W-7406-Eng-48 (H.-K.C., M.C., and R.W.L.) and the Office of Fusion Energy Sciences of the U.S. Department of Energy (Yu.R.).

Long pulse laser plasmas: Gold L-shell spectroscopy

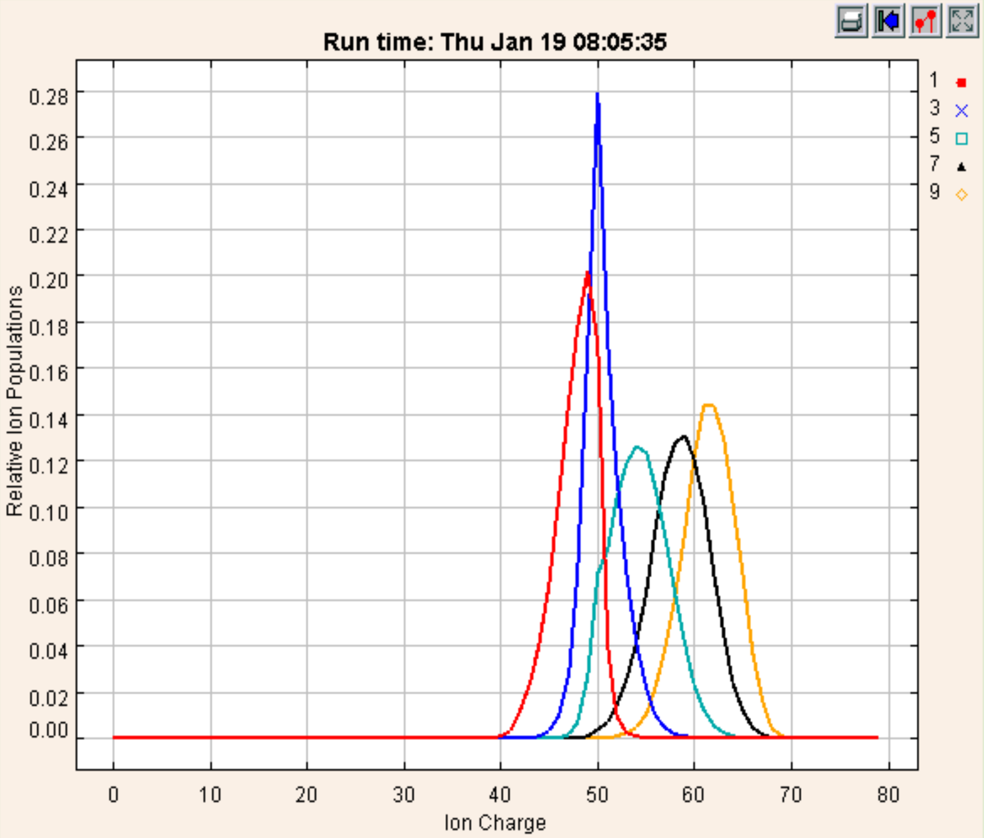
User: hchung

- Runfile Input
- Parameter Input
  - -Grid
  - -History
- Results
  - -Current
  - -Previous
- log out

Element: Au

Comments: Gold L-shell Spectra

The Java applet (PtPlot v.5.5) requires Java installed.



Static plots: PDF | PS

List of Selected Cases			
Case #	Temperature	Density	Data
1	4000.0	1.e+21	file
3	6000.0	1.e+21	file
5	8000.0	1.e+21	file
7	10000.0	1.e+21	file
9	12000.0	1.e+21	file

http://nlte.nis...

nist.gov

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45	6.12E-05
46	3.38E-04
47	1.63E-03
48	6.84E-03
49	2.67E-02
50	7.13E-02
51	8.13E-02
52	1.03E-01
53	1.19E-01
54	1.26E-01
55	1.23E-01
56	1.09E-01
57	8.78E-02
58	6.21E-02
59	3.99E-02
60	2.32E-02
61	1.23E-02
62	5.32E-03
63	2.08E-03
64	7.21E-04
65	2.19E-04
66	4.86E-05

Long pulse laser plasmas: Gold L-shell spectroscopy

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User: hchung

Runfile Input
Parameter Input
-Grid
-History
Results
-Current
-Previous
log out

Plot | Clear

Run time: Thu Jan 19 08:05:35

Run description: Gold L-shell Spectra

Plot spectrum for a specific E/λ range

Select parameter, x-axis units and range				
Parameter:	Intensity ◉	Emissivity ○ total	Opacity ○ bound-bound	Optical Depth ○
Units:	energy [eV] ◉			
Range:	low limit 9600		upper limit 10600	

Select either all cases (left) or a subset of cases (right)

Plot spectra for all cases: ☐

case	temperature	density
1 ☑	4000.0	1.e+21
2 ☐	4000.0	1.e+22
3 ☑	6000.0	1.e+21
4 ☐	6000.0	1.e+22
5 ☑	8000.0	1.e+21
6 ☐	8000.0	1.e+22
7 ☑	10000.0	1.e+21
8 ☐	10000.0	1.e+22
9 ☑	12000.0	1.e+21
10 ☐	12000.0	1.e+22

Plot options			
Log X ☐	X_{min} 9600	X_{max} 10600	Show data values on the plot ☐
Log Y ☐	Y_{min}	Y_{max}	Remove grid lines on the plot ☐

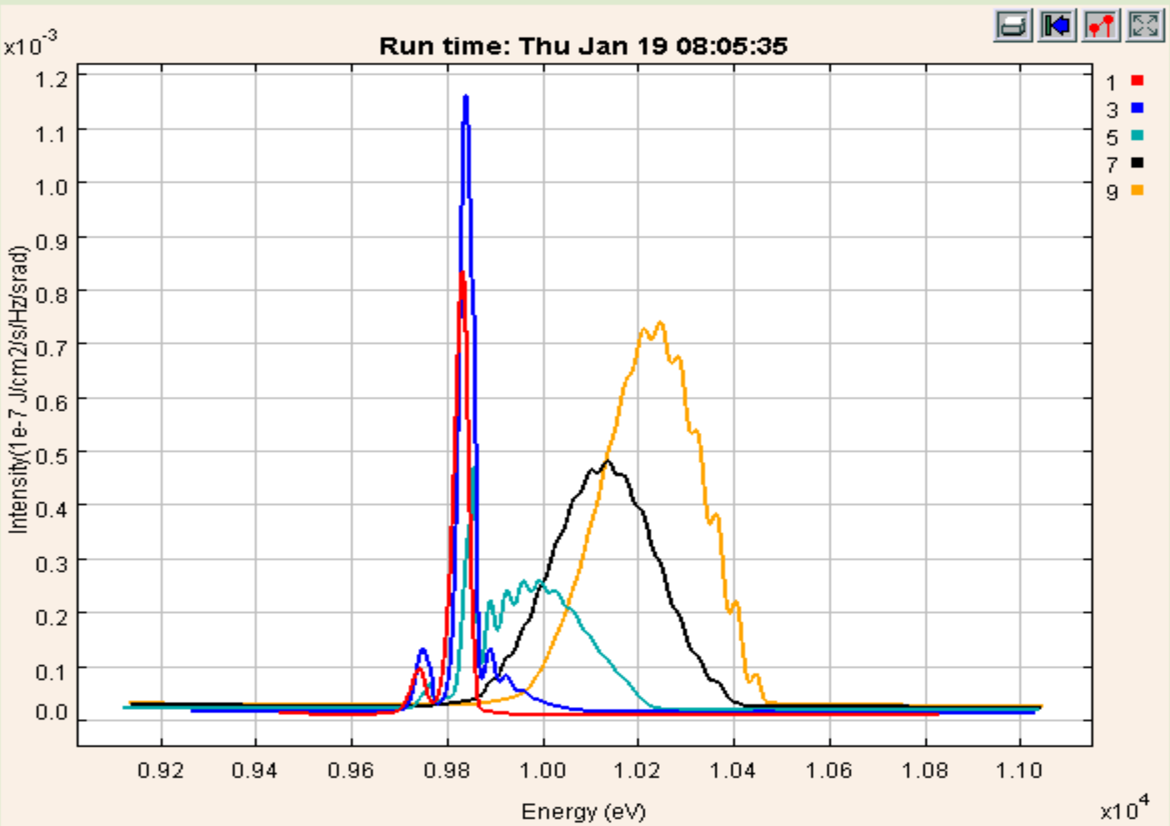
Plot | Clear

Long pulse laser plasmas: Gold L-shell spectroscopy

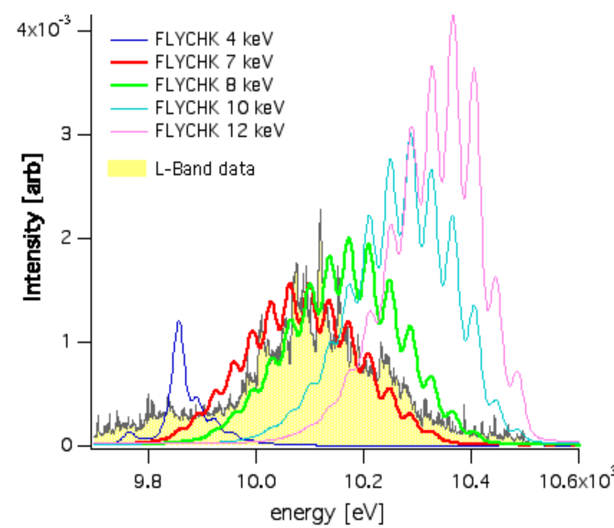
FLYSPEC is running...

Log file

The Java applet (PtPlot v.5.5) requires Java installed.



List of Selected Cases				
Case #	Temp	Dens	Spectrum	Lines
1	4000.0	1.e+21	file	lines
3	6000.0	1.e+21	file	lines
5	8000.0	1.e+21	file	lines
7	10000.0	1.e+21	file	lines
9	12000.0	1.e+21	file	lines
Opacities etc.			Spectra etc.	
All files in an archive:				zip



Long pulse laser plasmas: Gold L-shell spectroscopy

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User: hchung

Runfile Input
Parameter Input
-Grid
-History
Results
-Current
-Previous
log out

Plot Clear

Run time: Thu Jan 19 08:05:35

Run description: Gold L-shell Spectra

Plot approximate total emissivities for bound-bound transitions

Select x-axis units and range for total emissivities

Units: energy [eV]

Select either all cases (left) or a subset of cases (right)

Plot spectra for all cases: ☐

case	temperature	density
1 ☑	4000.0	1.e+21
2 ☐	4000.0	1.e+22
3 ☑	6000.0	1.e+21
4 ☐	6000.0	1.e+22
5 ☑	8000.0	1.e+21
6 ☐	8000.0	1.e+22
7 ☑	10000.0	1.e+21
8 ☐	10000.0	1.e+22
9 ☑	12000.0	1.e+21
10 ☐	12000.0	1.e+22

Plot options

Log X ☑	X_{min}	X_{max}	Show data values on the plot ☐
Log Y ☑	Y_{min}	Y_{max}	Remove grid lines on the plot ☐

Long pulse laser plasmas: Gold L-shell spectroscopy

User: hchung

Runfile Input

Parameter Input

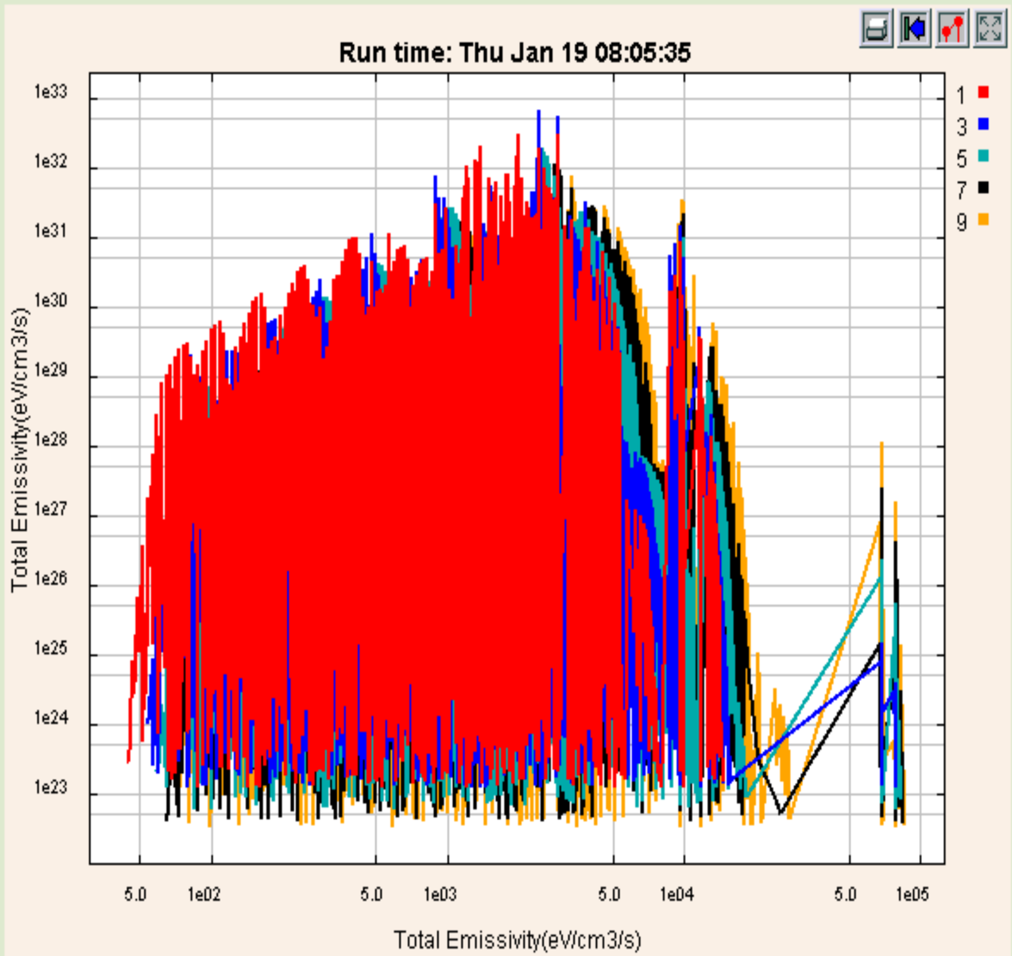
- -Grid
- -History

Results

- -Current
- -Previous

log out

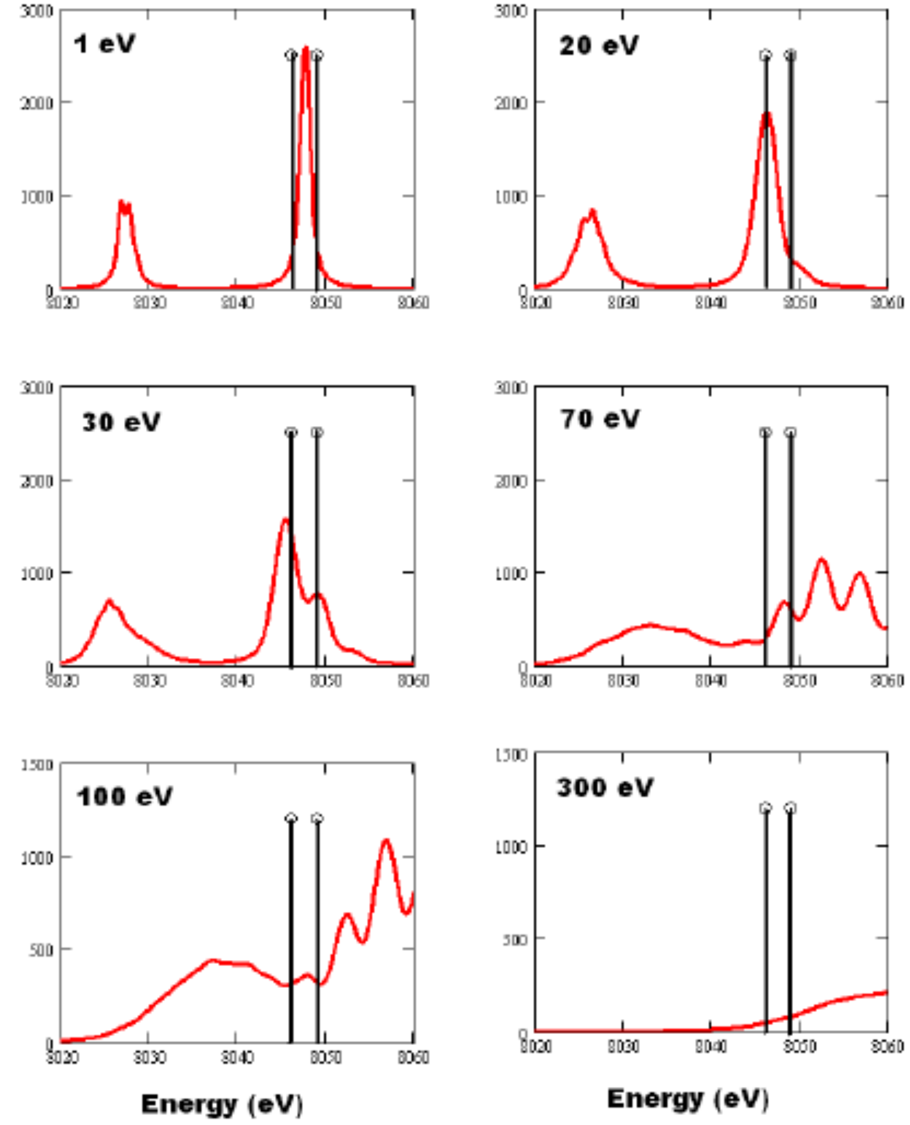
The Java applet (PtPlot v.5.5) requires Java installed.

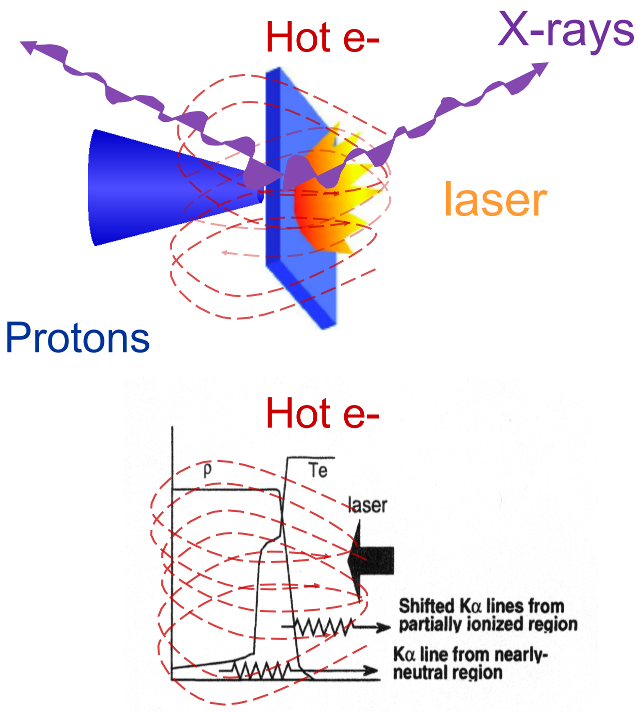


Help on spectra

List of Selected Cases			
Case #	Temp	Dens	Spectrum
1	4000.0	1.e+21	file
3	6000.0	1.e+21	file
5	8000.0	1.e+21	file
7	10000.0	1.e+21	file
9	12000.0	1.e+21	file
Opacities etc.		Spectra etc.	
All files in an archive:			zip

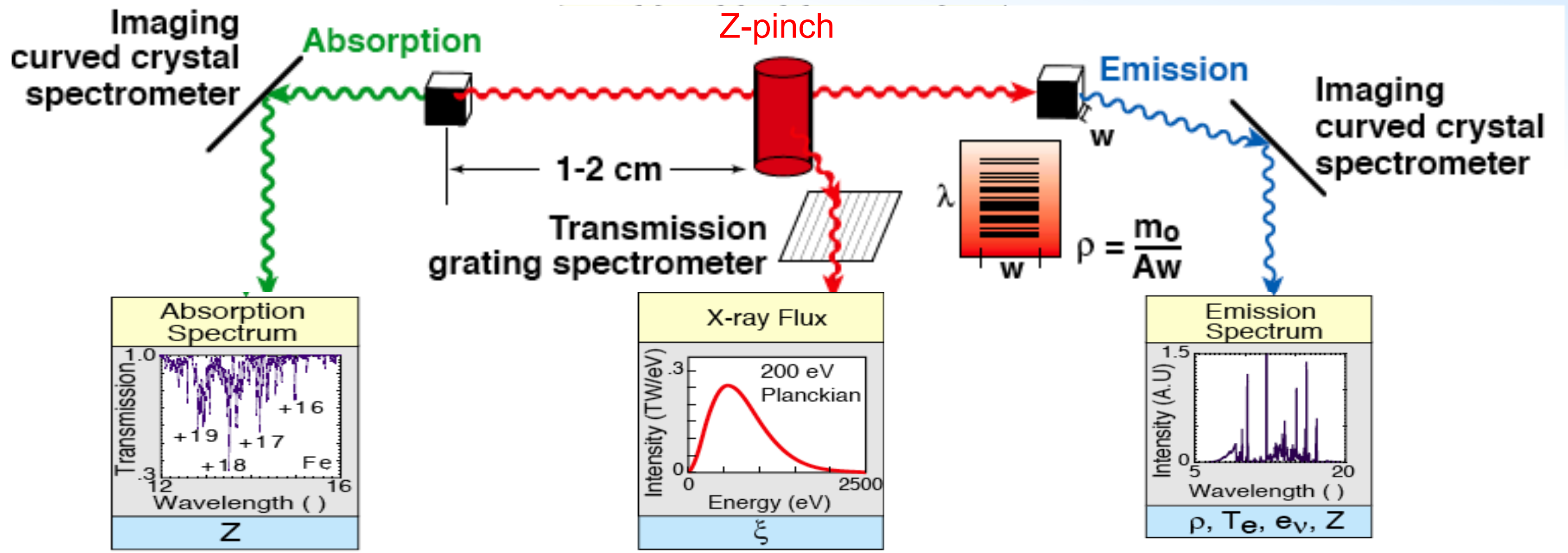
Short Pulse Laser Plasma: Shift and Broadening of K-shell line emission





Phys. Plasmas
14, 023102 (2007)

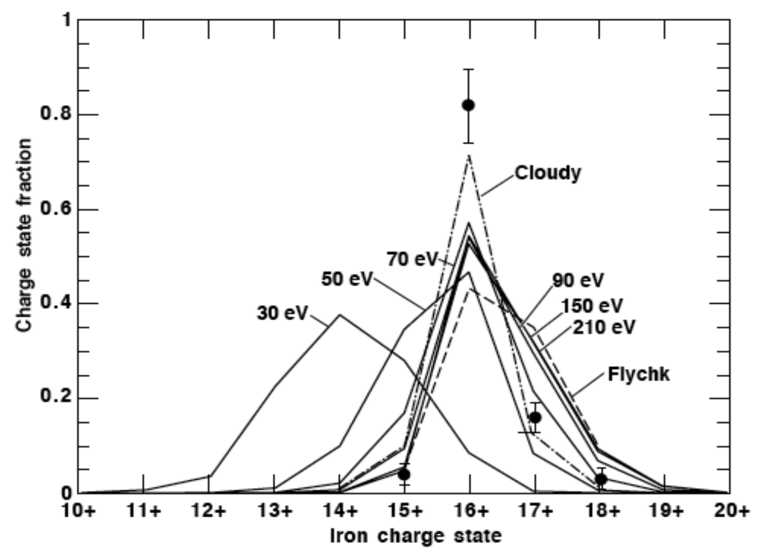
Z-pinch Photoionized Plasmas



ξ=20-25 ergs-cm/s

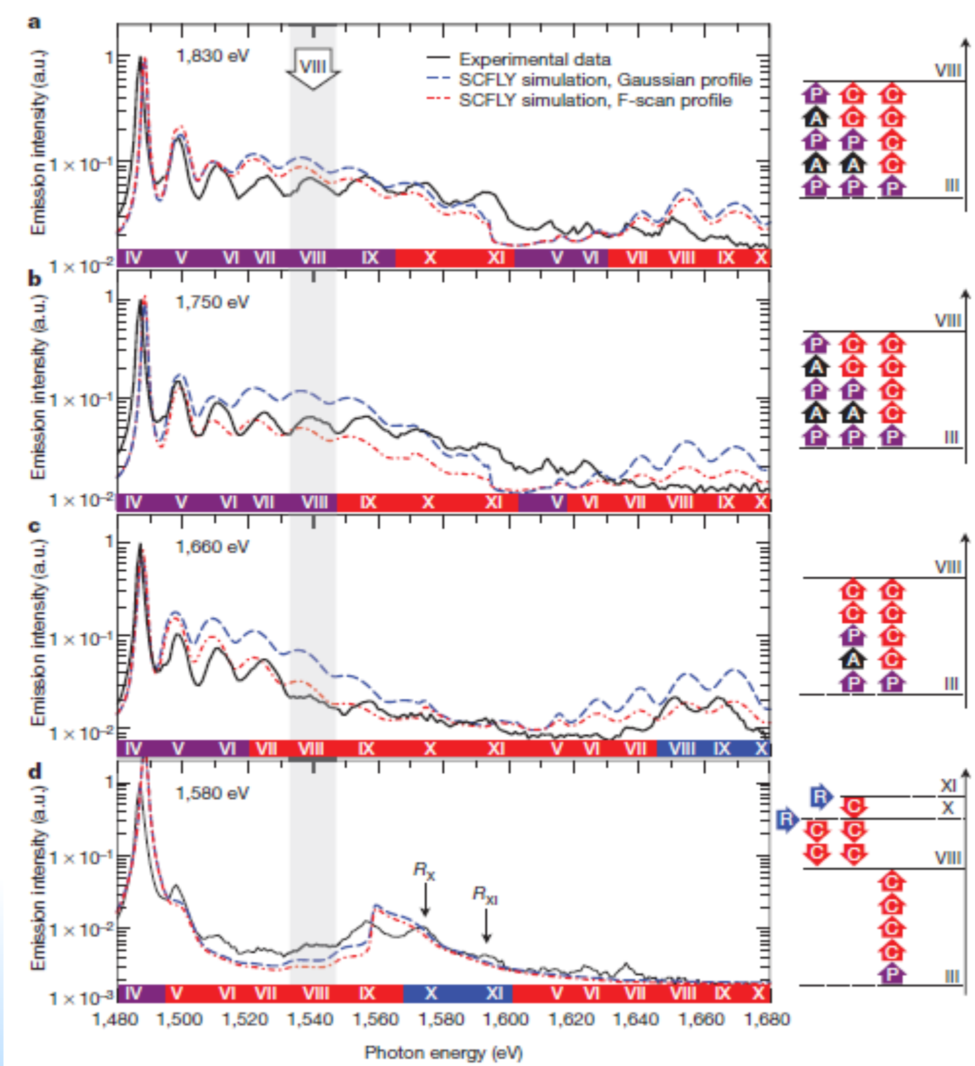
The agreement between measured and calculated CSDs is reasonable at T_e = 150 eV:

- Cloudy: Astrophysics code
- Galaxy: NLTE kinetics code
- FLYCHK: NLTE kinetics code



PRL 93 055002 (2004)

XFEL driven ionization processes in solid target (SCFLY)



- **P** - K-shell photoionization
- **A** - KLL Auger recombination
- **C** - L-shell collisional ionization
- **R** - K-L resonant excitation

- 1 micron thick Al foil (9.1±0.8 μm^2)
- 80 fs X-ray pulse at 1560-1830 eV
- 10^{12} photons w/ 0.4% bandwidth
- 1.1 ×10^{17} W/cm^2

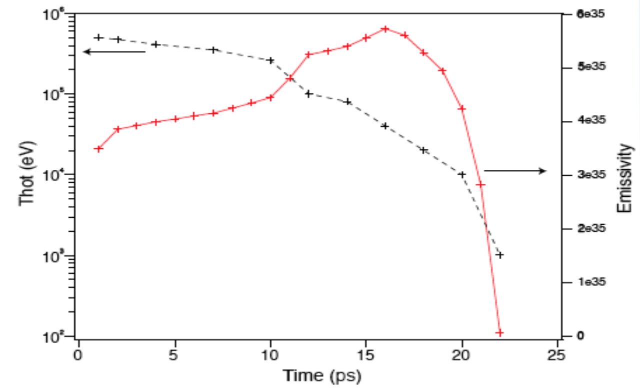
- With experimentally determined XFEL intensity distribution, the agreement of calculation and measurement is better

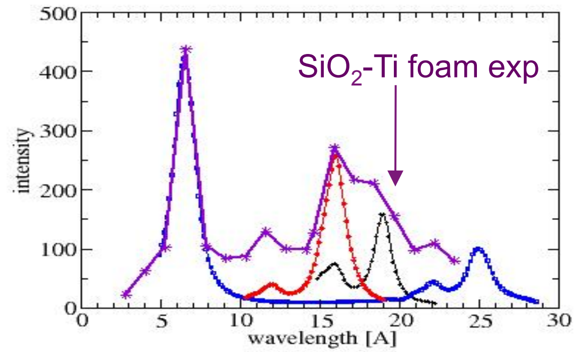
- S. Vinko, Nature 482, 59 (2012)
- Ciricosta, PRL, 109, 065002 (2012)
- B. I. Cho, PRL 109, 245003 (2012)
- D. S. Rackstraw, PRL 114, 015003 (2015)
- P. Sperling, PRL 115, 115001 (2015)

Applications to Plasma Research

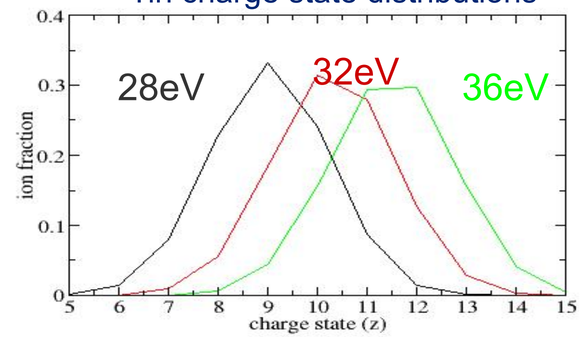
- **Short-pulse laser-produced plasmas**
  - Arbitrary electron energy distribution function
  - Time-dependent ionization processes
  - K-α shifts and broadening: diagnostics
- **Long-pulse laser-produced plasmas**
  - Average charge states
  - Spectra from a uniform plasma
  - Gas bag, Hohlraum (H0), Underdense foam
- **Z-pinch plasmas**: photoionizing plasmas
- **Proton-heated plasmas**: warm dense matter
- **EBIT**: electron beam-produced plasmas
- **EUVL**: Sn plasma ionization distributions
- **TOKAMAK**: High-Z impurities

Time-dependent Ti Kα emissivities





Tin charge state distributions



Advantages and Limitations

http://nlte.nist.gov/FLY

Advantages: simplicity and versatility→ applicability

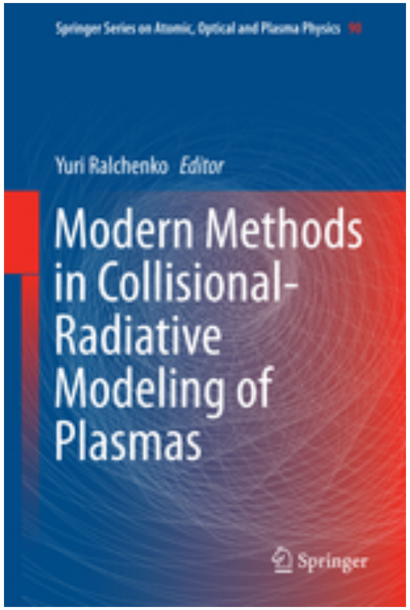
- <Z> for fixed any densities: electron, ion or mass
- Mixture-supplied electrons (eg: Argon-doped hydrogen plasmas)
- External ionizing sources : a radiation field or an electron beam.
- Multiple electron temperatures or arbitrary electron energy distributions
- Optical depth effects

Caveats: simple atomic structures and uniform plasma approximation

- Not valid for neutral and near neutral conditions
- Less accurate when $\Delta n = 0$ transitions become prevalent
- Less accurate when metastable states populations are important
- Less accurate spectral intensities for non-K-shell lines
- Less accurate for coronal and for LTE plasmas
- When spatial gradients and the radiation transport affect population significantly

Modern Methods in CR Modeling of Plasmas, Springer 2016 (Yu. Ralchenko)

- Balancing Detail and Completeness in Collisional-Radiative Models
- Self-consistent Large-Scale Collisional-Radiative Modeling
- Generalized Collisional Radiative Model Using Screened Hydrogenic Levels
- Collisional-Radiative Modeling for Radiation Hydrodynamics Codes
- Average Atom Approximation in Non-LTE Level Kinetics
- Spectral Modeling in Astrophysics—The Physics of Non-equilibrium Clouds
- Validation and Verification of Collisional-Radiative Models
- Collisional-Radiative Modeling and Interaction of Monochromatic X-Rays with Matter



http://www.springer.com/in/book/9783319275123

IAEA

60 Years

Atoms for Peace and Development

Thank you!

The Abdus Salam International Centre for Theoretical Physics

www.ictp.it

Joint ICTP-IAEA School on Atomic Processes in Plasmas

27 February – 3 March 2017

(ICTP, Miramare - Trieste, Italy)

The Abdus Salam International Centre for Theoretical Physics (ICTP) and the International Atomic Energy Agency (IAEA) will jointly organize this School to be held at ICTP in Miramare, Trieste, Italy, from 27 February to 3 March 2017. The event will provide advanced training in theoretical and computational methods for atomic processes in plasmas. The schedule will feature lectures by international experts, exposure to modern scientific computer codes, posters and discussion sessions, with good time available for personal interaction. We expect participants from around the world.

PURPOSE

The conditions in laboratory and industrial plasmas, laser-produced plasmas, astrophysical plasmas, and warm and hot dense matter are determined by numerous atomic processes including electron-ion and heavy particle collisions, photon-induced processes, and radiation emission and transport. Even in fully ionized plasmas, which are typical for fusion energy research, atomic processes are very important as they underlie all impurity-based spectroscopic diagnostics.

The school will assist qualified Ph.D. students and early career researchers to develop their quantitative understanding of collisional and radiative atomic processes in plasmas with applications to fusion energy research, astrophysical science, laser-produced plasmas and other plasma environments. Participants will become acquainted with their international peers and will have a unique opportunity to establish links for their mutual support. Knowledge transfer will be facilitated between individuals from developed and developing countries.

TOPICS

- Principles of spectroscopic diagnostics of plasma;
- Collisional-radiative modelling and calculation of plasma spectra;
- Computational methods for atomic structure and collisions;
- Simulations of non-Maxwellian and highly transient plasmas;
- Radiation transport effects on plasma properties and plasma diagnostics;
- Methods for analysis of spectral line shapes and profiles;
- Online codes for calculation of ionization distributions and spectra.

The School will consist of lectures, computer labs and participant presentations. For the most up-to-date information please see the meeting web page at IAEA: https://www-amdis.iaea.org/Workshops/ICTP2017/

GRANTS

A limited number of grants are available to support the travel and living expenses of selected participants, with priority given to participants working in a developing country and who are at the early stages of their career.

There is no registration fee for attending the school.

HOW TO APPLY FOR PARTICIPATION

The Online Application can be accessed at: http://indico.ictp.it/event/7950/ Comprehensive instructions will guide you step-by-step on how to fill out and submit the application form. After your profile information is complete and before submitting the application you will be asked to attach a one-page abstract of a scientific contribution to the poster session of the school. Kindly send all file attachments in Word or PDF format.

Secretariat: *Ms. Rosa del Rio (smr 3105)*
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ICTP Home Page: http://www.ictp.it

September 2016

In cooperation with IAEA
International Atomic Energy Agency

IAEA 60 Years Atoms for Peace and Development

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DEADLINE
to request participation

20 October 2016