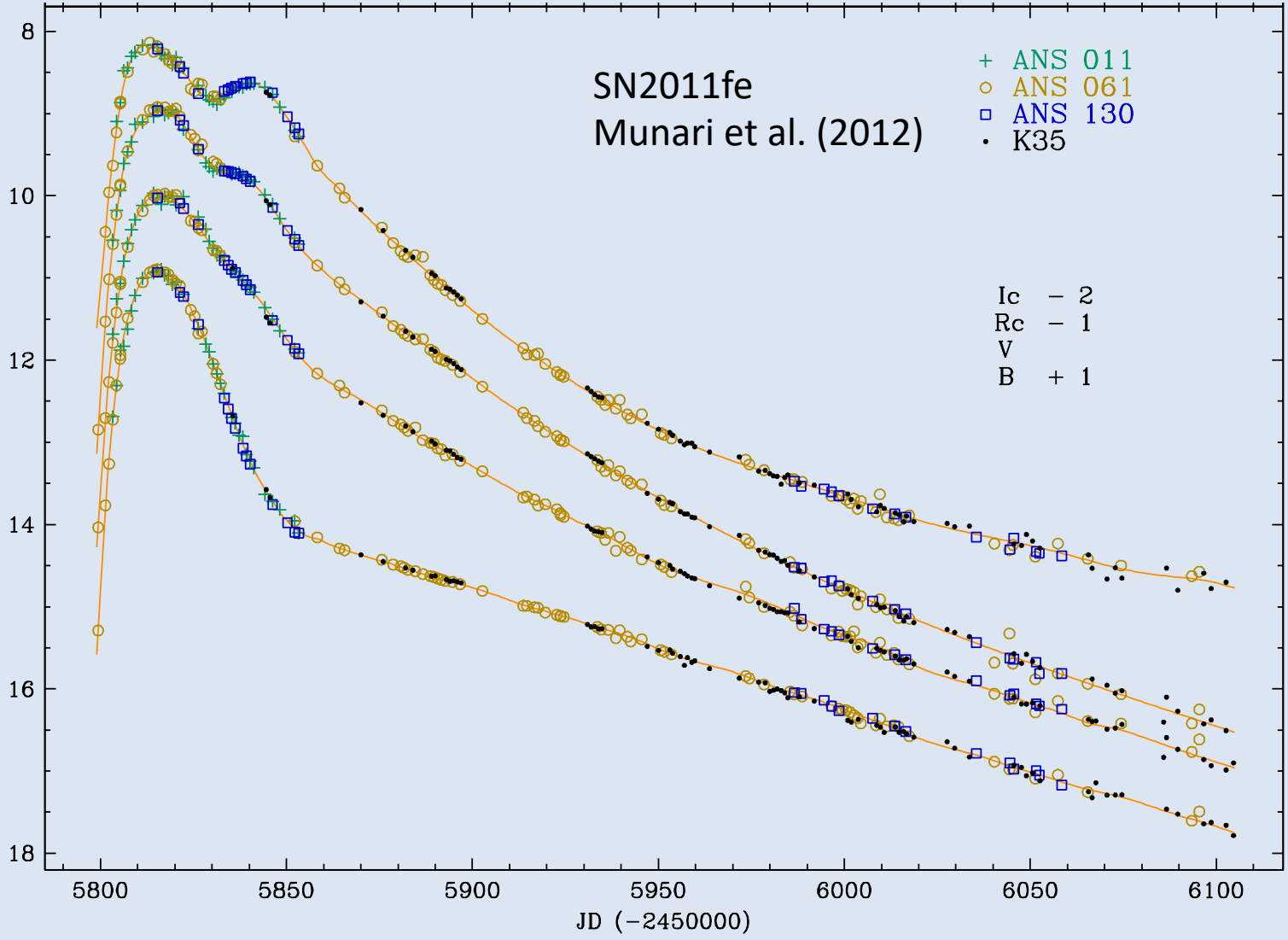
Light curves and spectra for astrophysical explosions

Stuart Sim
(Queen's University Belfast)
SAMCSS 2019

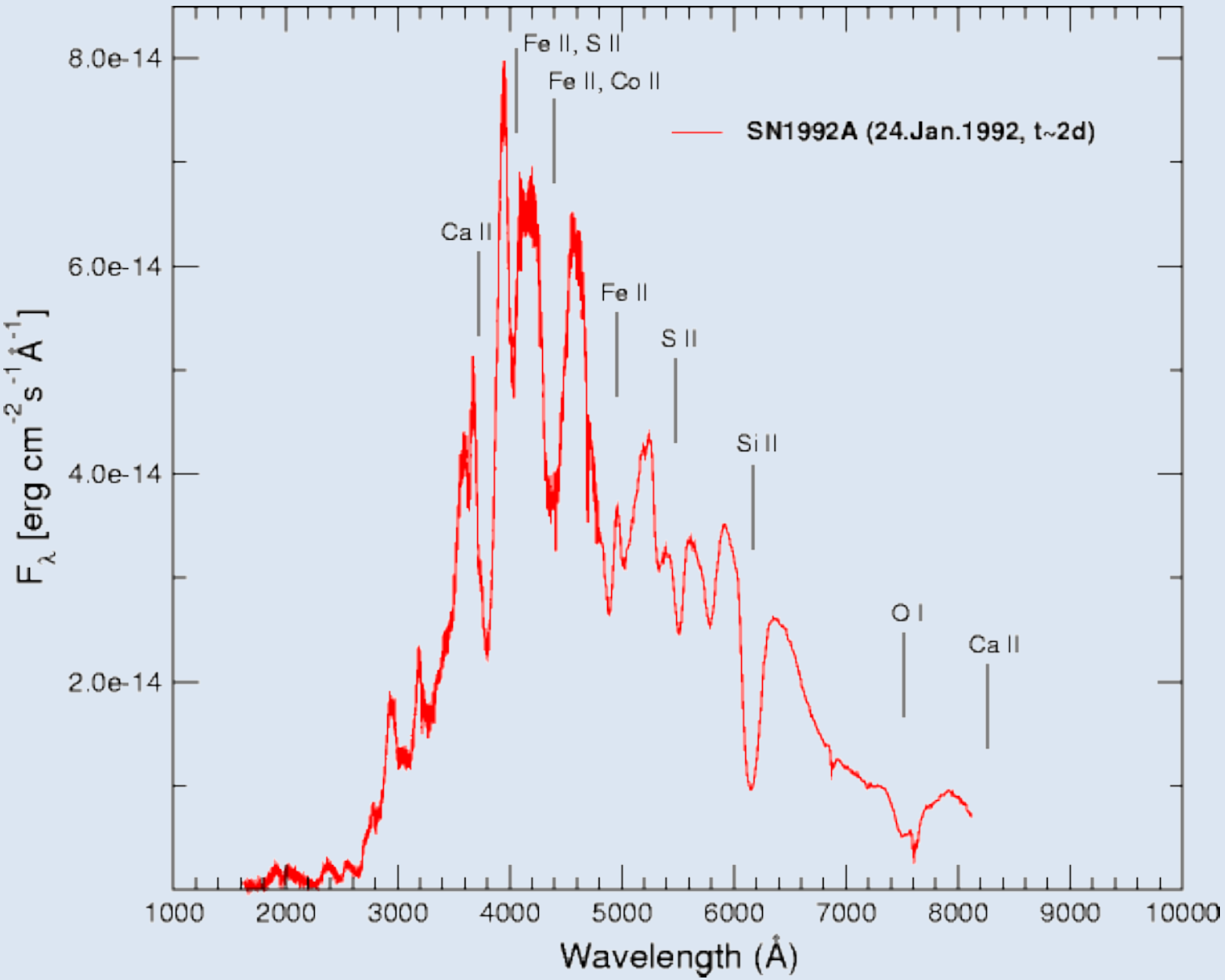
Overview:

- Brief introduction to supernovae
  - Observations to study
- Considerations for modelling radiation transport for supernovae
  - Suitability of MCRT techniques
- Light curve calculations (Lecture 1)
  - Simple 1D example
- Spectrum calculations (Lecture 2; Wed afternoon)
  - Sobolev treatment of lines
  - Macro Atom methods for radiative equilibrium

Supernova (Type Ia) lightcurves



Supernova (Type Ia) spectrum



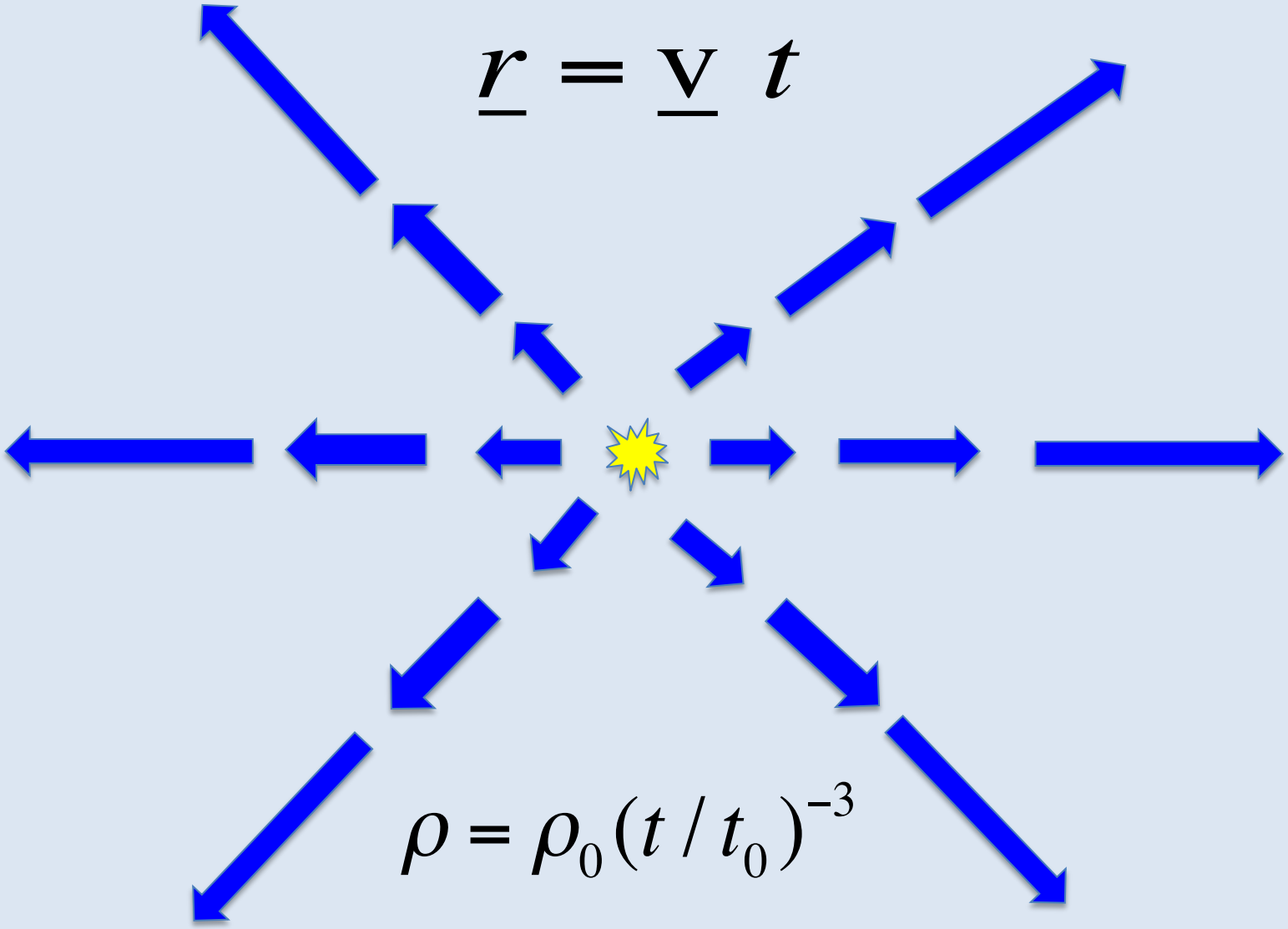
Spectral modelling

Need to consider:

- Velocity field (for supernovae, homologous flow assumption often sufficient)
  - not necessarily need for full dynamical coupling in calculation
  - …but kinematics are critical to shaping spectrum
- Realistic opacity
- Non-LTE needed for accurate treatment of emission and reprocessing

Homologous flow

normally established within seconds to hours



Non-grey opacity

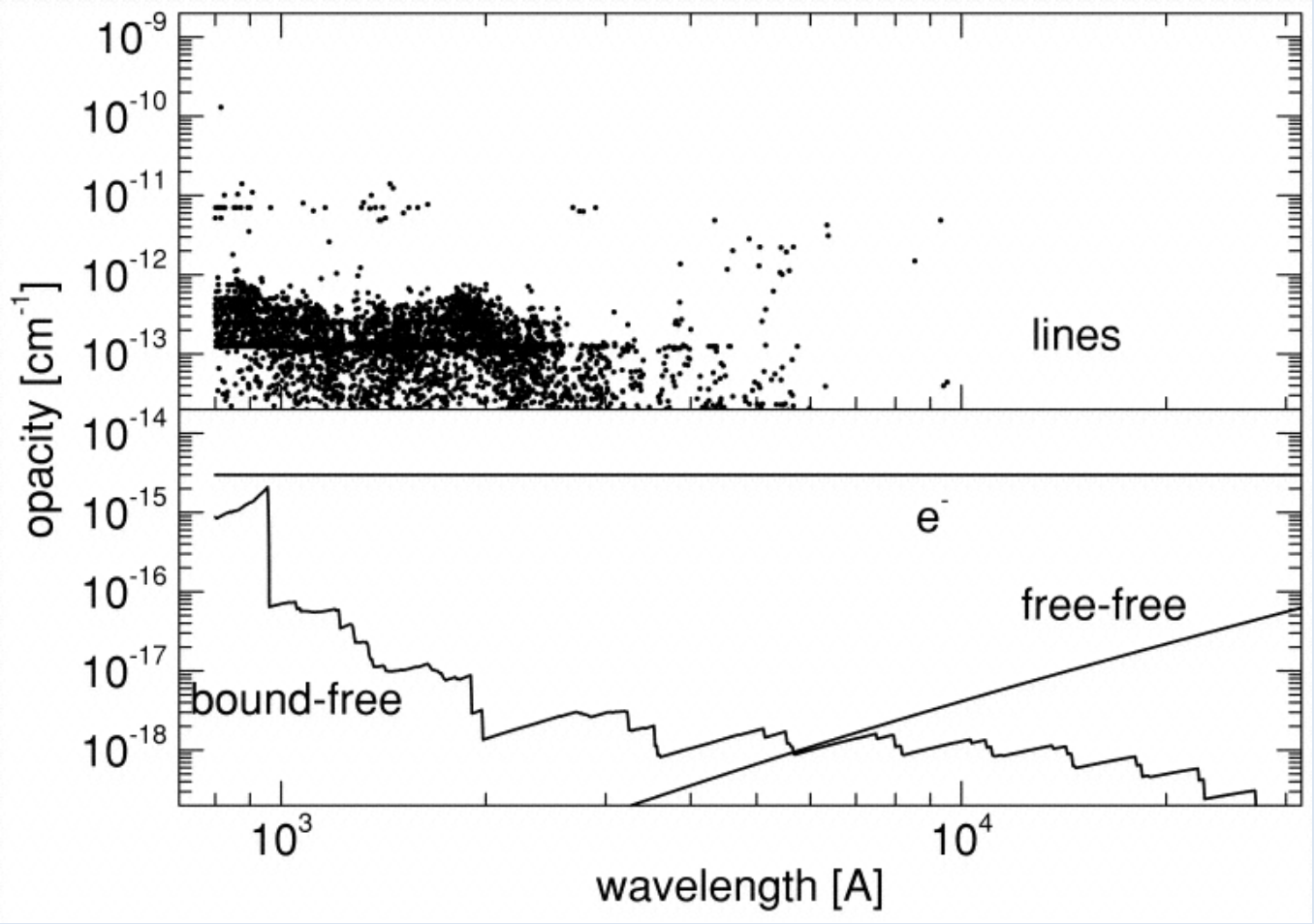
Finding interaction points for MCRT method:

- Need to be able to compute rate at which optical depth is accumulated by propagating MC packet

$$\mathrm{d}\tau = \kappa\rho\mathrm{d}s$$

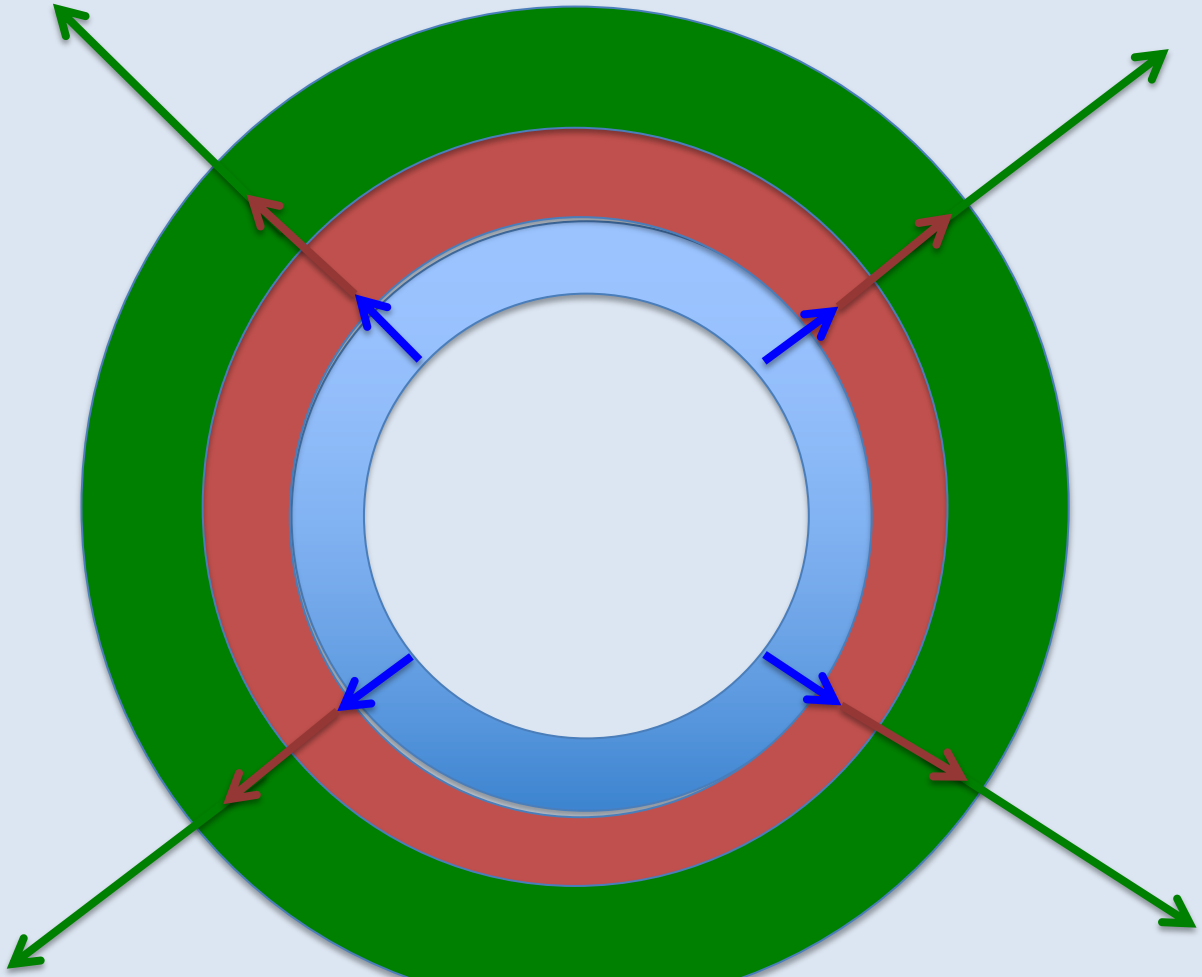
- Was trivial for grey opacity assumed in light curve …
- …but still easily accomplished thanks to conditions / approximations appropriate to homologous supernovae ejecta

Non-grey opacity



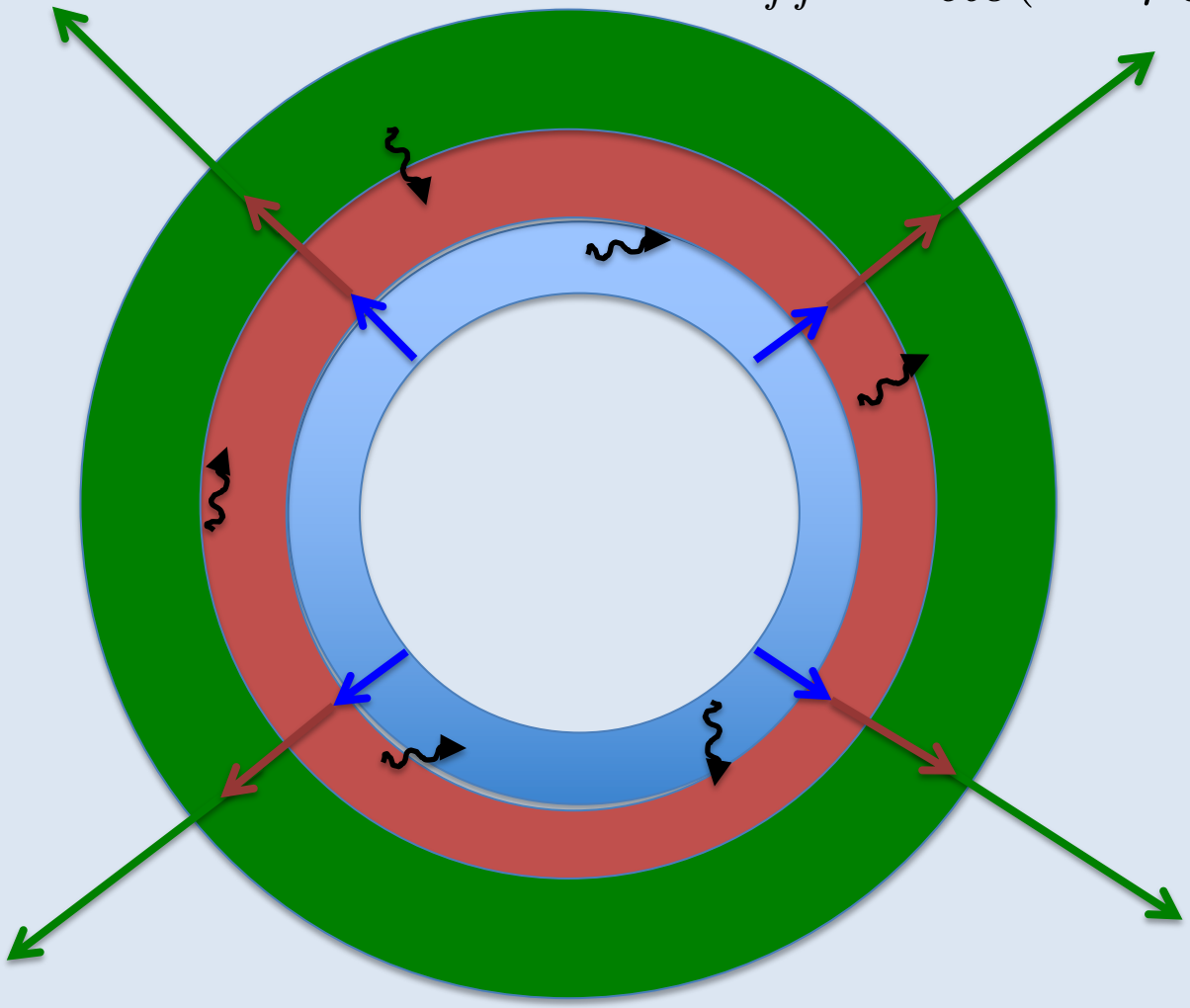
Pinto & Eastman 2000

Photons in expanding media



Photons in expanding media

$$\nu_{ff} = \nu_{obs}(1 - \mu_{obs}\beta)$$



Photons in expanding media

$$\nu_{ff} = \nu_{obs}(1 - \mu_{obs}\beta)$$

Fluid-frame frequency evolves in remarkably simple way for radial velocities:

$$\frac{\mathrm{d}\nu_{ff}}{\mathrm{d}s} = -\frac{\nu_{obs}}{c}\frac{\mathrm{d}}{\mathrm{d}s}\left(\mu_{obs}v(r)\right)$$

Use cosine rule to differentiate direction cosine along a path:

$$\frac{\mathrm{d}\nu_{ff}}{\mathrm{d}s} = -\frac{\nu_{obs}}{c}\left(\frac{v(r)}{r}(1-\mu_{obs}^2) + \mu_{obs}^2\frac{\mathrm{d}v(r)}{\mathrm{d}r}\right)$$

Provided speed is positive (outflow) and increases outward, always negative!
For homologous flow, even simpler: independent of position and direction:

$$\frac{\mathrm{d}\nu_{ff}}{\mathrm{d}s} = -\frac{\nu_{obs}}{ct}$$

Photons in expanding media

Implication:

- Fluid-frame frequency of a propagating packet evolves (at a near-constant rate) to the red
- Will successively Doppler-shift in and out of resonance with line transitions in (inverse) frequency order

Sobolev approximation

Sobolev approximation:

- Simplification for dealing with line opacity in high velocity-gradient flows

Sobolev approximation

Sketch derivation (Sobolev 1957; see e.g. Lamers & Cassinelli 1999):
The absorption coefficient for a bound-bound line can be written:

$$\kappa\rho = \frac{B_{lu}h\nu_0}{4\pi} n_l \left(1 - \frac{n_u}{n_l}\frac{g_l}{g_u}\right) \phi(\Delta\nu_{ff})$$

The optical depth traversed by a photon along a short path is:

$$\mathrm{d}\tau = \kappa\rho \mathrm{d}s$$

So integrating along a path element

$$\tau_{ul} = \int_{s_0}^{s_1} \frac{B_{lu}h\nu_0}{4\pi} n_l \left(1 - \frac{n_u}{n_l}\frac{g_l}{g_u}\right) \phi(\Delta\nu_{ff})\, \mathrm{d}s$$

Use fact that frequency and path-length are related in flow

$$\tau_{ul} = \int_{\nu_{ff}(s=s_0)}^{\nu_{ff}(s=s_1)} \frac{B_{lu}h\nu_0}{4\pi} n_l \left(1 - \frac{n_u}{n_l}\frac{g_l}{g_u}\right) \frac{\mathrm{d}s}{\mathrm{d}\nu_{ff}} \phi(\Delta\nu_{ff})\, \mathrm{d}\nu_{ff}$$

If resonance region is small

$$\tau_{ul} = \frac{B_{lu}h\nu_0}{4\pi} n_l \left(1 - \frac{n_u}{n_l}\frac{g_l}{g_u}\right) \frac{\mathrm{d}s}{\mathrm{d}\nu_{ff}} \int_{\nu_{ff}(s=s_0)}^{\nu_{ff}(s=s_1)} \delta(\Delta\nu_{ff})\, \mathrm{d}\nu_{ff}$$

Sobolev approximation

Resulting optical depth for homologous flow:

$$\tau_{ul}^{S} = \frac{B_{lu} hct\nu_0}{4\pi\nu_{obs}} n_l \left(1 - \frac{n_u}{n_l}\frac{g_l}{g_u}\right)$$

Leads to dramatic simplification:

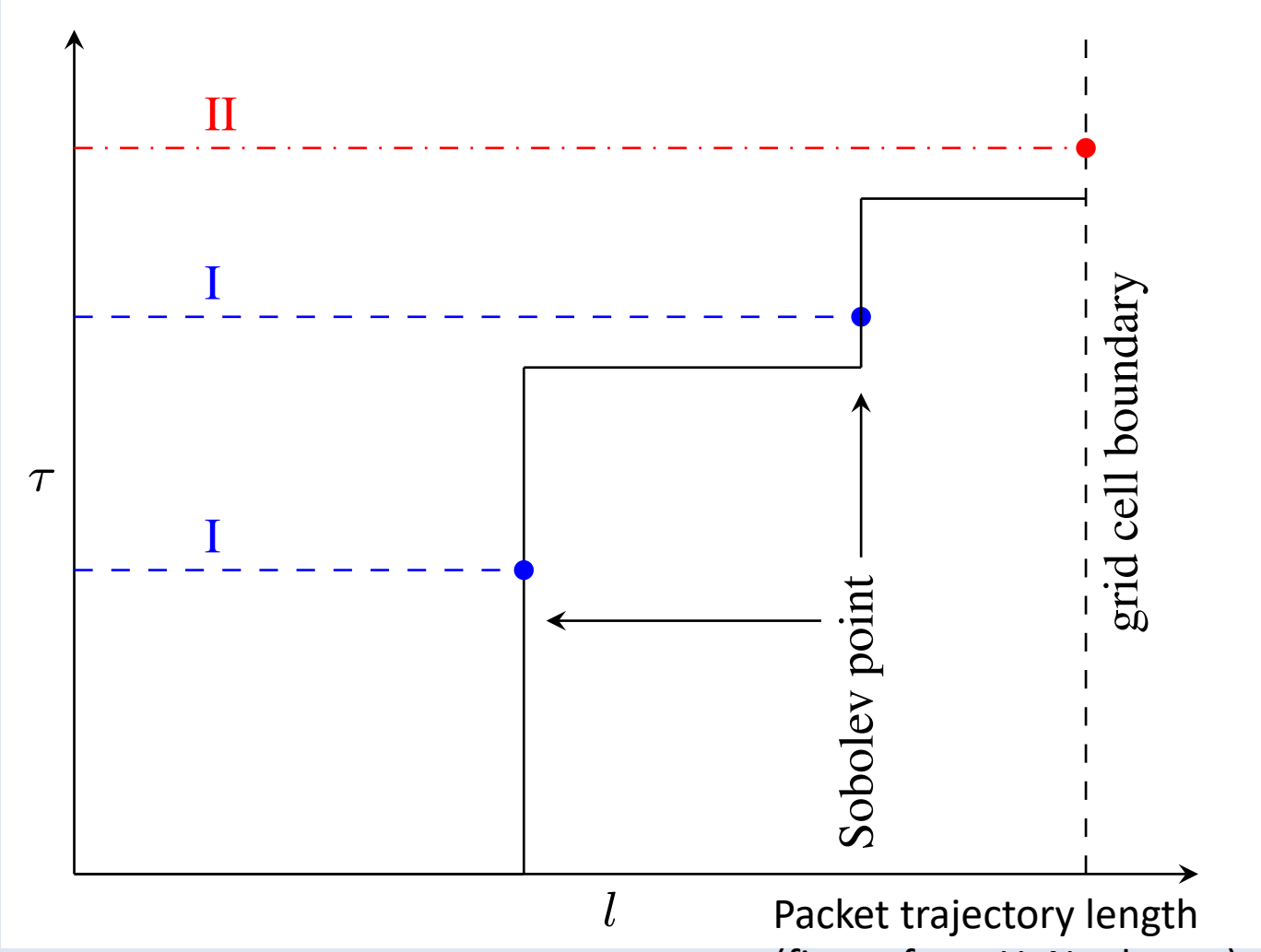
- Easy to compute total optical depth accumulated by packet that passes through resonance with a line
- In Sobolev limit, all this opacity encountered in spatially small region (approximated as Sobolev point in codes)
- Can be fairly-easily generalized e.g. to include continuum opacity
- …together with continuous red-shifting lends itself to simple algorithm with frequency-ordered line list

Issues:

- Overlapping lines
- Still need good level populations!

Sobolev approximation

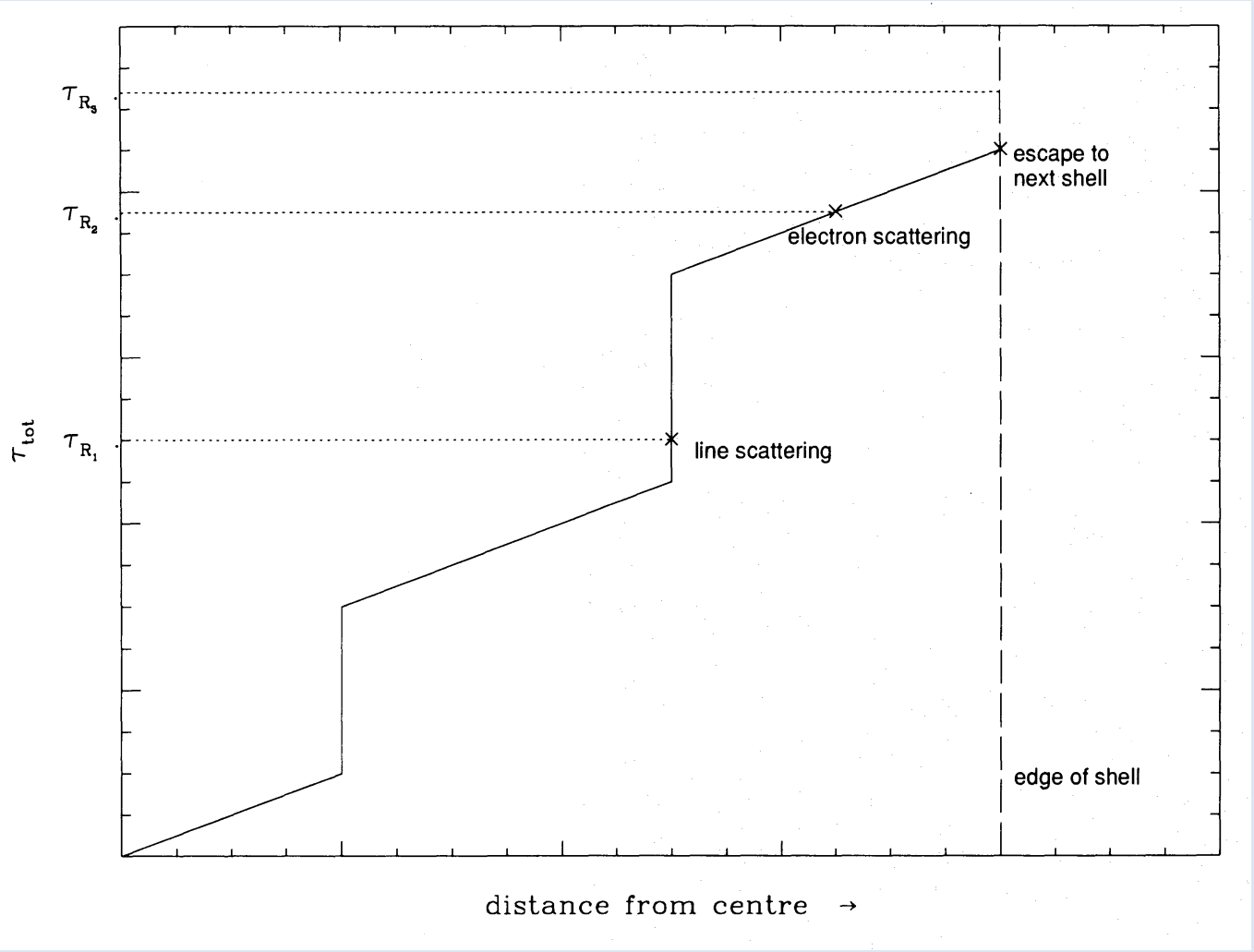
Algorithm for finding interaction point (only lines):



(figure from U. Noebauer)

Sobolev approximation

Process for finding interaction point (generalized to include continuum):

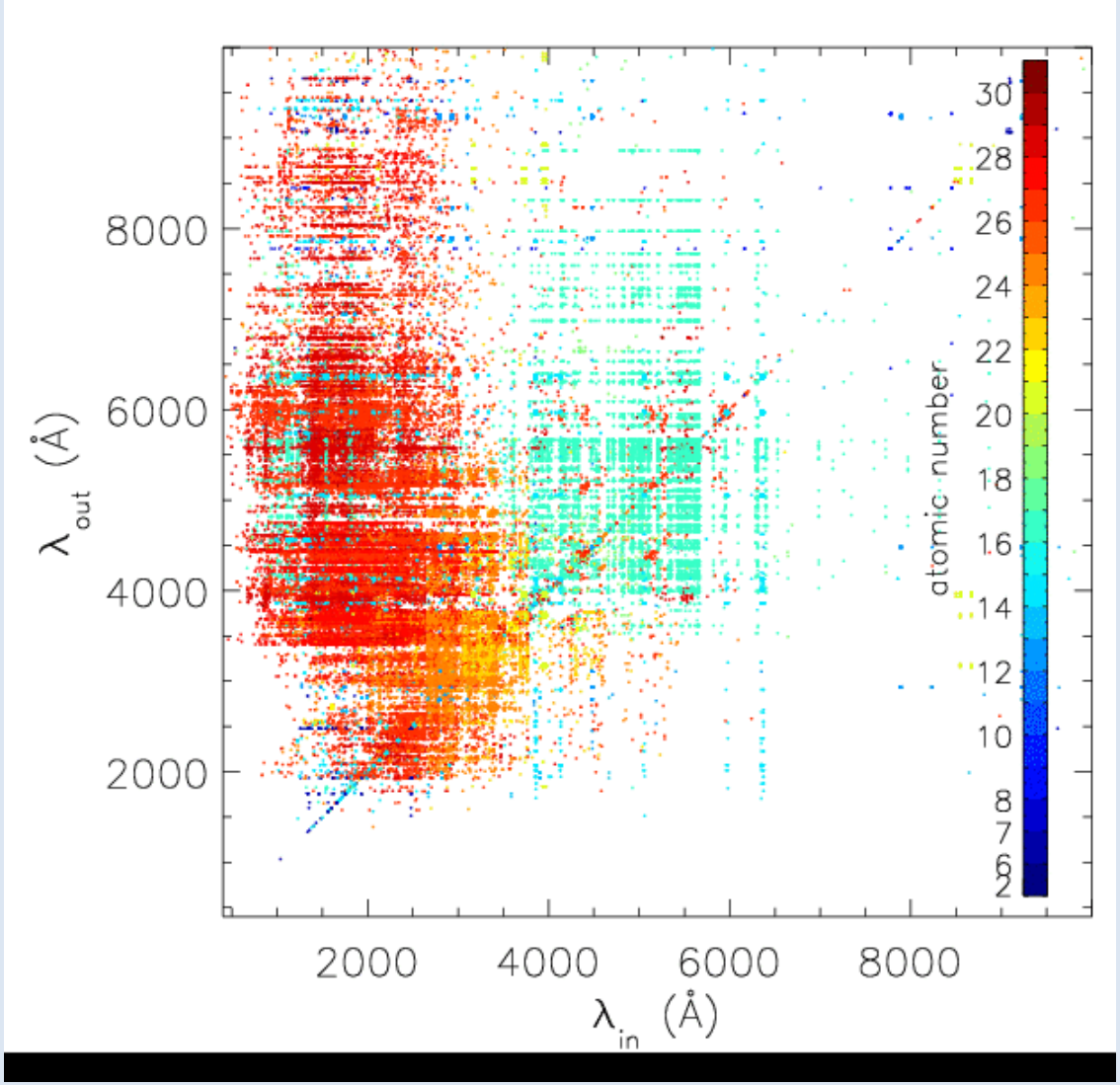


Packet trajectory length
(figure from Mazzali & Lucy 1993)

Line interaction events

…what to do when absorption occurs….

Redistribution in metal lines



(figure from Kromer & Sim 2009)

Line interaction events

Radiative equilibrium means any Monte Carlo packet absorbed by a line transition must be replaced.

An attractive way to handle this is by insisting packets are *indestructible* and *indivisible* (Lucy method). To implement this need rules to govern packet interactions.

Extremely simple to use resonance scattering approximation:

- In homologous flow Sobolev escape probabilities are isotropic
- Empirically seems to do quite well for optical spectra of SNe Ia

Alternative schemes based on “down branching” (Mazzali & Lucy 1993) and Lucy’s (2002, 2003) “macro atom” / “k-packet” methods give more physical realism.

Macro atom methods

(Lucy 2002/2003)

"Macro atom" is terminology introduced by Lucy (2002,2003) as part of a scheme designed to handle non-LTE interactions between radiation and matter (Monte Carlo energy packet scheme).

- Packets are *indestructible* and *indivisible*.
- Rules governing the interaction of packets with atomic energy levels are set up to enforce some desirable set of conservation laws: initially (and usually) statistical equilibrium (the construct for this is the "macro atom").
- Similar rules set up to enforce energy flow to/from the thermal energy reservoir of the gas, typically based on thermal equilibrium (described by the "k-packet" reservoir).

Macro atom methods

(Lucy 2002/2003)

"Macro atom" is terminology introduced by Lucy (2002,2003) as part of a scheme designed to handle non-LTE interactions between radiation and matter (Monte Carlo energy packet scheme).

- Packets are *indestructible* and *indivisible*.
- Rules governing the interaction of packets with atomic energy levels are set up to enforce some desirable set of conservation laws: initially (and usually) statistical equilibrium (the construct for this is the "macro atom").
- Similar rules set up to enforce energy flow to/from the thermal energy reservoir of the gas, typically based on thermal equilibrium (described by the "k-packet" reservoir).

Power of the method is that:

- ensures energy conservation conditions are exactly fulfilled locally within the simulation
- places energy conservation on a "higher footing" that current values of simulation properties (temperature, populations etc.)

Macro atom background

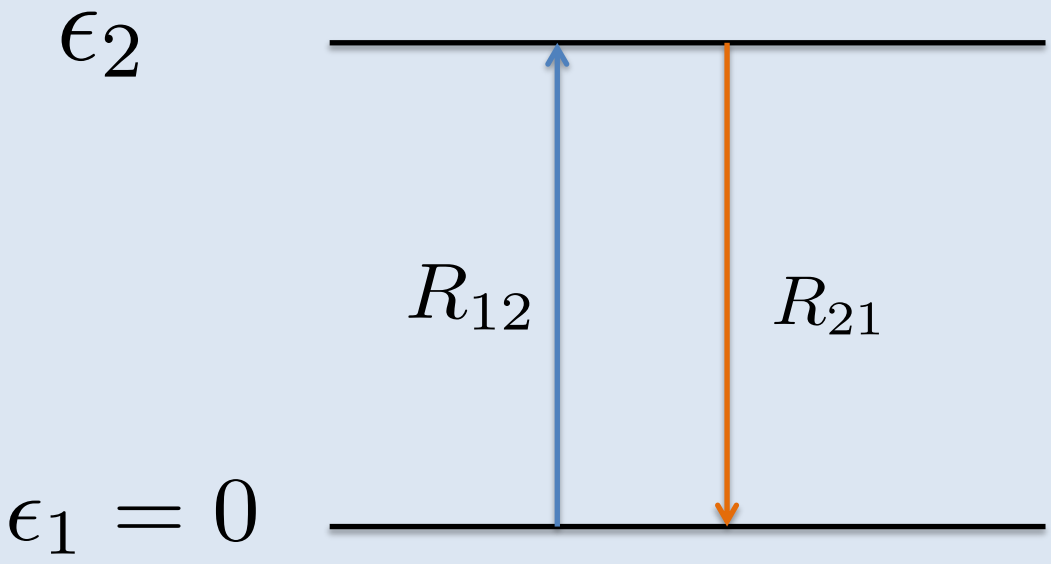
(Lucy 2002/2003)

For full derivation of scheme, see Lucy 2002/2003 (further comments in our review article, Noebauer & Sim 2019).

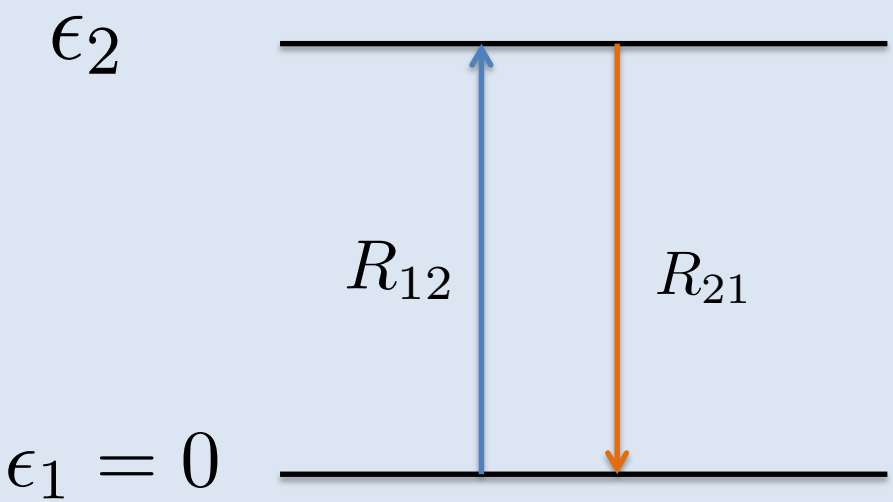
To illustrate principle here, will instead work with some simple examples: two- and three-level radiation dominated atoms…

Two-level atom

(radiation dominated)



Two-level atom



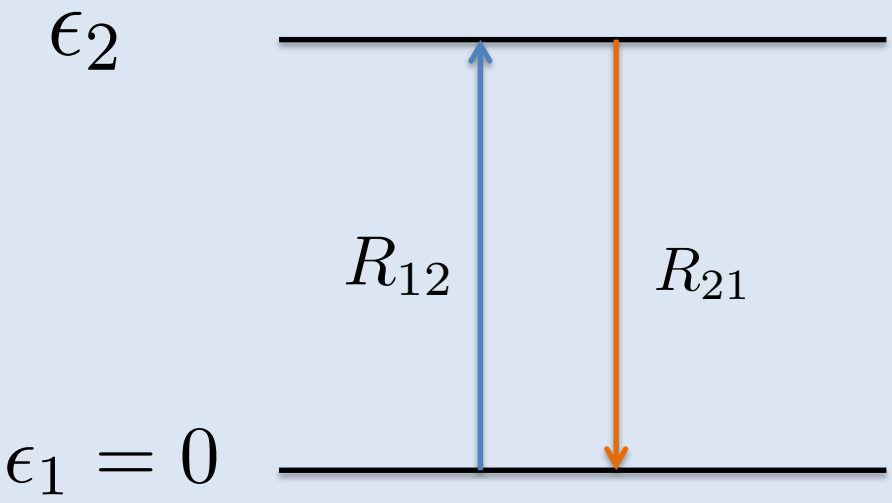
For homologous flow:

$$R_{21} = n_2 A_{21} p_{\mathrm{sob}}$$

$$p_{\mathrm{sob}} = \frac{1 - \bar{e}^{\tau_s}}{\tau_s}$$

$$R_{12} = n_1 \; B_{12} \; p_{\mathrm{sob}} \; J_b \; \left(1 - \frac{n_2}{n_1} \frac{g_1}{g_2} \right)$$

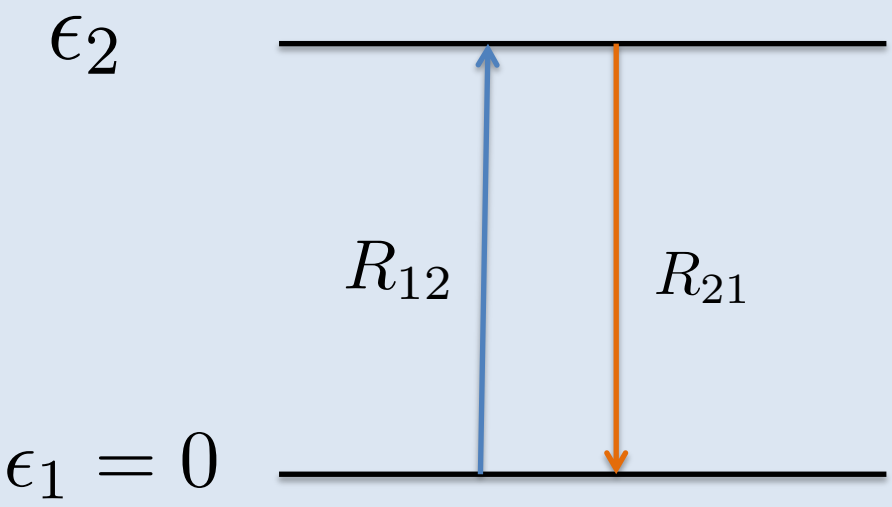
Two-level atom



Statistical equilibrium:

$$\frac{\mathrm{d}n_2}{\mathrm{d}t} = R_{12} - R_{21} = 0 \rightarrow R_{12} = R_{21}$$

Two-level atom



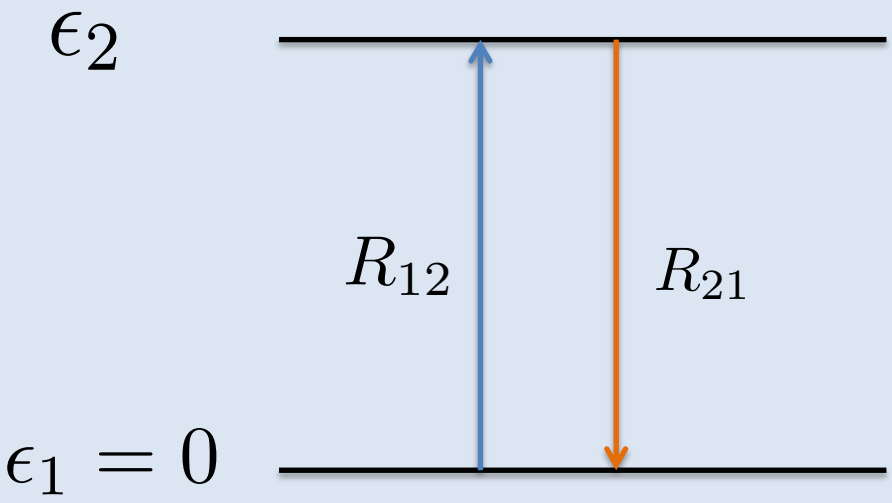
Statistical equilibrium:

Absorbing MC packets

$$\frac{\mathrm{d}n_2}{\mathrm{d}t} = R_{12} - R_{21} = 0 \rightarrow R_{12} = R_{21}$$

Re-emitted MC packets

Two-level atom

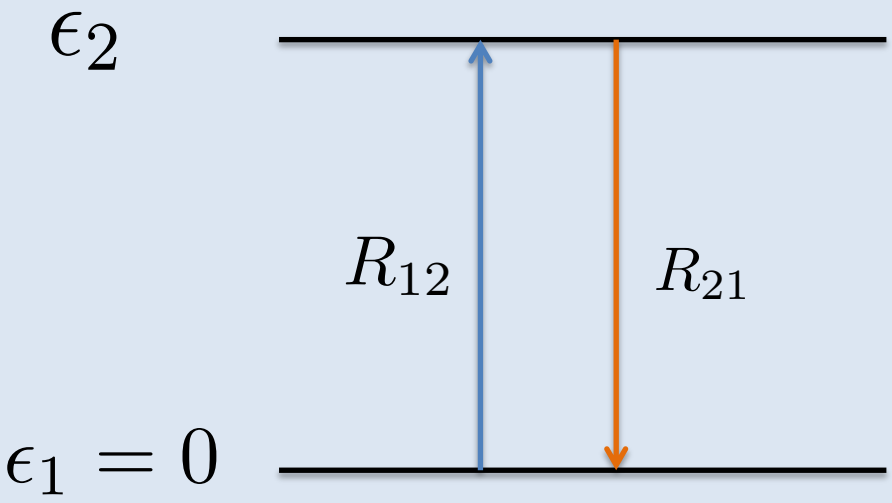


Simple algorithm ("scatter"):

Every time a line absorbs an energy packet immediately replace it with a new energy packet emitted by the same line. Effectively a scattering event – just need a new direction.

[Some codes generalize to include collisional destruction (e.g. Long & Knigge 2002)]

Two-level atom



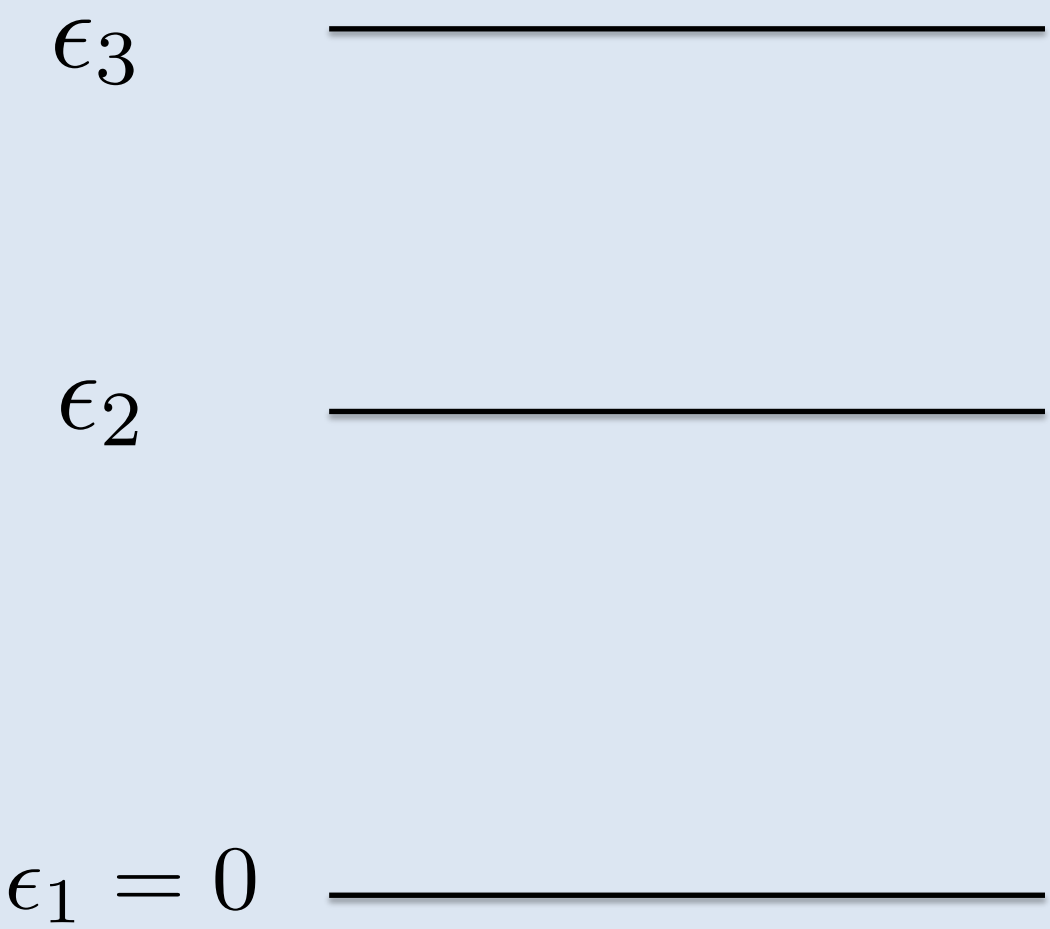
Note: This algorithm means that the rate of emission in the line is set by the rate of absorption, not an estimate of the upper level population (which would depend on an accurate non-LTE level population).

Simple algorithm ("scatter"):

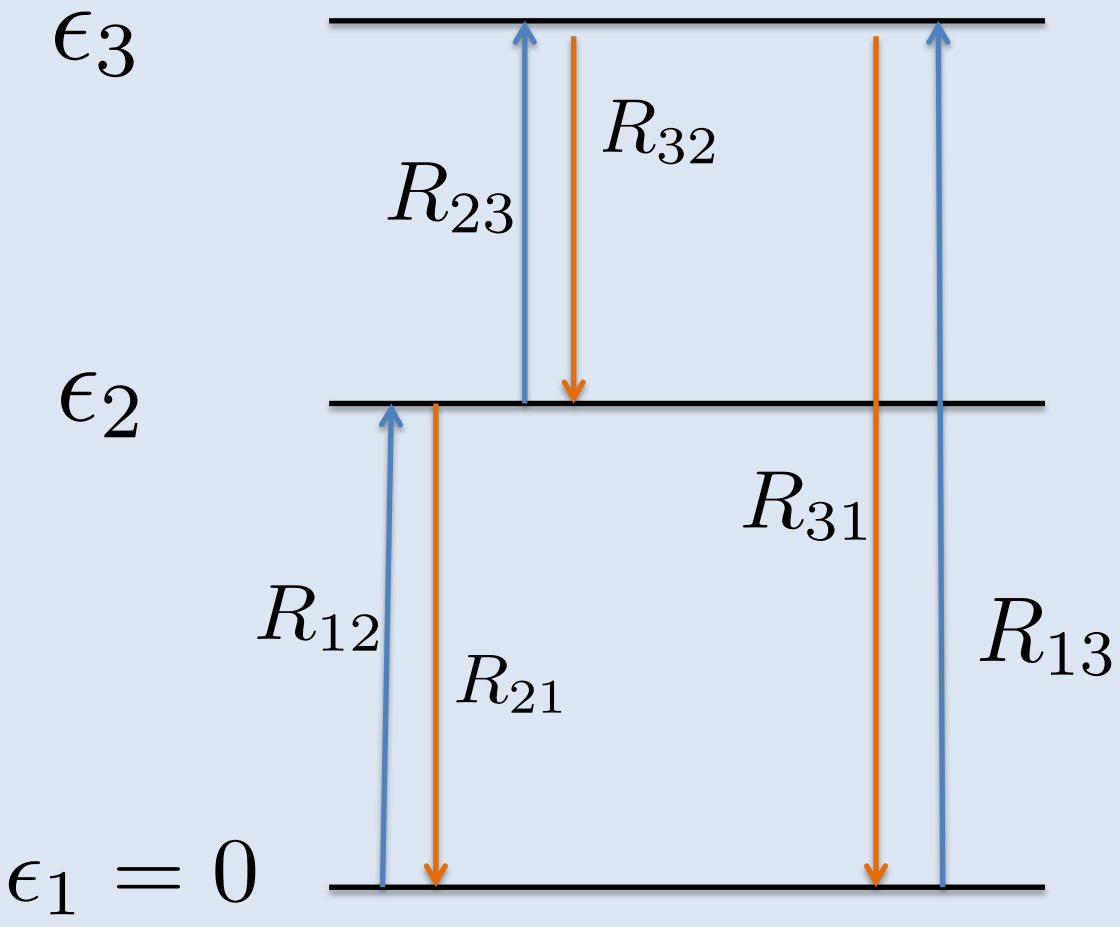
Every time a line absorbs an energy packet immediately replace it with a new energy packet emitted by the same line. Effectively a scattering event – just need a new direction.

[Some codes generalize to include collisional destruction (e.g. Long & Knigge 2002)]

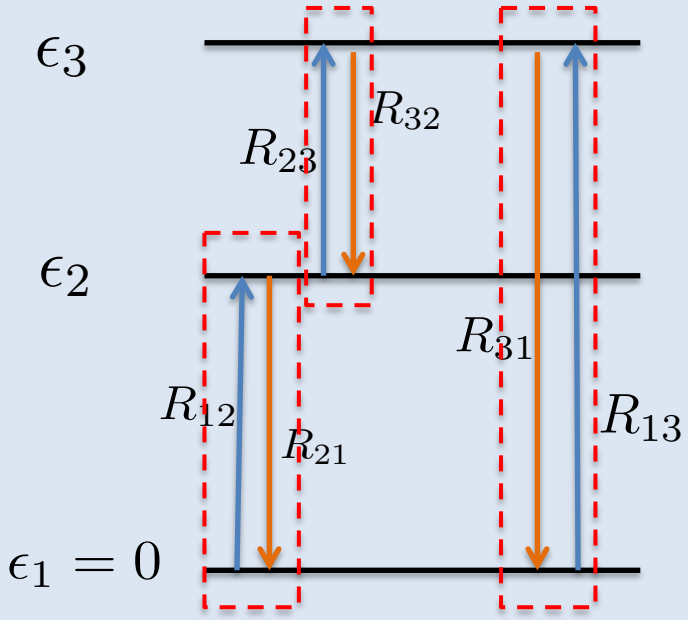
Radiation-dominated example



Radiation-dominated example



Radiation-dominated example



Resonance line scattering assumption:

$$R_{12} = R_{21}$$

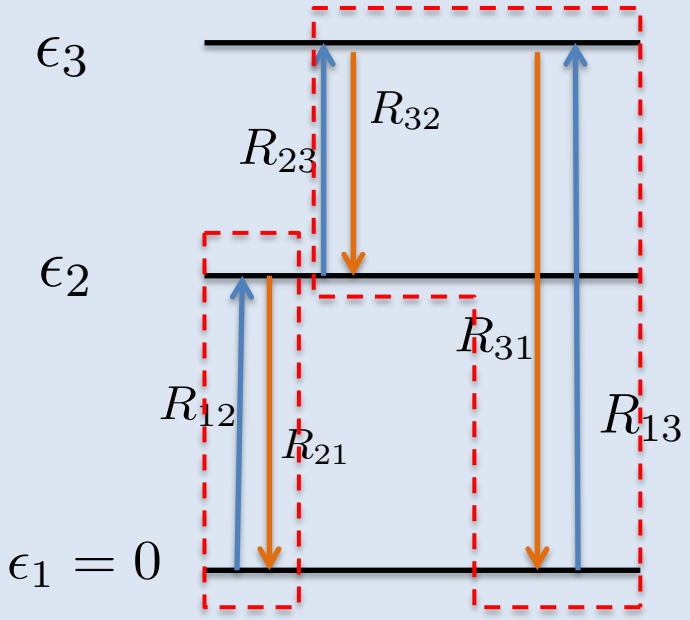
$$R_{23} = R_{32}$$

$$R_{13} = R_{31}$$

Advantages:
Very simple to implement in MCRT
Should be reasonable for many cases

Problem:
Neglects a lot of atomic physics!

Radiation-dominated example



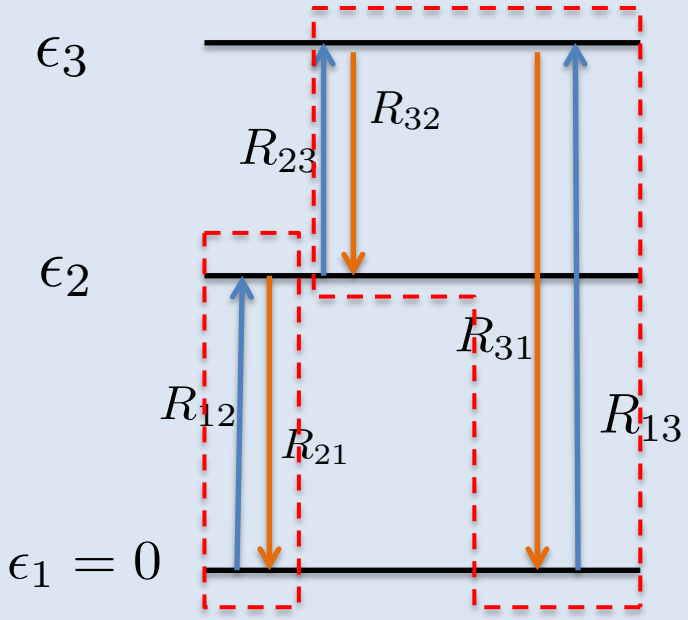
"Down-branching" approach:

Following excitation to an atomic level:

1. Randomly select a transition out of that level based on energy flow rates (Lucy 1999)

2. Emit an energy packet in that transition (energy equal to absorbed packet energy)

Radiation-dominated example



"Down-branching" approach:

E.g., following excitation to level 3, choose remission with

$$p_{31} = \frac{R_{31}\epsilon_3}{R_{31}\epsilon_3 + R_{32}(\epsilon_3 - \epsilon_2)}$$

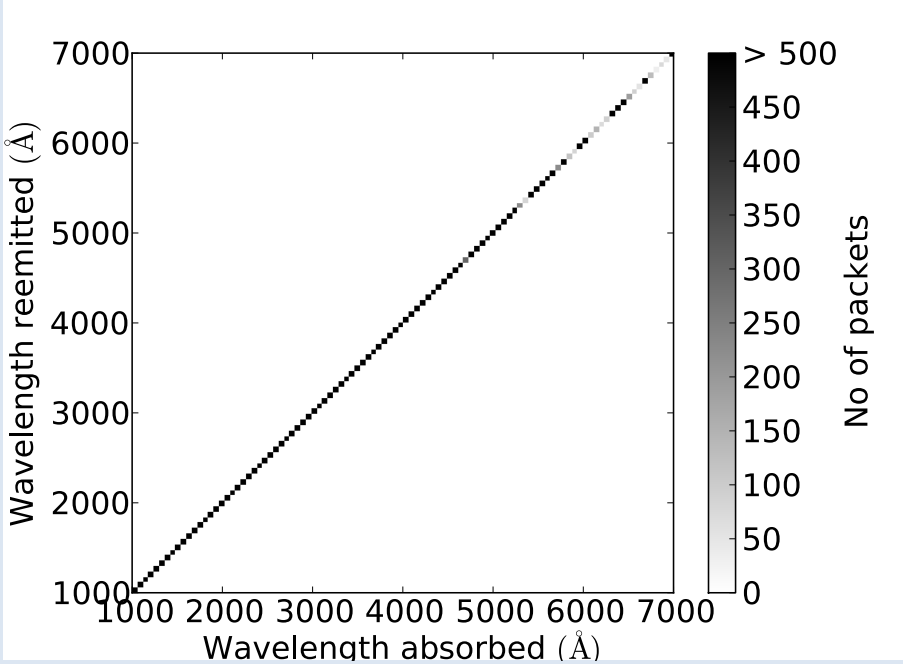
$$p_{32} = \frac{R_{32}(\epsilon_3 - \epsilon_2)}{R_{31}\epsilon_3 + R_{32}(\epsilon_3 - \epsilon_2)}$$

Advantages:
Only minor complication to MCRT
Major improvement for many cases

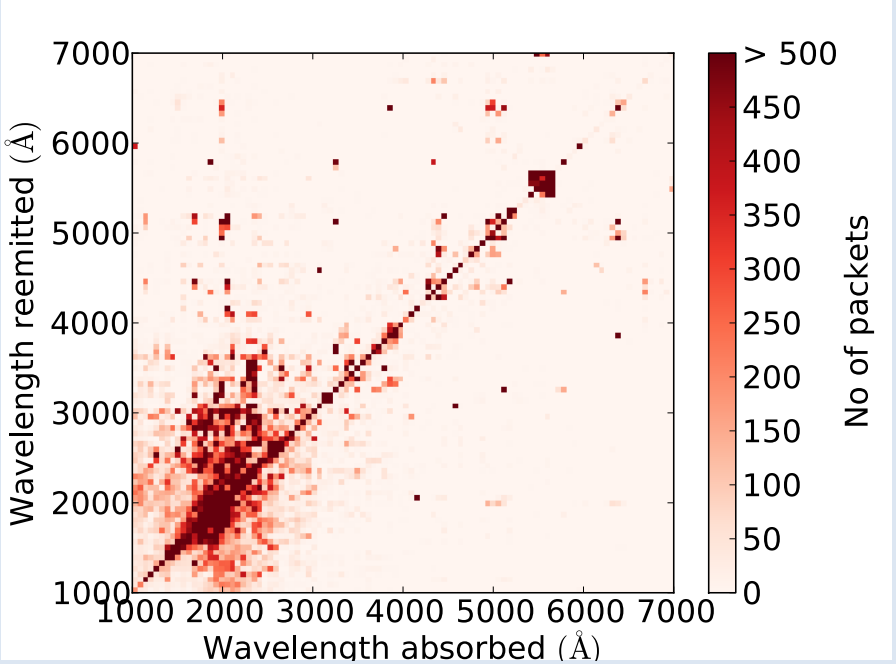
Problem:
Still neglects a lot of atomic physics!

Radiation-dominated example

Kerzendorf & Sim (2014)

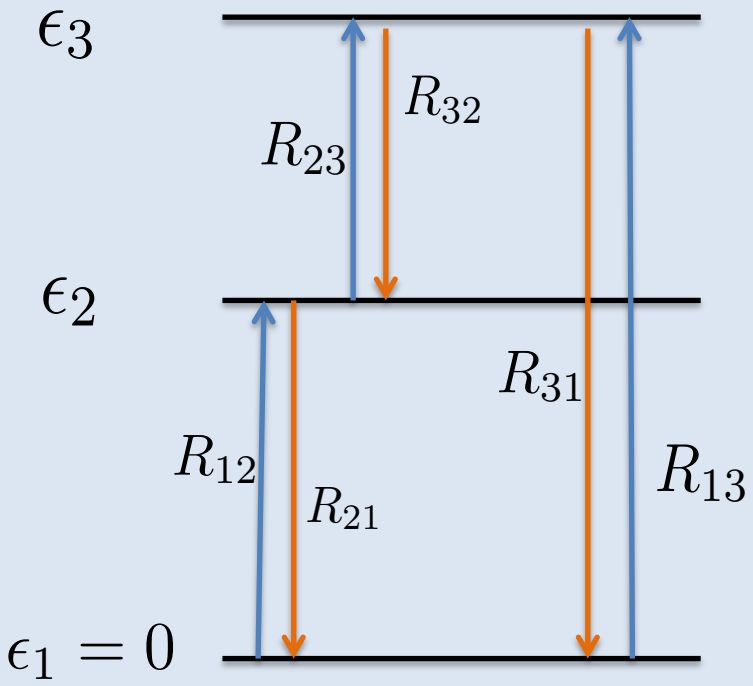


Resonance scattering



Downbranching

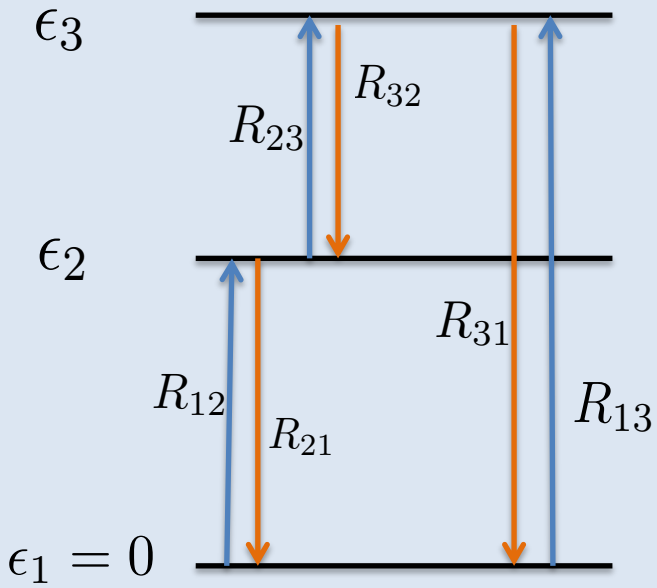
Radiation-dominated example



General solution can be found; e.g. via Lucy's "**Macro Atom**"

(see Lucy 2002)

Radiation-dominated example



Statistical equilibrium:

$$R_{13} + R_{23} - R_{31} - R_{32} = 0$$

$$R_{12} + R_{32} - R_{21} - R_{23} = 0$$

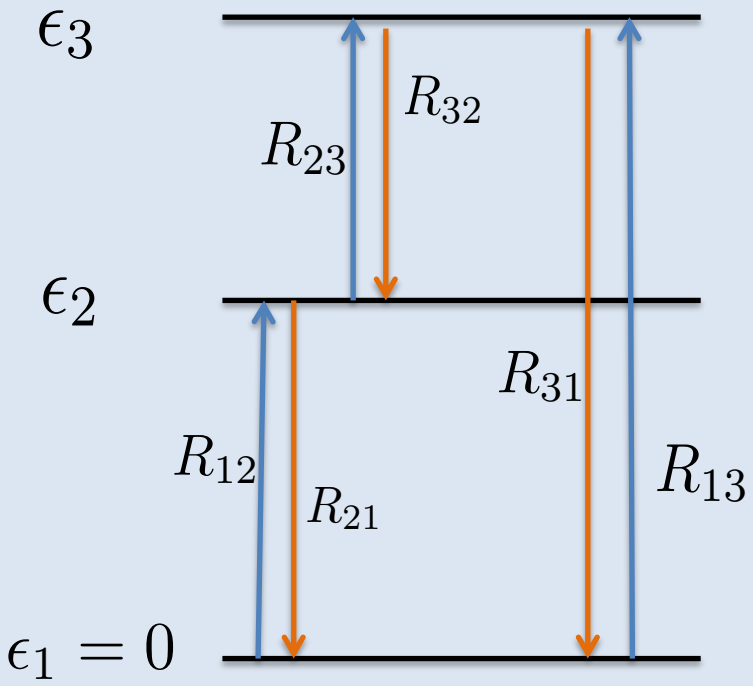
Energy "flow" rates:

$$\dot{A}_2 = R_{12}\epsilon_2 \qquad \dot{A}_3 = R_{13}\epsilon_3 + R_{23}(\epsilon_3 - \epsilon_2)$$

$$\dot{E}_2 = R_{21}\epsilon_2 \qquad \dot{E}_3 = R_{31}\epsilon_3 + R_{32}(\epsilon_3 - \epsilon_2)$$

(see Lucy 2002)

Radiation-dominated example



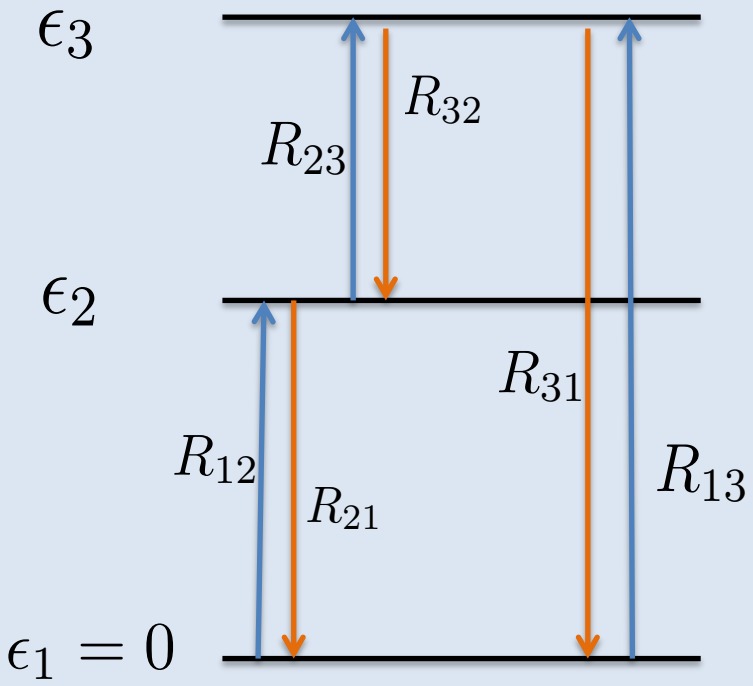
Algebra with rates and stat. eqm. from last slide:

$$\dot{A}_3 + R_{23}\epsilon_2 = \dot{E}_3 + R_{32}\epsilon_2$$

$$\dot{A}_2 + R_{32}\epsilon_2 = \dot{E}_2 + R_{23}\epsilon_2$$

Interpret as traffic flow problem: "Macro Atom" (see Lucy 2002)

Radiation-dominated example



Algebra with rates and stat. eqm. from last slide:

$$\dot{A}_3 + R_{23}\epsilon_2 = \dot{E}_3 + R_{32}\epsilon_2$$

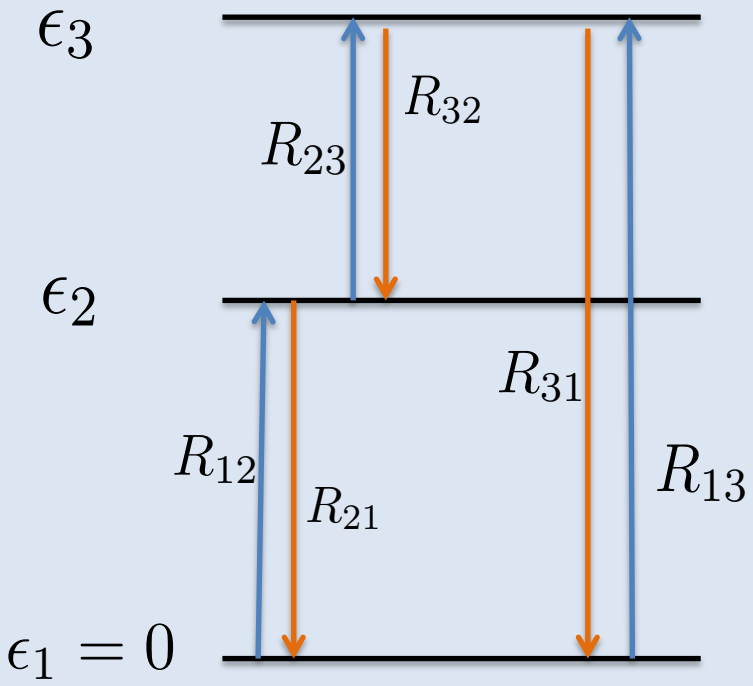
$$\dot{A}_2 + R_{32}\epsilon_2 = \dot{E}_2 + R_{23}\epsilon_2$$

Interpret as traffic flow problem: "Macro Atom" (see Lucy 2002)

Absorption of radiation packets

Emission of packets

Radiation-dominated example



Algebra with rates and stat. eqm. from last slide:

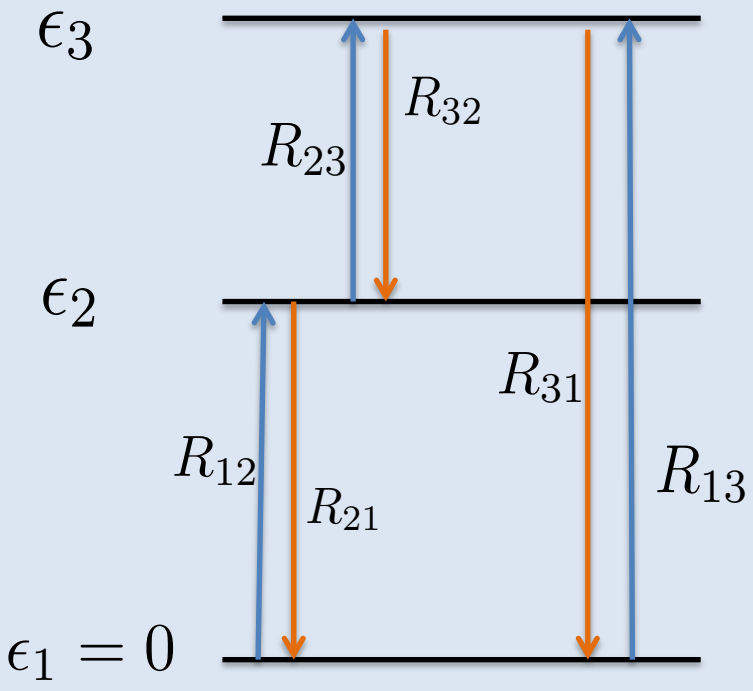
$$\dot{A}_3 + R_{23}\epsilon_2 = \dot{E}_3 + R_{32}\epsilon_2$$

$$\dot{A}_2 + R_{32}\epsilon_2 = \dot{E}_2 + R_{23}\epsilon_2$$

Interpret as traffic flow problem: "Macro Atom" (see Lucy 2002)

Absorption of radiation packets
Emission of packets
Internal macro atom (radiationless) transition out of level
Internal macro atom (radiationless) transition into level

Radiation-dominated example



Algebra with rates and stat. eqm. from last slide:

$$\dot{A}_3 + R_{23}\epsilon_2 = \dot{E}_3 + R_{32}\epsilon_2$$

$$\dot{A}_2 + R_{32}\epsilon_2 = \dot{E}_2 + R_{23}\epsilon_2$$

Interpret as traffic flow problem: "Macro Atom" (see Lucy 2002)

Algorithm:

1. Following activation of some state, select either an emission or internal transition (probabilities proportion to terms above)

2a. If select emission emit a photon (as in "down-branch" scheme)

2b. If select an internal transition, change the macro atom state and GOTO 1

Radiation-dominated example

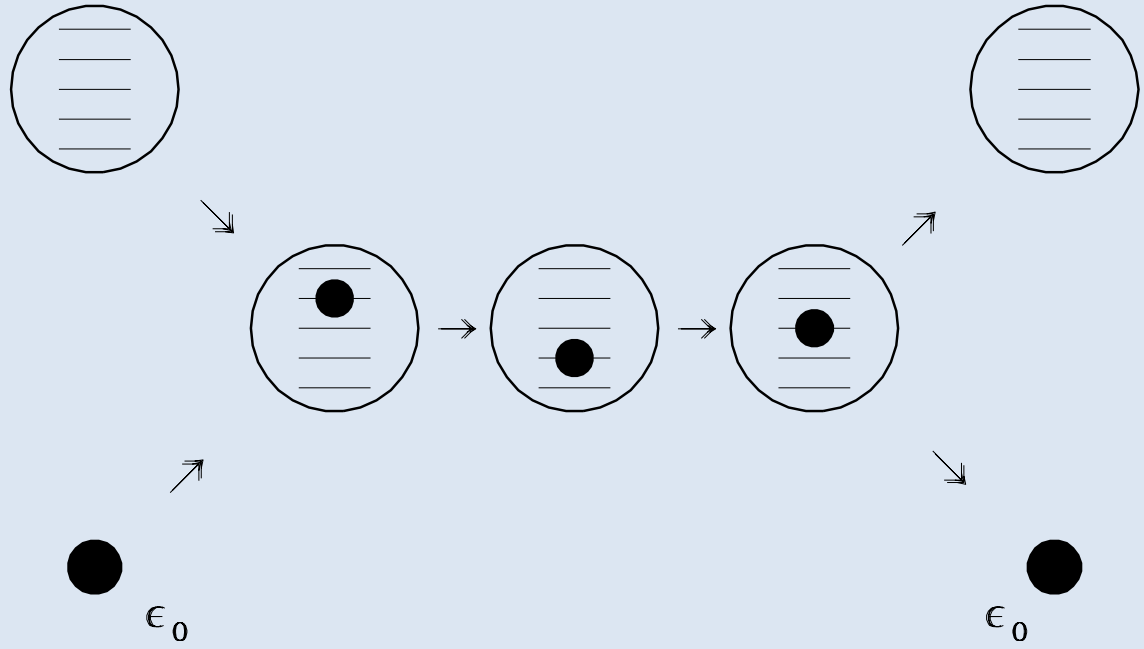
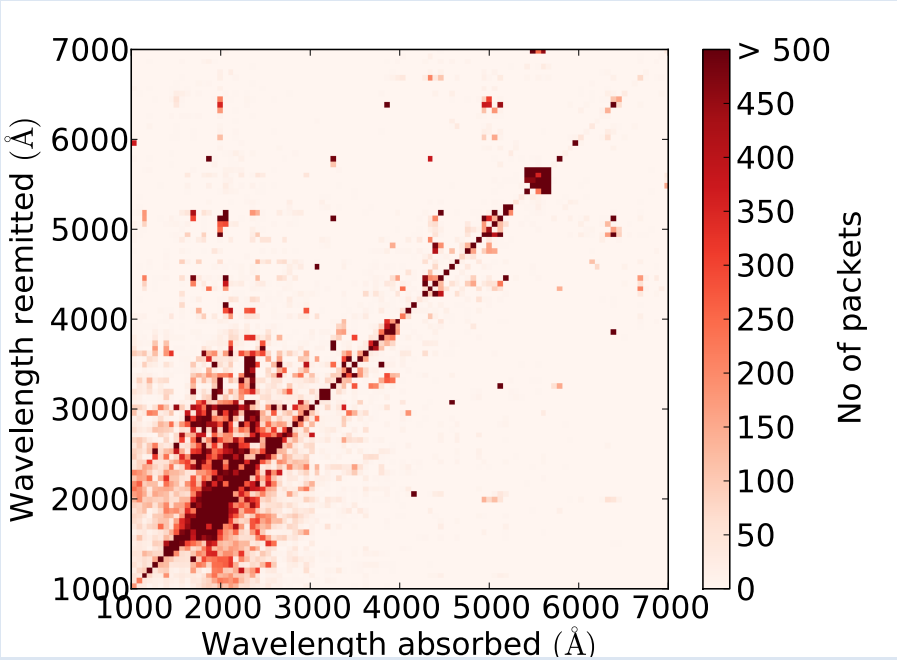


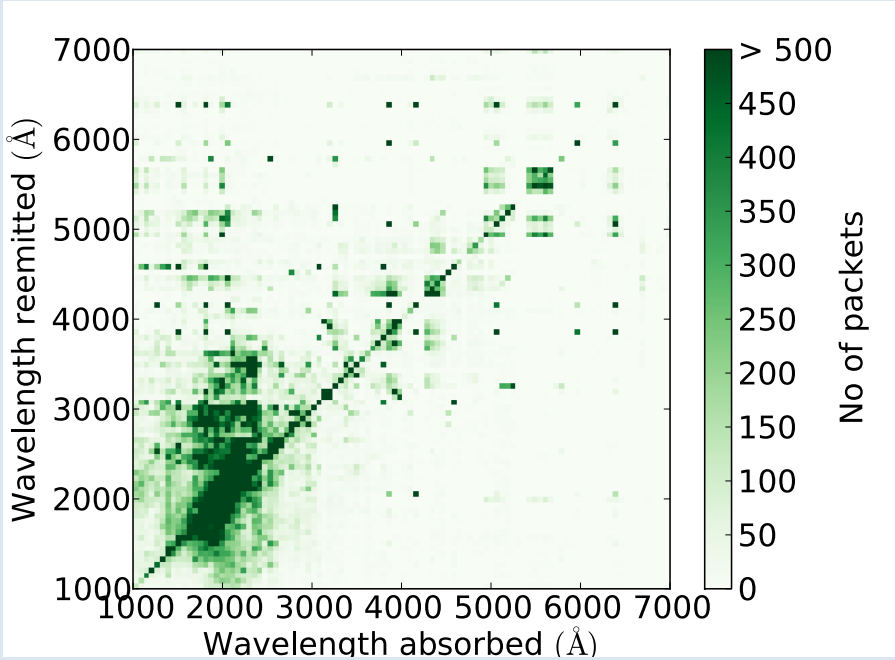
Fig. 1. Schematic representation of the interaction of a macro-atom with a packet of energy ϵ_0. The macro atom is activated by absorbing the energy packet, makes two internal transitions, and then de-activates by emitting a packet of energy ϵ_0.

Lucy 2002

Radiation-dominated example

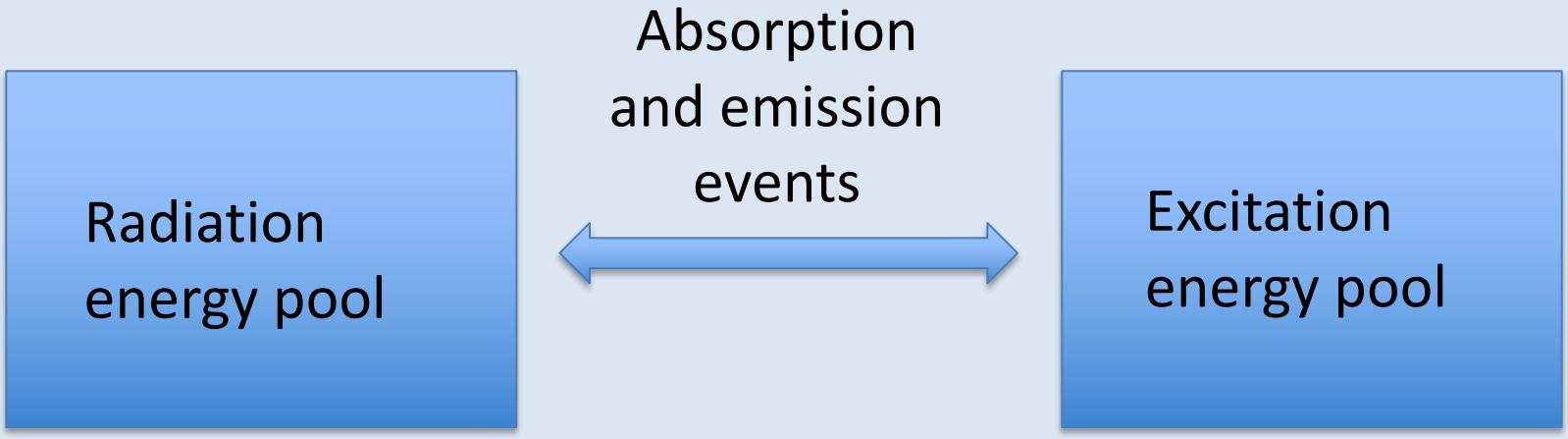
Kerzendorf & Sim (2014)





Downbranch v Macro Atom

Radiation-dominated example



Governed by radiative packet transport algorithm

Governed by macro atom internal transition rules

Generalization (Lucy 2003)

For full solution in radiative and thermal equilibrium can extend to include third energy pool:

… coupling to energy in the thermal pool of random particle velocities ("*k*-packe"t pool).

Transfer of energy to/from this reservoir is governed by heating/cooling processes:

- Some processes (e.g. free-free) can be viewed as transferring energy from radiation energy pool to thermal pool
- Others (e.g. inelastic collisions between electrons and atoms) transfer energy between atomic excitation pool and thermal pool

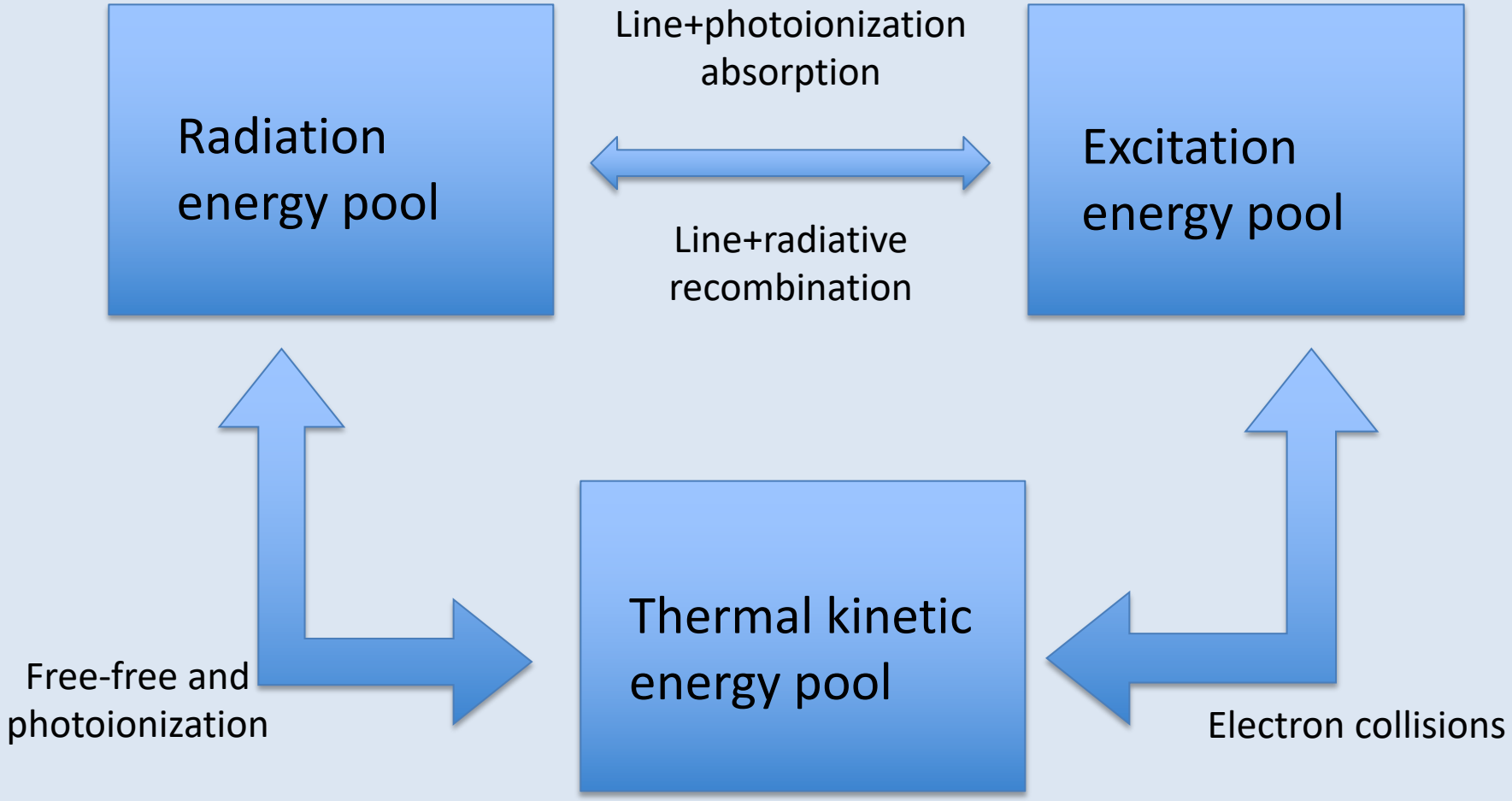
Governing equation is thermal balance:

$$H_{\mathrm{R}} + H_{\mathrm{C}} = C_{\mathrm{R}} + C_{\mathrm{C}}$$

…also lends itself to traffic flow interpretation of thermal pool: heating rates are flow to thermal pool, cooling rates are flows out from thermal pool.

Generalization (Lucy 2003)

For full solution in radiative and thermal equilibrium can extend to include third energy pool:
(for SNe implementation e.g. Kromer & Sim 2009)



Macro Atom implementation

- Use Macro Atom implementation in our ARTIS supernova code (Kromer & Sim 2009) and TARDIS spectral synthesis code (Kerzendorf & Sim 2014)

TARDIS: open source code for spectral synthesis of supernovae

On public release (regular updates):

- Available on github,

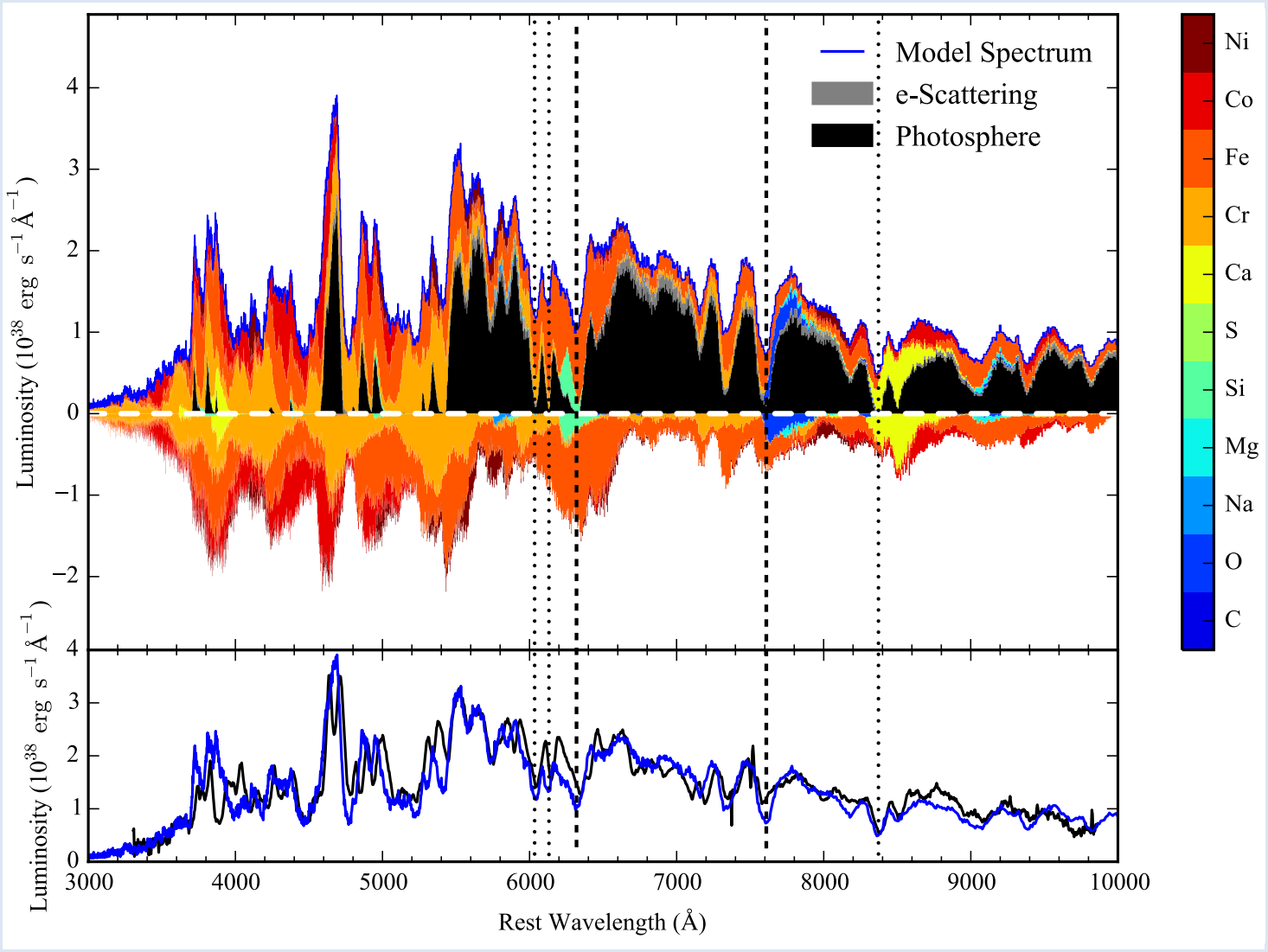
http://github.com/tardis-sn/tardis

http://tardis.readthedocs.org/

- Also implemented now in non-homologous flow codes, both Python (Long & Knigge 2002) and Sim et al. (2008, 2010)

- Implemented by Ergon et al. (2018) in full time-dependent SN code – uses additional step to avoid explicit sampling of internal transitions.

TARDIS example work (Magee et al. 2016):



SN2015H
Magee+2016
(22 days)

Summary

- **Lecture 1:**
  - MCRT methods work well for rapidly expanding environments
  - Critical ingredients are the special relativistic effects associated with frame transformations
  - For time dependent applications (e.g. light curves) tracking photon flight times is central (but trivial).
- **Lecture 2:**
  - Opacity in expanding media can be complicated due to Doppler shifting of photons – particularly relevant for line absorption
  - Sobolev approximation to line opacity provides huge simplification and lends itself to very efficient algorithms
  - Macro Atom formalism of Lucy is effective way of dealing with non-LTE emissivities based on strict energy conservation.