Kilonovae and the origin of the R-process elements

Lanthanide atomic structure and Non-LTE spectral modelling

Knut och Alice Wallenbergs Stiftelse

UPPSALA UNIVERSITET

Jon Grumer

Theoretical Astrophysics
Uppsala University

The CompAS collaboration

CompAS

Kilonovae and the origin of the ~~R-process~~ n-capture elements

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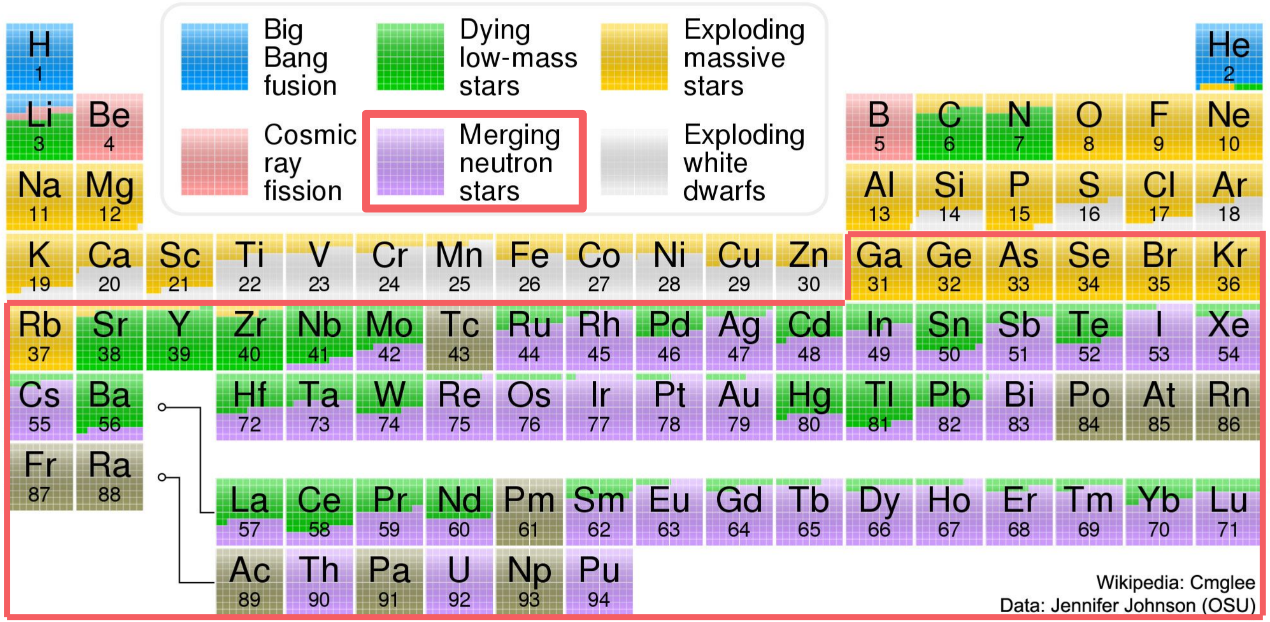
Kilonovae and the origin of the ~~R-process~~ n-capture elements



Kilonovae and the origin of the ~~R-process~~ n-capture elements


Gediminas Gaigalas
Professor
Vilnius University
Lithuania


Jacek Bieroń
Professor
Jagiellonian University
Poland


Charlotte Froese Fischer
Professor
Vanderbilt University &
NIST, Gaithersburg, USA
Publications in Google Scholar


Ian Grant
Professor
Oxford University
Great Britain
Publications in Google Scholar


Alan Hibbert
Professor
Queens University
Northern Ireland


Per Jönsson
Professor
Malmö University
Sweden
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Michel Godefroid
Professor
Université Libre de Bruxelles, Belgium
Publications in Google Scholar


Tomas Brage
Professor
Lund University
Sweden

CompAS

The international collaboration on atomic structure

Atomic structure and processes

and many more post-docs, phd's

Experiments (FTS)
Henrik Hartman ++ (LUMCAS, Malmö/Lund)
\+ the rest of the FTS community!

NLTE modelling and data (Uppsala)

Paul Barklem

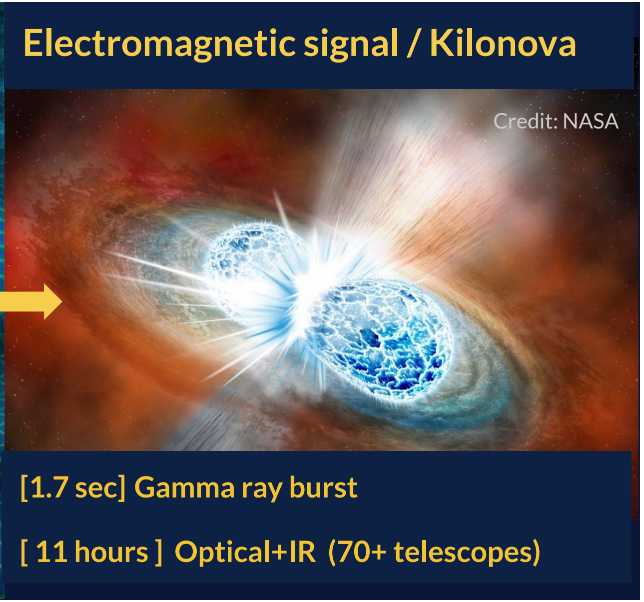
Spectral SNe modelling (Stockholm)

Anders Jerkstrand
Astronomy department, Stockholm University

Sofie Liljegren
Astronomy department, Stockholm University

Jon Grumer / jon.grumer@physics.uu.se

Kilonovae and the origin of the n-capture elements - 2 x neutron stars



Suggested Kilonova reviews: **Tanaka** 2016, **Metzger** 2017, **Cowan, Sneden & Lawler** ++ 2019

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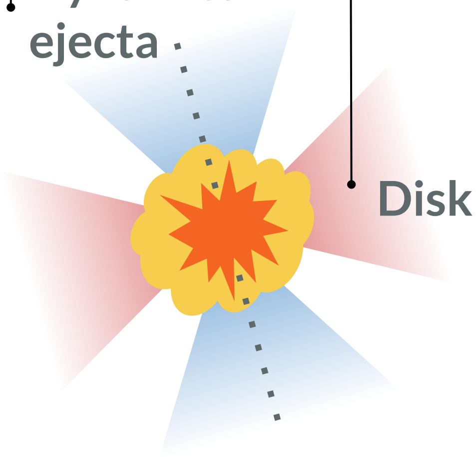
Merger → R-process → Radioactive decay

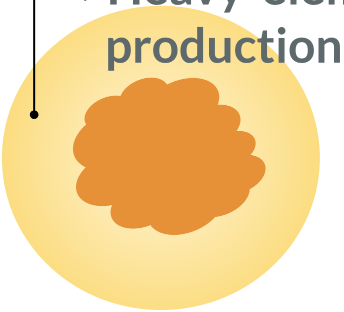
< 10 ms	≲ 100 ms	< 1s	Late phase ~ days

Dynamical ejecta

Disk Wind



Decompression → Heavy-element production



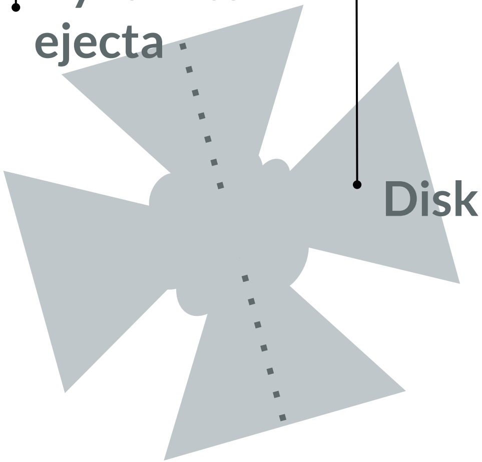
Outwards diffusion kept warm for weeks

Merger → R-process → Radioactive decay

Late phase ~ days

Dynamical ejecta

Disk Wind

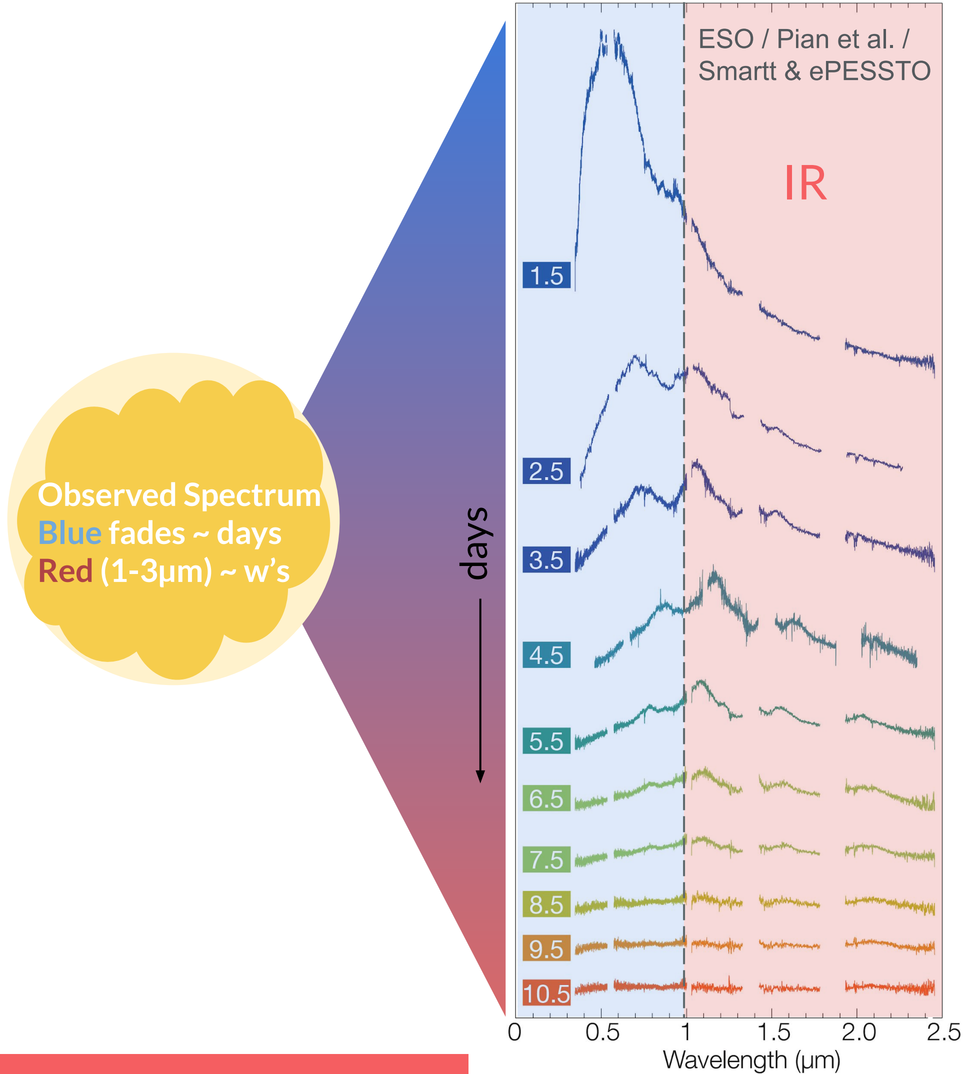


Decompression
→ Heavy-element production

Outwards diffusion
kept warm for weeks

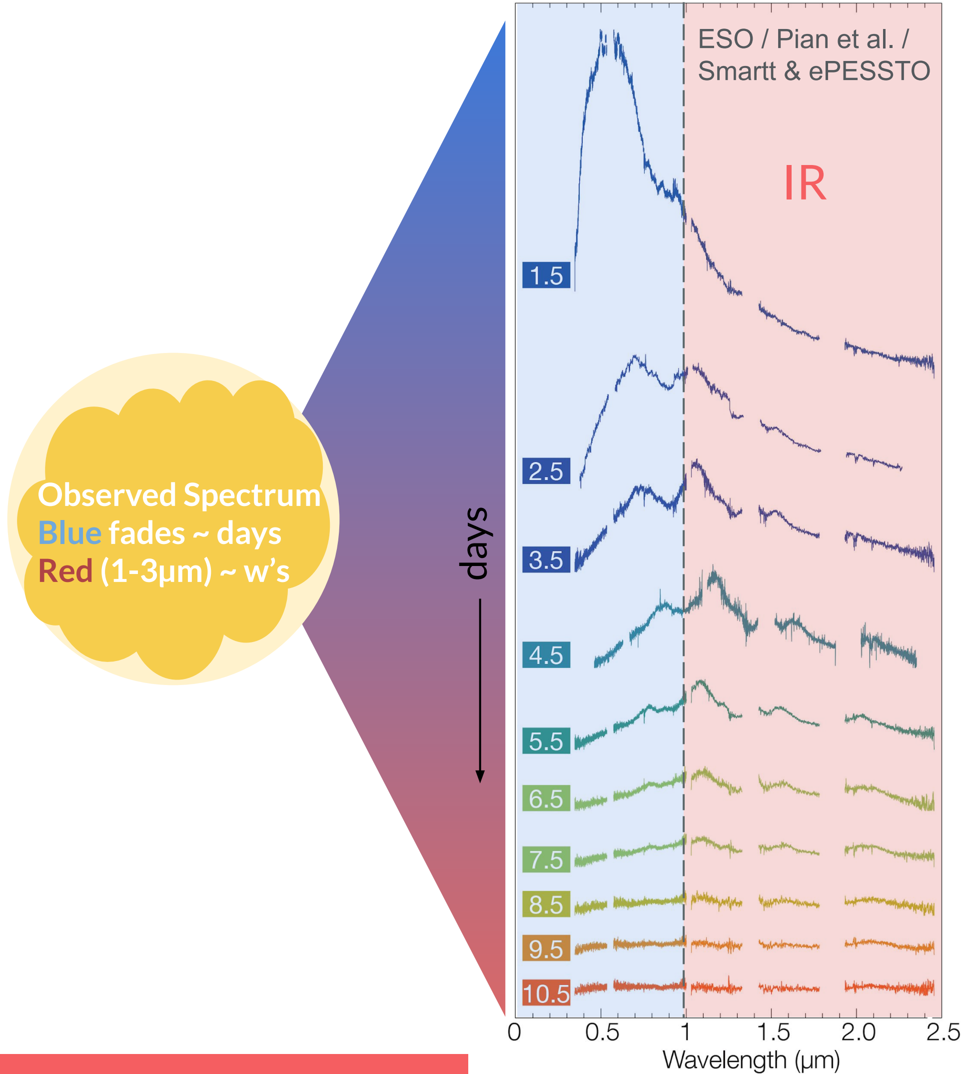
Observed Spectrum
Blue fades ~ days
Red (1-3μm) ~ w's

Jon Grumer / jon.grumer@physics.uu.se

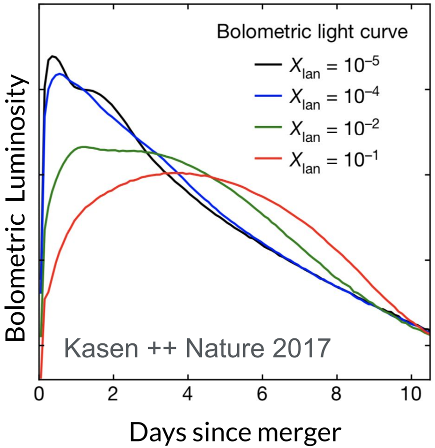


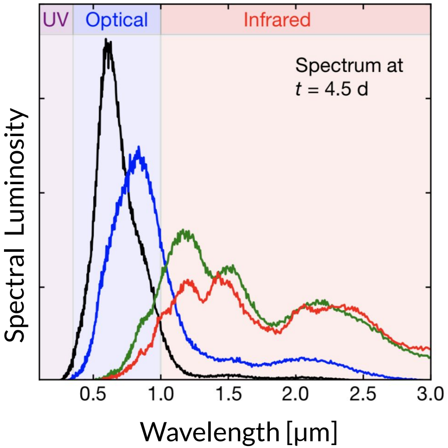
Observations showed a strong reddening as the object faded over two weeks

Jon Grumer / jon.grumer@physics.uu.se



Observations showed a strong reddening as the object faded over two weeks



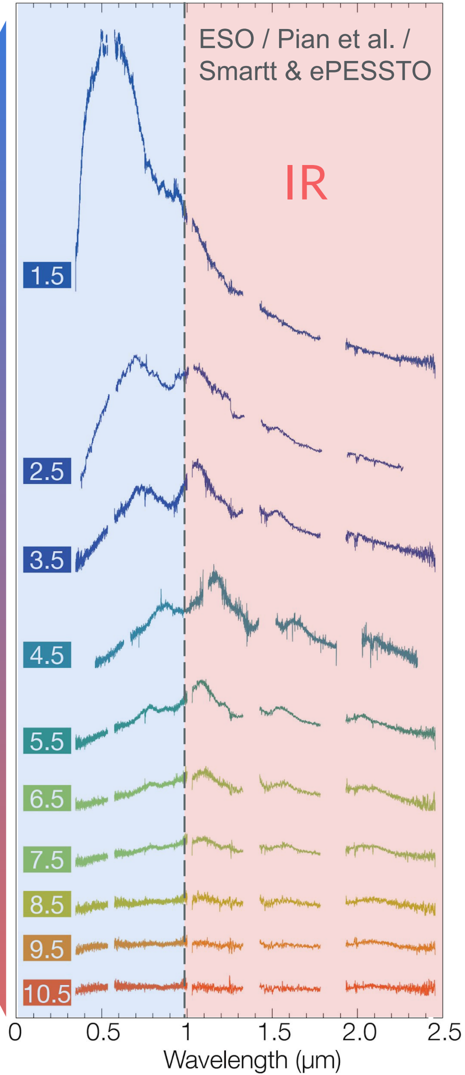


Black | Lanthanide mass fraction | Red

10^{-5} → 10^{-1}

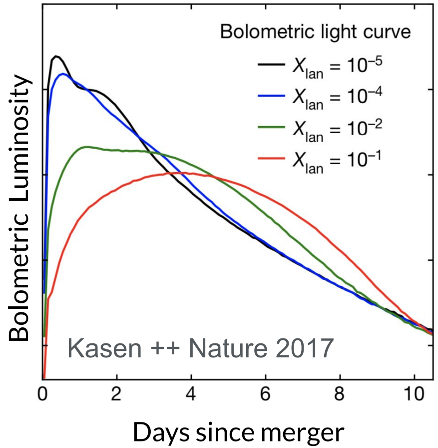
Jon Grumer / jon.grumer@physics.uu.se

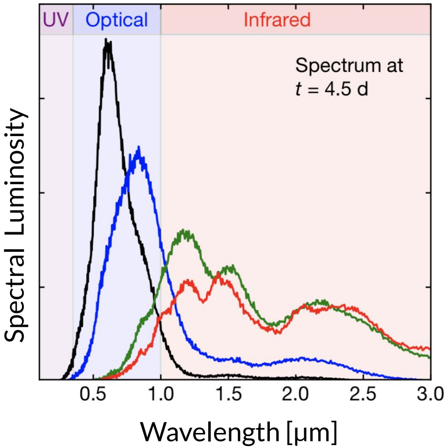
Observed Spectrum
Blue fades ~ days
Red (1-3μm) ~ w's



Observations showed a strong reddening as the object faded over two weeks → **Lanthanides?**

La 57 | Ce 58 | Pr 59 | Nd 60 | Pm 61 | Sm 62 | Eu 63 | Gd 64 | Tb 65 | Dy 66 | Ho 67 | Er 68 | Tm 69 | Yb 70 | Lu 71





Black **Lanthanide mass fraction** Red

10^{-5} → **10^{-1}**

General long term KN goals

- **Fundamental KNe parameters** (ejecta mass, explosion energy, densities, velocities, temperatures)
- ~~**First identification of r-process**~~ **elements in KNe** (if possible? NS-BH merger for lower velocities?)
- **Progenitor/NS-NS properties** (from KNe parameters)

General long term KN goals

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- **Progenitor/NS-NS properties** (from KNe parameters)

"Short term" for atomistic people...

- **Atomic structure models and processes** have to be fully adopted for **$4f^n$** systems
- Combine with **experimental data** (**FTS experiments**, IR → e.g **NIST, Imperial, Lund, Lawler**)
- Interface with databases (**NIST**, **VALD/VAMDC**)
- Create first generation of KNe **opacity tables** for various applications
- **Model KNe spectra** - test **Non-LTE effects** - **SUMO** (Jerkstrand, Stockholm/Max Planck)
- Push atomic data and models towards **spectroscopic accuracy..**

Lanthanides/rare earths | earlier work

As Chris mentioned yd - a lot have been done, motivated by the lighting industry
- but, in generally **limited to the optical, and we need n-IR!**

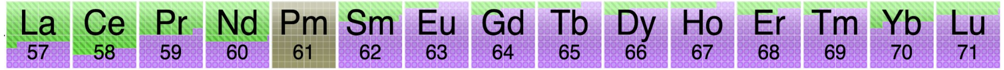
Significant works on rare-earth elements:

- A lot of exp. work done on neutrals and singly ionized species in the optical decade long rare-earth FTS study of **Jim Lawler** ++ in Wisconsin
- The **D.R.E.A.M database** (Biémont, Palmeri and Quinet)
- More recently, **large-scale accurate calculation projects** - mainly by Gaigalas++ (Vilnius)
- ++ many more (e.g. Los Alamos/Fontes++, Japan/Tanaka&Kato++, UC Berkley/Kasen++)

Jon Grumer / jon.grumer@physics.uu.se

Lanthanides/rare earths | properties

- Z = 57 → 71 with open f-shell configurations



- 4f orbital collapse:
- → 4f, 5d, 6s and 6p have similar binding energies
- → overlapping configurations
- → high levels densities even at a few eV

TABLE 20-1. LOW CONFIGURATIONS OF NEUTRAL AND SINGLY IONIZED LANTHANIDE ATOMS[a]

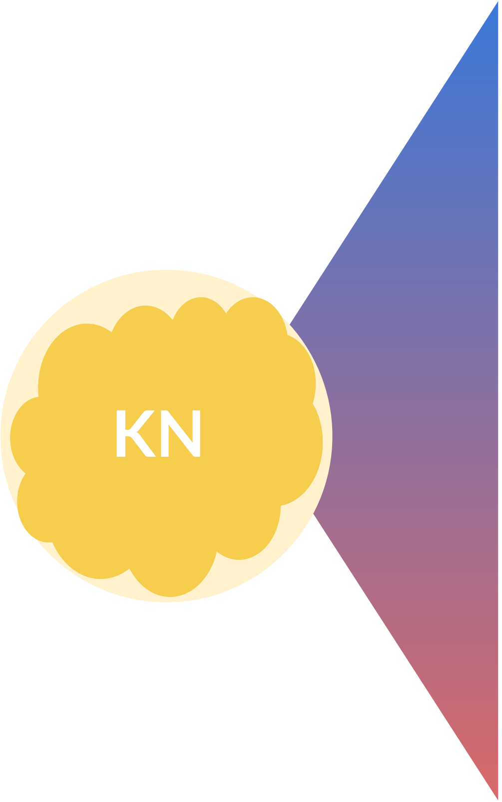
$4f^w 6s^2$	$4f^w 6s6p$
$4f^{w-1} 5d6s^2$	$4f^{w-1} 5d6s6p$
$4f^w 5d6s$	$4f^w 5d6p$
$4f^{w-1} 5d^2 6s$	$4f^{w-1} 5d^2 6p$
$4f^{w+1} 6s$	$4f^{w+1} 6p$
$4f^{w+1} 5d$	

[Cowan Ch. 20]

Open f-shell atomic models | requirements

Goal: an consistent well-defined **overall picture**
but also **individual spectral** lines

1. **Scalability** - order of 10k levels (at once?) and many millions of lines.
2. **Efficient electron correlation** - must be able to handle half-filled f-shells
3. **Relativistic** - high-Z elements
4. **Spectral modelling requires specifically:**
    a. **High-lying states**
    b. **Non-LTE** data - rad. and collisional excitation and ionization processes



Employed theoretical methods:

- MCDHF **`GRASP2018`** [github.com/compas/grasp]
  C. F. Fischer++ CPC 2019

  Accurate structure and radiative properties, (very) non-black box

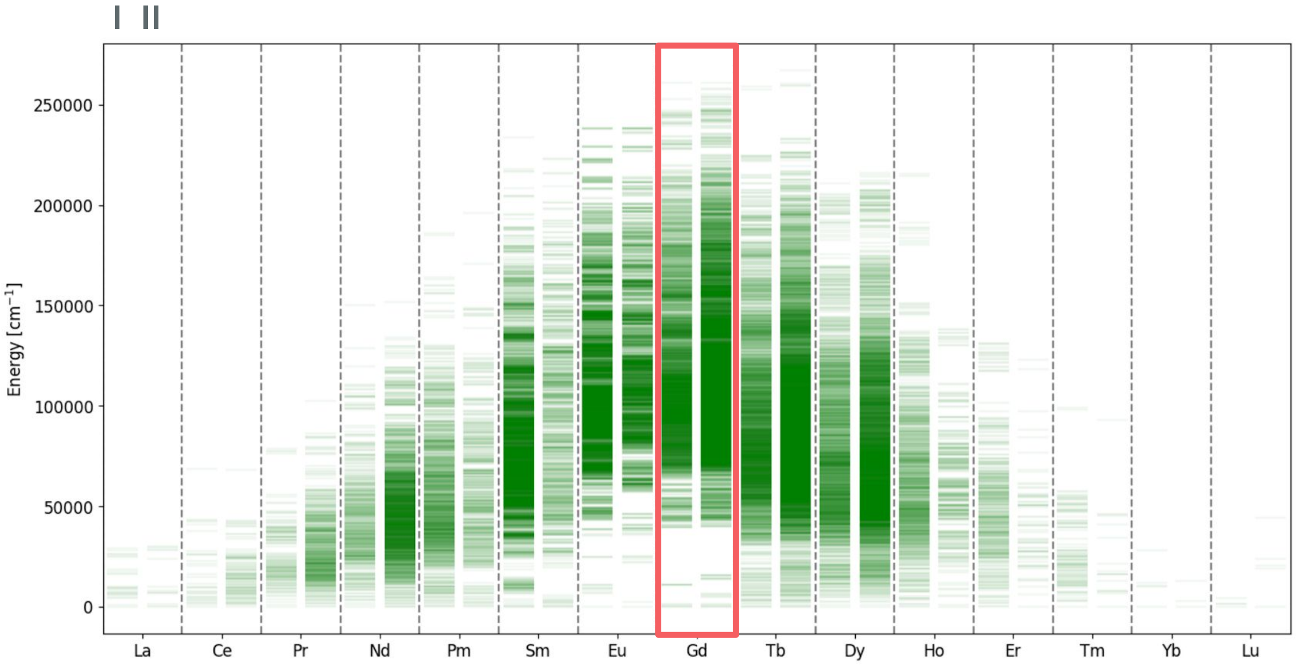
- CI+RMBPT **`FAC`** [github.com/flexible-atomic-code/fac]
  M. F. Gu Can J Phys 2008

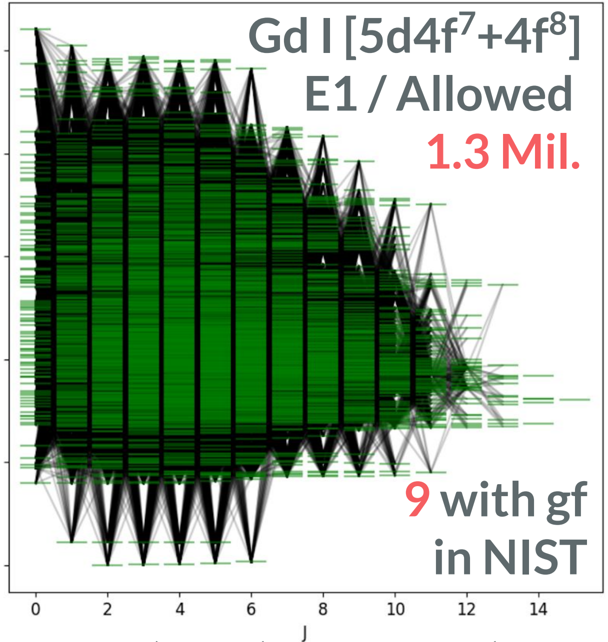
  More black-box, but scales better and can be used to determine Non-LTE data (PI/RR, CE, CI)

\+ the non-LTE radiative transfer code **`SUMO`** by Jerkstrand++

Preliminary results | levels

Goal: Atomic data of reasonable quality for all neutrals to triply ionized species (Fe to U)





Preliminary MCDHF/GRASP calculations (see e.g. Gaigalas ApJS 240:29 (2019) for Nd II-IV)

Jon Grumer / jon.grumer@physics.uu.se

Preliminary results | levels

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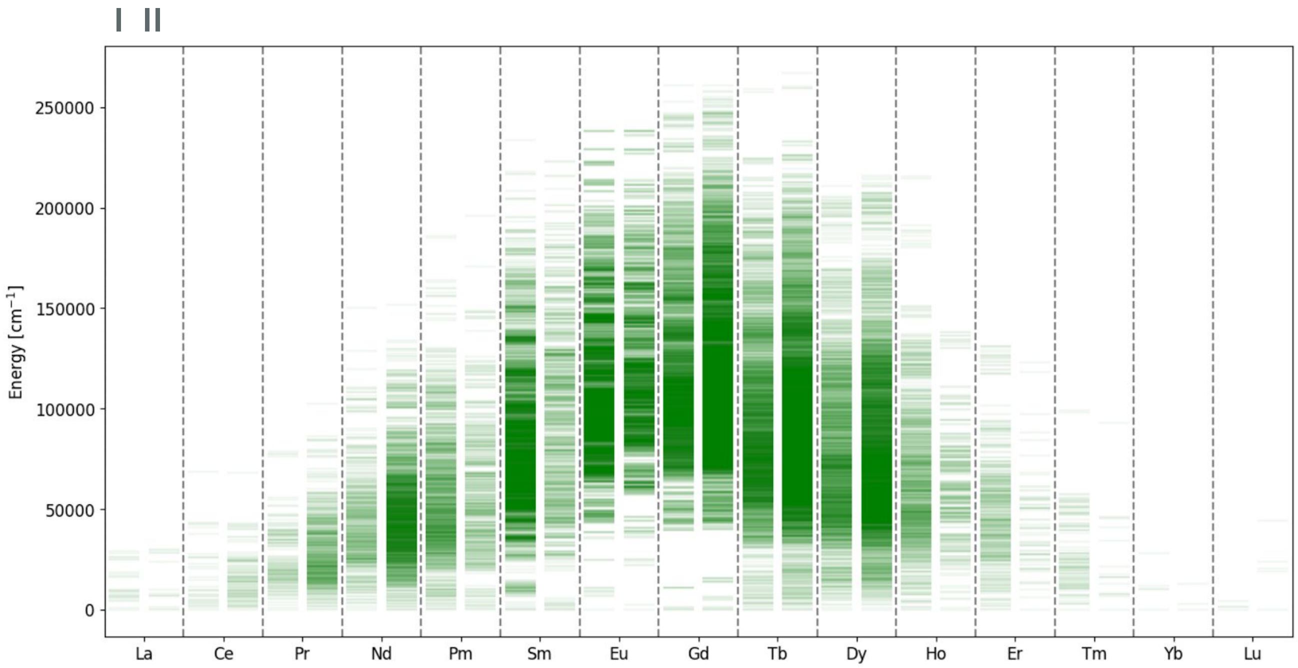

- The small radii of the 4f electrons lead to strong interactions, and $4f^w$ will thus cover unusually large energy ranges of around 12 ev / 100k cm^{-3}

$4f^w6s^2$
$4f^{w-1}5d6s^2$
$4f^w5d6s$
$4f^{w-1}5d^26s$
$4f^{w+1}6s$
$4f^{w+1}5d$
$4f^w6s6p$
$4f^{w-1}5d6s6p$
$4f^w5d6p$
$4f^{w-1}5d^26p$
$4f^{w+1}6p$

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Preliminary results | levels

Goal: Atomic data of reasonable quality for all neutrals to triply ionized species (Fe to U)

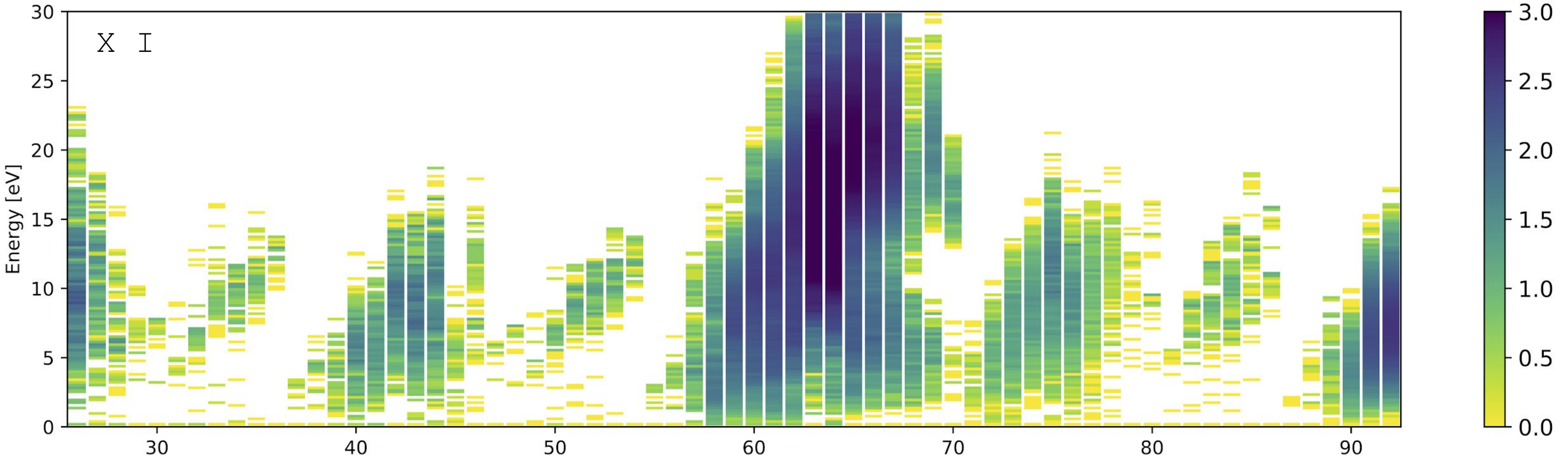
GRASP is accurate, but tedious to adopt ↣ run simpler model to get KNe machinery going.

Preliminary results | levels

Goal: Atomic data of reasonable quality for all neutrals to triply ionized species (Fe to U)

For starters, instead: DF-Slater + RCI +QED on "all" bound states (FAC):

- Level densities (0.2 ev bin size) for neutral atoms



Preliminary results | levels

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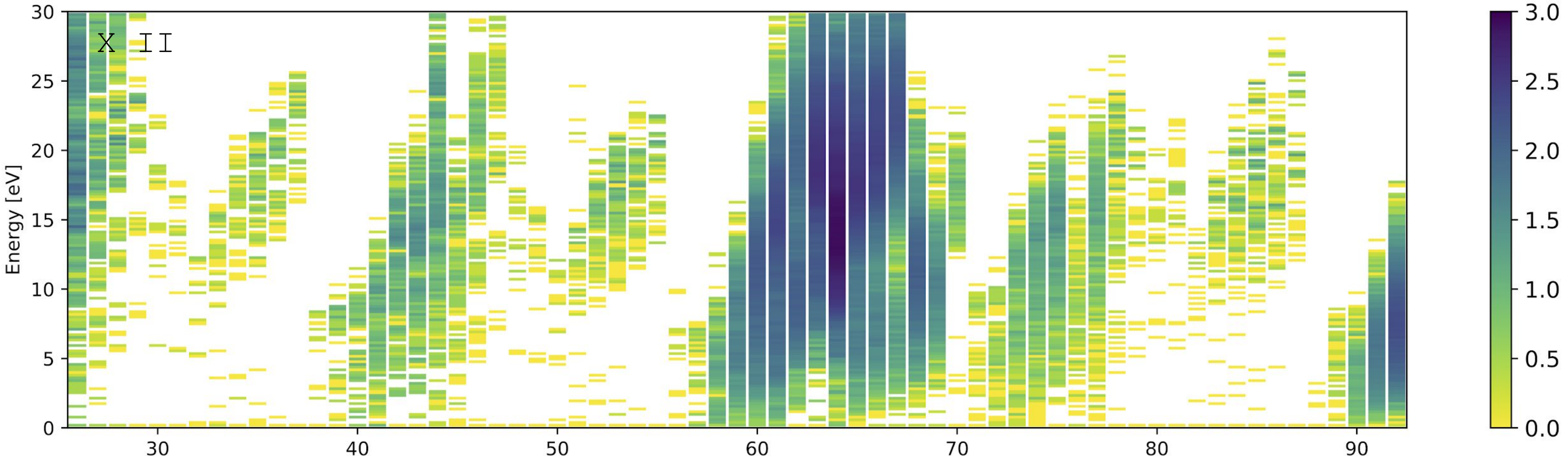
For starters, instead: DF-Slater + RCI +QED on "all" bound states (FAC):

- Level densities (0.2 ev bin size) for singly ionized ions



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Preliminary results | levels

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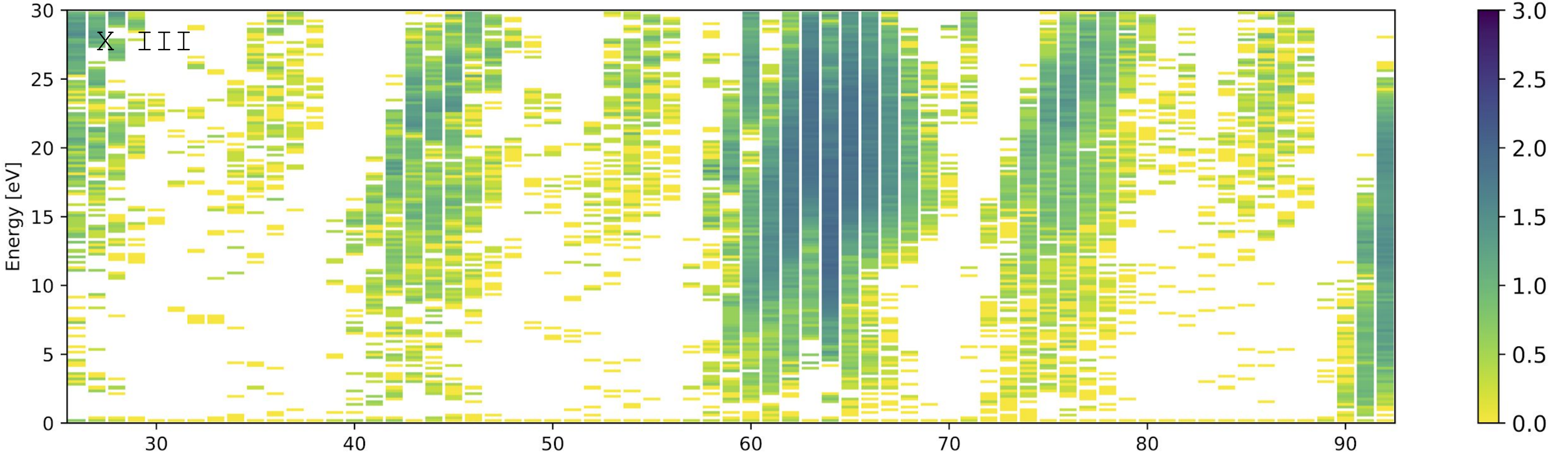
- Level densities (0.2 ev bin size) for doubly ionized ions



Preliminary results | levels

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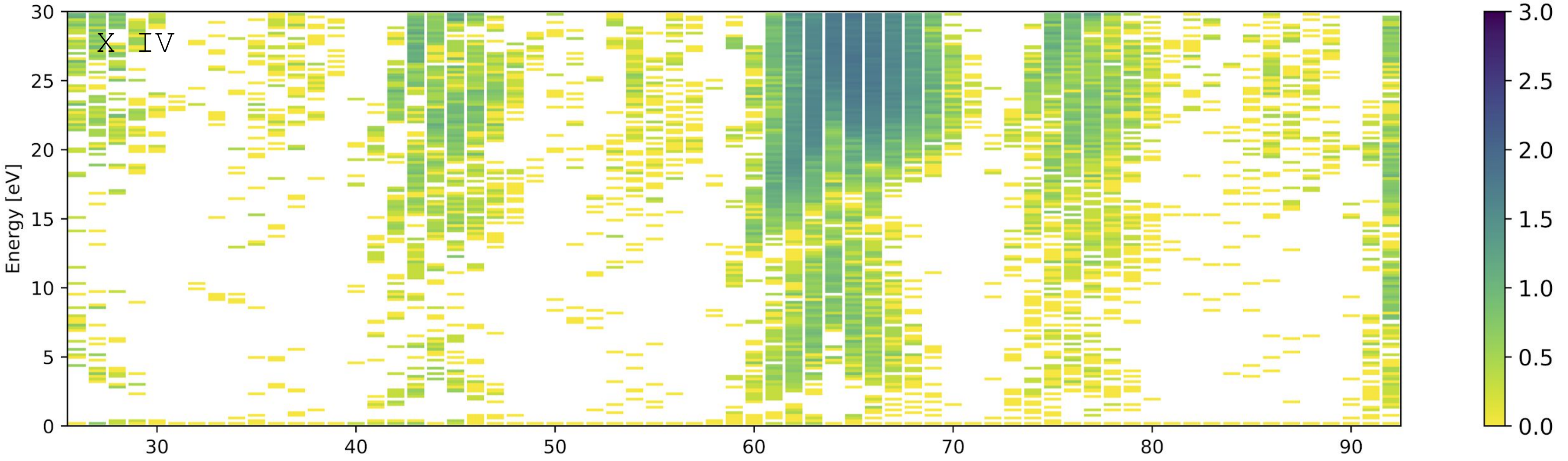
- Level densities (0.2 ev bin size) for triply ionized ions



The level densities agree relatively well with Tanaka++ 2019 arXiv:1906.08914 (HULLAC)

Jon Grumer / jon.grumer@physics.uu.se

Preliminary results | lines

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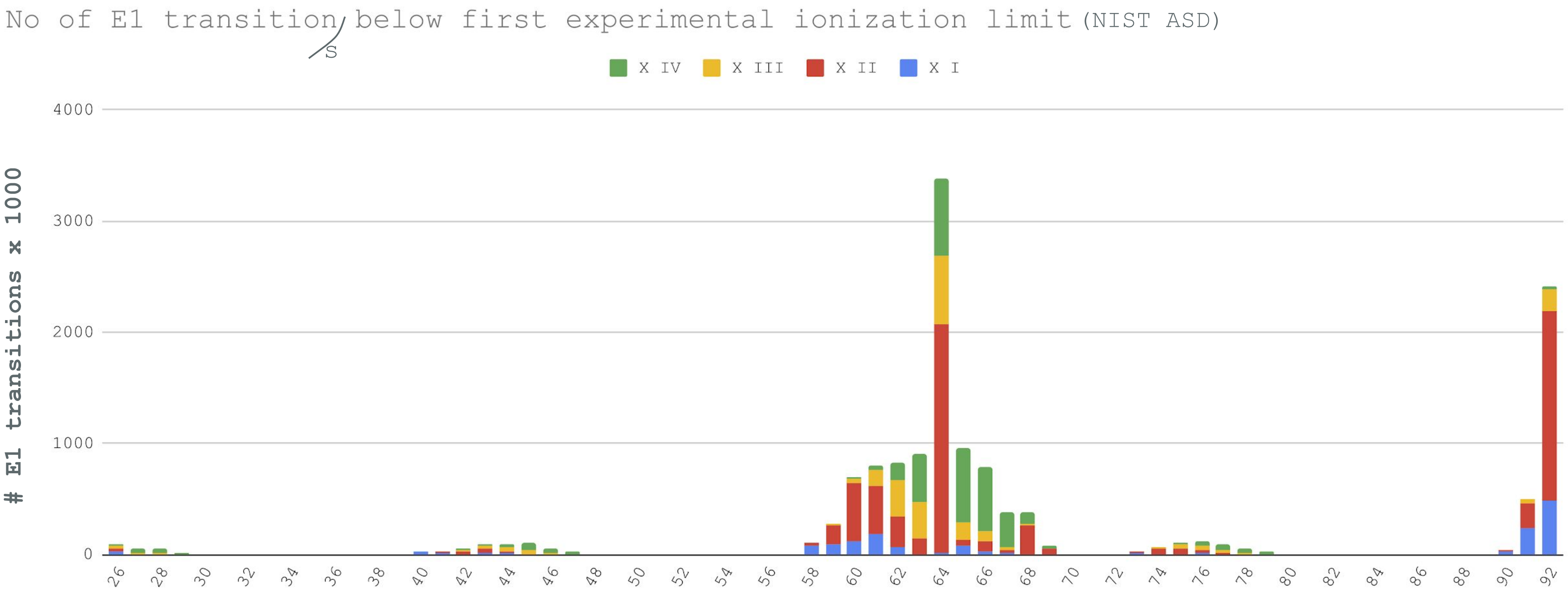

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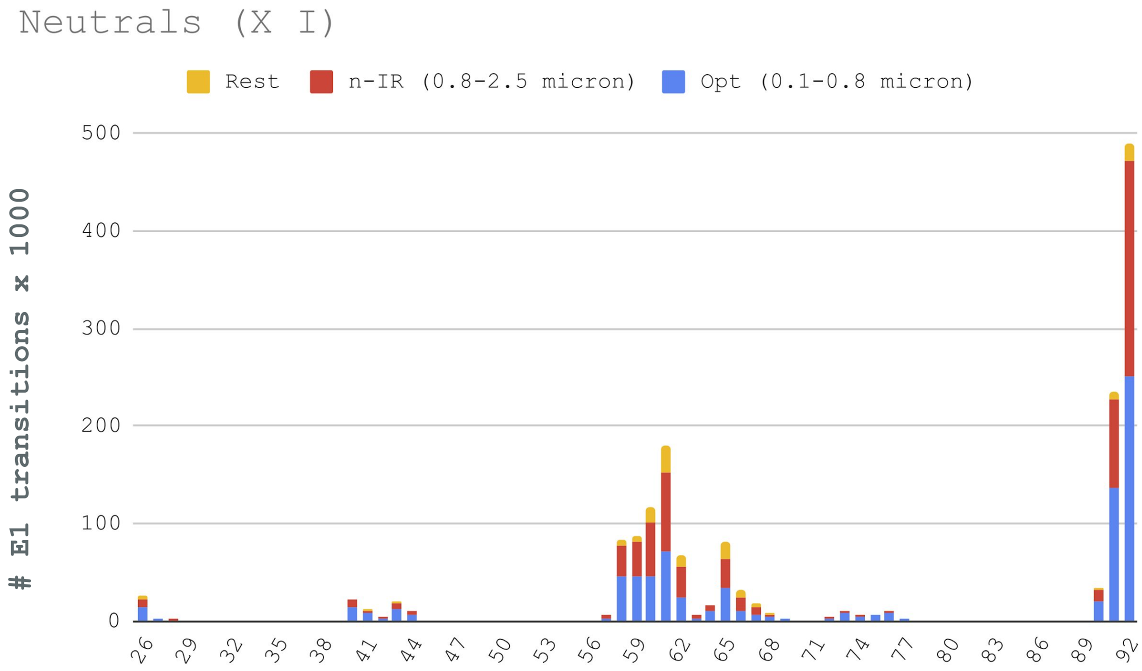


Preliminary results | expansion opacities

Eg. as input to light curve models...

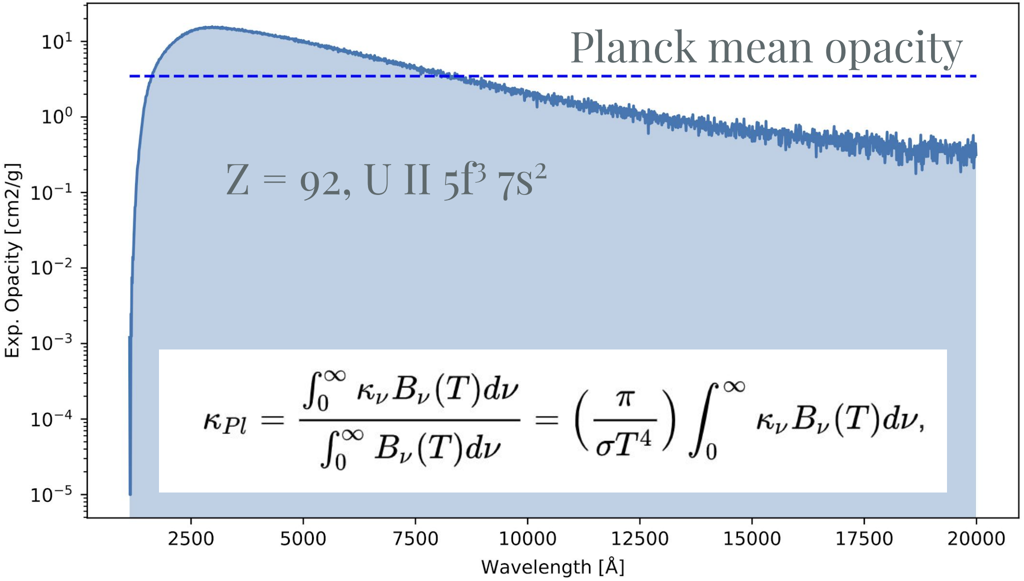
Expansion opacity: $$\kappa_{\rm exp}(\lambda) = \frac{1}{ct\rho}\sum_l \frac{\lambda_l}{\Delta\lambda}(1 - e^{-\tau_l})$$

In the bound-bound Sobolev approximation: $$\tau_l = \frac{\pi e^2}{m_e c} f_l n t \lambda_l$$

Preliminary results | expansion opacities

Goal: Atomic data of reasonable quality for all neutrals to triply ionized species (Fe to U)

Sobolev expansion opacities @ t = 1 day | T = 5000K | ρ = 1E10-13 g/cm3



$$\kappa_{Pl} = \frac{\int_0^\infty \kappa_\nu B_\nu(T) d\nu}{\int_0^\infty B_\nu(T) d\nu} = \left(\frac{\pi}{\sigma T^4}\right) \int_0^\infty \kappa_\nu B_\nu(T) d\nu,$$

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Preliminary results | expansion opacities

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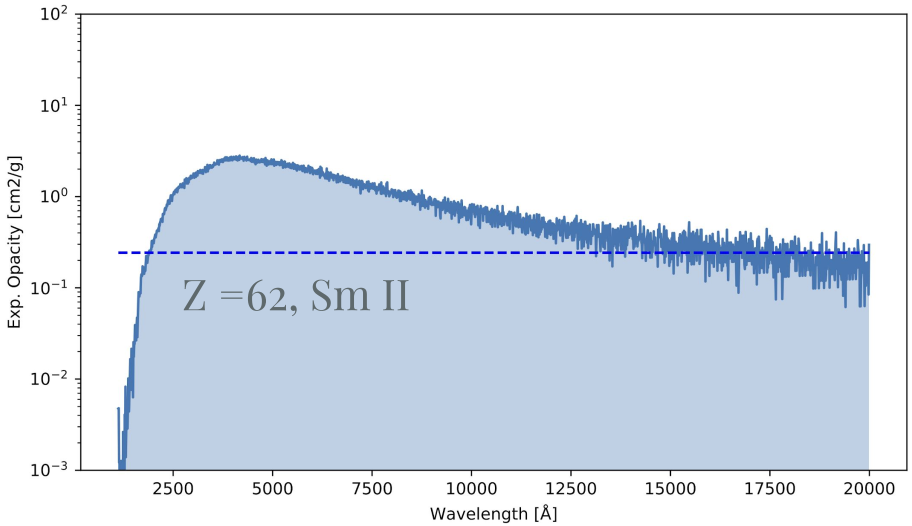
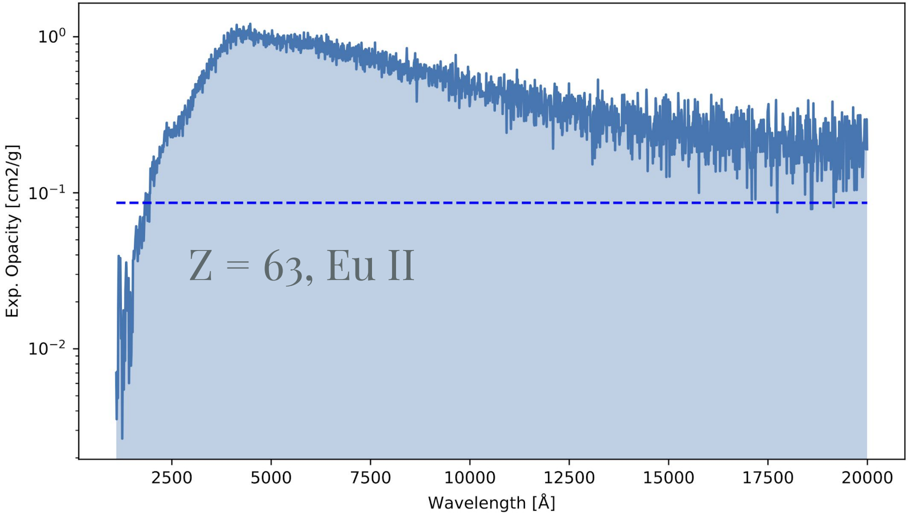




SUMO (Jerkstrand++, Stockholm Uni./MaxPlanck Garching)

A Monte-Carlo non-LTE spectral model for supernovae from atomic data

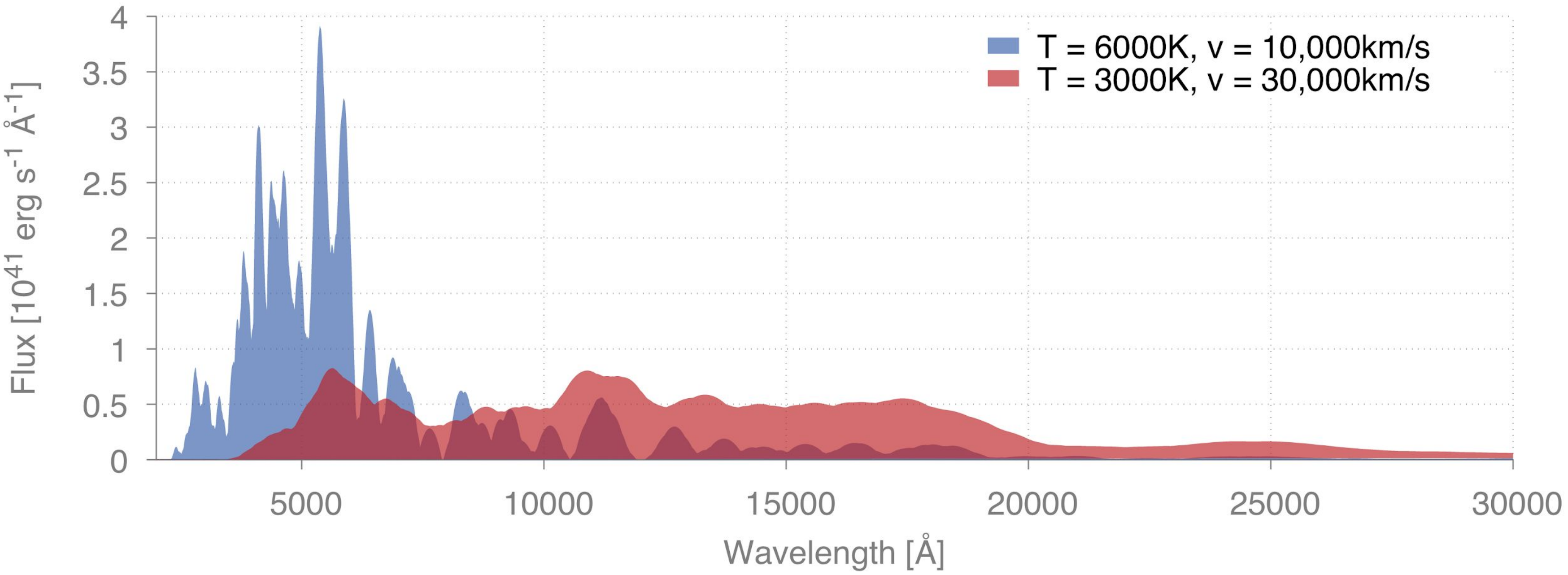
Self-consistent loop: Fueled by radioactive decay (g-rays, compton heating)

- Compton electron distribution (Spencer-Fano)
- Radiative Transfer
  - Monte-Carlo, multi-shell, Sobolev approx
  - Support for most relevant radiative and collisional processes
- NLTE statistical equilibrium (current SNe model, X I - X III up to Ni)

Jon Grumer / jon.grumer@physics.uu.se

KNe Models: Preliminary results

GRASP + SUMO (Jerkstrand): Ce I KNe NLTE spectra



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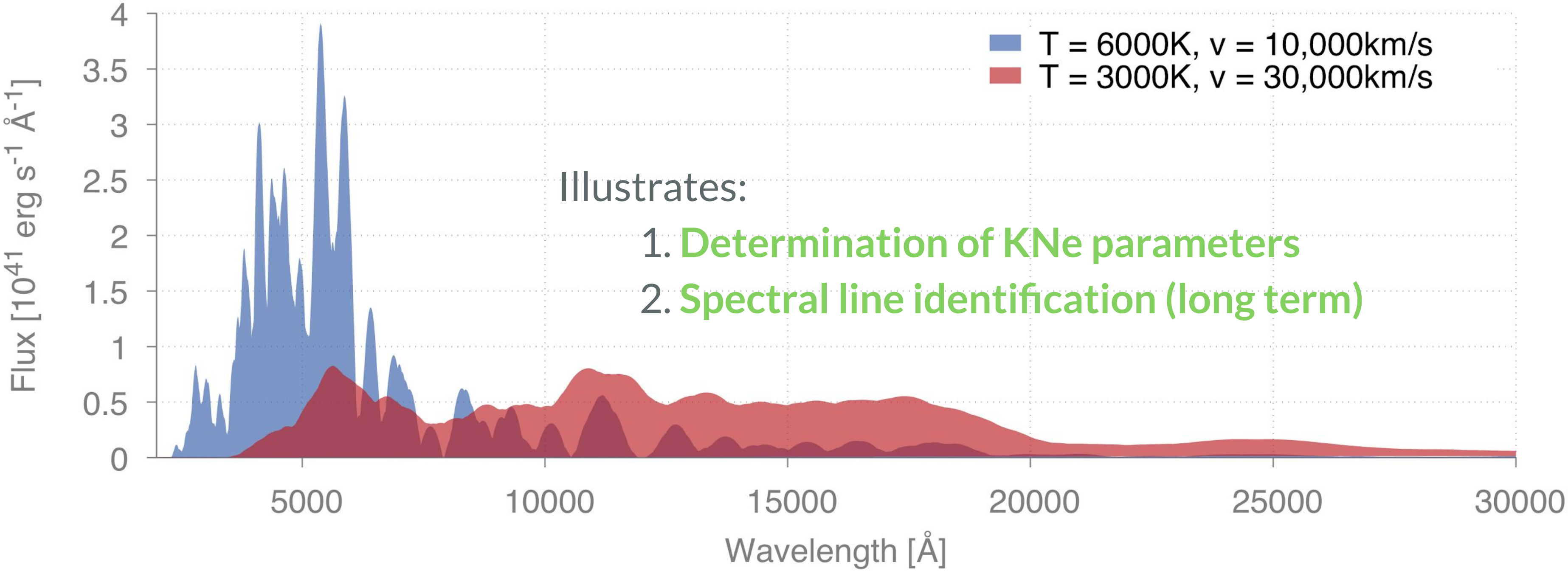
KNe Models: Preliminary results

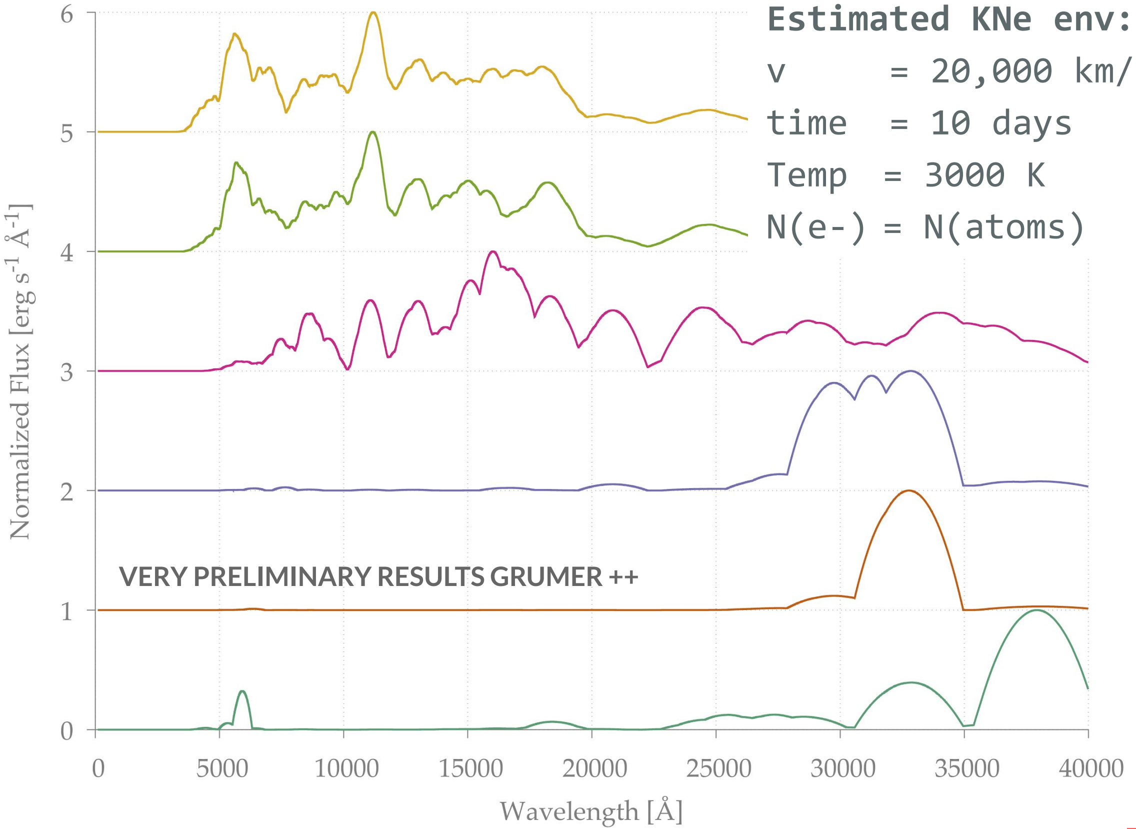
GRASP + SUMO (Jerkstrand): Ce I KNe NLTE spectra



Illustrates:

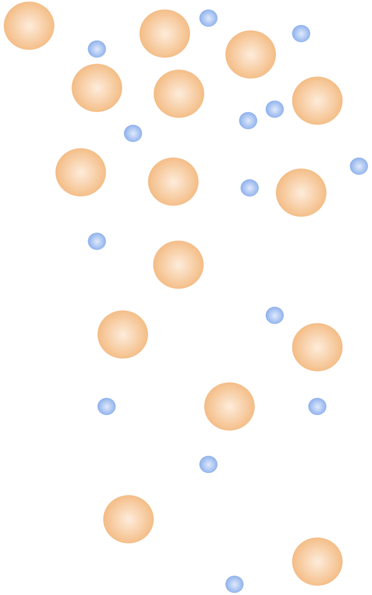
1. Determination of KNe parameters
2. Spectral line identification (long term)

KNe Models: Preliminary results NLTE/density




```
Estimated KNe env:
v      = 20,000 km/s
time   = 10 days
Temp   = 3000 K
N(e-) = N(atoms)
```


```
Simple model:
Thermal e-collisions
+ spont. emission
```



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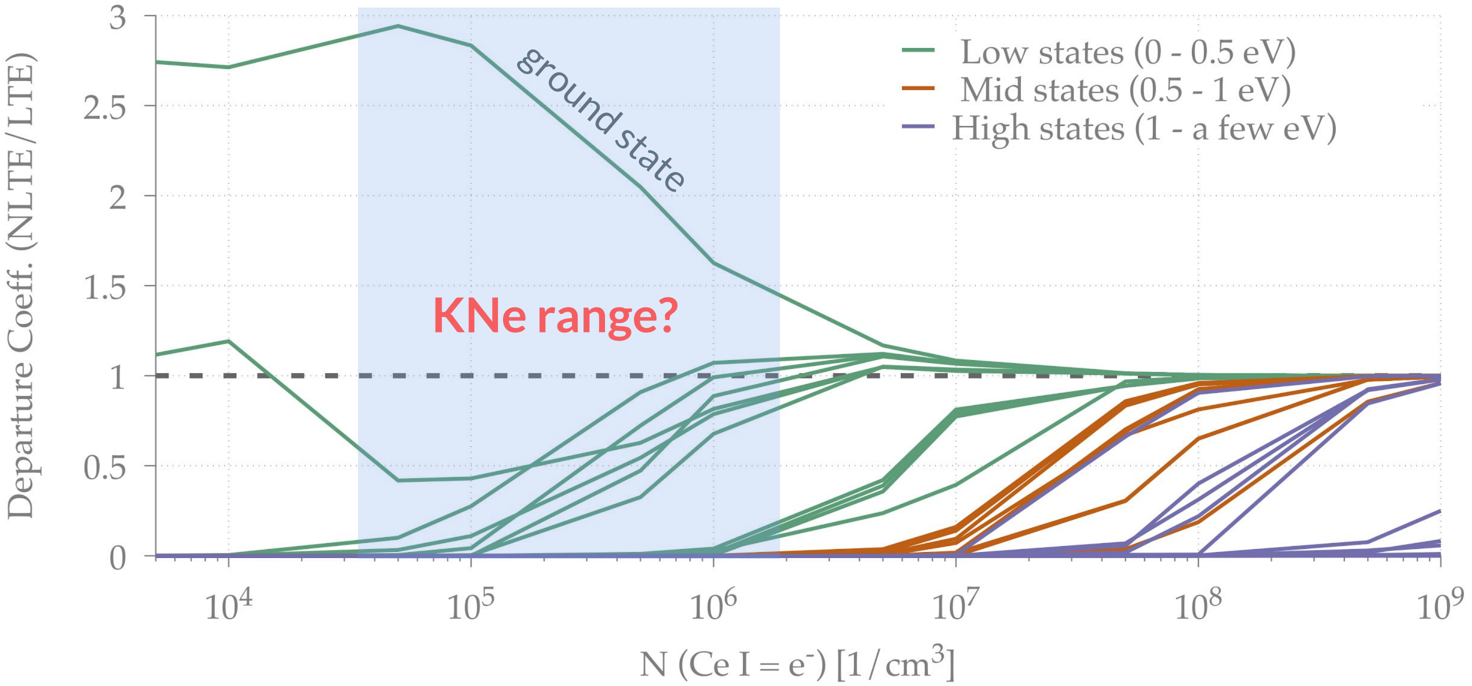
KNe Models: Preliminary results

Ce I NLTE vs LTE: departure coefficients

Simple model:
Thermal e-collisions
+ spont. emission



Outlook

- **Working on a "complete" grid of neutrals to triply ionized neutron capture elements**
  Energy levels + radiative transition rates + NLTE processes - prel. model done

- **From this:**
  - Finish grid of expansion opacities as function of temperature, density and expansion time and make available to e.g. light curve modellers (+static op. for e.g. Stellar evol. models)
  - Finish atomic NLTE data - also PI/RR + CE
  - Find a way to get all this data into SUMO and work towards NLTE spectral modelling
  - (+1D->3D modelling, and connect with hydro-models)
  - Improve atomic data - exp + theory

  repeat