What every astronomer should know about atmosphere modeling and about `PHOENIX` in particular

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- What is a stellar atmosphere?
    - Atmosphere vs. Spectrum
    - General physics
        - The Radiative Transfer Equation
        - Equation of State
        - Convection in 1D
    - Computation of 1D Model Atmospheres
    - Computation of 3D Model Atmospheres

- What is PHOENIX?
    - Important Physics
    - Example applications
    - Almost a tutorial
        - PHOENIX/3D
        - PHOENIX/1D

- Summary

Atmosphere vs. Spectrum

Atmosphere:

- $T, P, \rho, v, \ldots$

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1D: e.g. SYNTHE
3D: e.g. Asplund et al.

The Radiative Transfer Equation

The radiative transfer equation (RTE) in its general form:

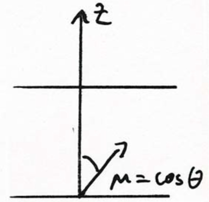
$$\begin{aligned} \frac{1}{c}\frac{\partial I_\nu}{\partial t} + \vec{n} \cdot \nabla I_\nu &= \epsilon_\nu - \chi_\nu I_\nu \\ &= \chi_\nu (S_\nu - I_\nu) \end{aligned}$$

where

- ϵ_ν: emission coefficient (account for the net rate of change of photons)
- χ_ν: extinction coefficient (account for the net rate of change of photons)
- $S_\nu = \frac{\epsilon_\nu}{\chi_\nu}$: source function, in (L)TE $= B_\nu$
- in general $\epsilon = \epsilon(I) \rightarrow$ Scattering problem

RTE in different Geometries

Plane parallel:



$$\mu \frac{dI_\nu}{dz} = \chi_\nu (S_\nu - I_\nu)$$

With $d\tau_\nu = -\chi_\nu \, dz$, the pp RTE becomes

$$\mu \frac{dI_\nu}{d\tau_\nu} = I_\nu - S_\nu$$

Spherical symmetric:

$$\mu \frac{\partial I}{\partial r} + \frac{1-\mu^2}{r} \frac{\partial I}{\partial \mu} = -\chi \, (I - S)$$

Radiation Flux F_ν

- net flux of radiation through a surface element $d\sigma$:

$$\vec{F_\nu} = \oint_{4\pi} I_\nu \vec{n}\, d\Omega$$

- in 1D the vector $\vec{F_\nu}$ reduces to

$$F_\nu = \int \mu I_\nu \, d\mu d\varphi$$

so that (I_ν independent of φ!)

$$F_\nu = 2\pi \int \mu I_\nu \, d\mu$$

- old literature: 'astrophysical flux'

$$\pi\mathcal{F} = F_\nu$$

RT for Synthetic Spectra

radiative transfer equation $\forall\lambda$

- absorption & scattering coefficients

$$\sum \sigma_i^j n_i^j$$

  - j: ionization stage
  - i: energy level within each ionization stage
  - σ_i^j: cross section [cm^2] incl. line profile
  - n_i^j: population density [1/cm^3]
- $\sum$ over all elements, processes, ionization stages, level
- σ_i^j from QM, measurements
- tables of data, fit formulae etc.

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→ how is scattering treated?

RT for Model Atmospheres

Three possibilities:

- Actually do all the calculations and the RTE line by line (PHOENIX)
- Use appropriate approximations for the frequency sampling (typical atmosphere codes)
  - Opacity Distribution Functions
  - Opacity Sampling
- Use optically thick or grey approximations

Equation of state

- n_i^j depend on
  - temperature
  - gas pressure
  - abundances
  - *radiation field*

→ in general: NLTE
rate equation for all population and de-population processes

- gives relation $(T, P_{\mathrm{gas}}, \rho)$
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How is NLTE implemented? (in 3D?)

The Saha Equation

With

- n_k: number density of ionization stage k (summed over all energy levels)
- n_e: electron density
- Q_k: partition function of state k
- $\chi_{k\to k+1}$: ionization energy (ground state to ground state)

$$n_k = n_{k+1} n_\mathrm{e} \frac{Q_k}{Q_{k+1} 2} \left(\frac{h^2}{2\pi m_e k T} \right)^{3/2} \exp\left(\frac{\chi_{k\to k+1}}{kT} \right)$$

The Saha Equation

The system is closed by

- particle conservation:

$$n_i = \epsilon_i \left(P_{\mathrm{gas}}/kT - n_{\mathrm{e}}\right)$$

  ϵ_i: normalized abundance (by number) of this element

- charge conservation:

$$n_{\mathrm{e}} = \sum_i \sum_j q_{ij} n_{ij}$$

Ultimatively: root of high order polynomial in n_{e} for (T, P_{gas})
With all n_{ij}

$$\rho = (n_{\mathrm{e}} m_e + \sum_i n_{ij} m_{ij})$$

Boltzmann Formula

With

- n_i: population density (particles /cm^3)
- $N = \sum n_i$
- g_i: statistical weights (number of degenerate quantum states)
- χ_i: excitation energy ($\chi_1 \equiv 0$)
- $Q = \sum g_i \exp\left(-\frac{\chi_i}{kT}\right)$: partition function

$$\frac{n_i}{N} = \frac{g_i}{Q} \exp\left(-\frac{\chi_i}{kT}\right)$$

Convection (in 1D)

- no real theory of convective energy transport!
- comparatively simplistic model for convection
- especially bad in optically thin media!

Basic picture:

- convection = buoyant bubbles
- bubbles are allowed to form in *any* environment
- if buoyancy increases → convection occurs

Mixing Length Theory

Assumptions:

- bubbles rise an average distance $l_m = \alpha_m h_p$
    - h_p is the pressure scale height $h_p := -P\frac{dr}{dP} = \frac{P}{\rho g}$
- estimate convective flux

$$F_{conv} = \rho c_p \overline{v \Delta T}$$

- ... and all necessary quantities
    - T (and ρ) difference (ΔT) to surroundings increases linearly
    - work of buoyancy goes into kinetic energy (v)
    - energy loss due to radiation (e.g. diffusion approximation)
- system of equations

$\rightarrow$ cubic equation for $\frac{dT}{d\tau}$

Computation of 1D Model Atmospheres

- minimum independent variables/parameters:
  - effective temperature T_{eff}
  - gravity $g = GM/R^2$ (or $g(r) = GM/r^2$ if not constant)
  - mass M or radius R or luminosity $L = 4\pi R^2 \sigma T_{\mathrm{eff}}^4$
  - abundances of all elements
- additional parameters may exist (B-fields, irradiation etc)
- necessary prelims:
  - discretize the radial coordinate

Computation of 1D Model Atmospheres

step 1:

- select a grid of $\tau_{\rm std}$ points
- guess (approximate or scale) a temperature structure $T(\tau_{\rm std})$
- integrate hydrostatic equation

$$\frac{dP_{\rm gas}}{d\tau_{\rm std}} = \frac{g\rho}{\chi_{\rm std}}$$

(ignoring $P_{\rm rad}$ and setting $g = {\rm const.}$ for simplicity)

Computation of 1D Model Atmospheres

- need initial value for $P_{\mathrm{gas}}(\tau_{\mathrm{std}} = 0)$!
- need $\rho(T, P_{\mathrm{gas}}) \rightarrow$ equation of state, e.g.,

$$\rho = \frac{\mu}{\mathcal{R}} \frac{P_{\mathrm{gas}}}{T}$$

- $\mathcal{R} = k/m_{\mathrm{H}}$
- μ: mean molecular weight
- ρ and μ from Saha-Boltzmann

Computation of 1D Model Atmospheres

step 2a:

- compute convective $\frac{dT}{d\tau}$ via MLT

step 2b:

- compute total radiative flux

$$F_{\mathrm{rad}}(\tau_{\mathrm{std}}) = \int_0^\infty F_\lambda(\lambda, \tau_{\mathrm{std}})\, d\lambda$$

  for *each* layer!
- → need to know $F_\lambda(\lambda)$ ...
- → need to solve radiative transfer problem $\forall\lambda$
- → must know all $\sigma_i^j(T, P_{\mathrm{gas}}, \lambda)$
- *and* must know all $n_i^j(\tau_{\mathrm{std}})$
- alternatively invoke ODF or opacity sampling formalism

Computation of 1D Model Atmospheres

step 3:

- in general we will find that

$$F_{\mathrm{rad}}(\tau_{\mathrm{std}}) \neq \sigma T_{\mathrm{eff}}^4$$

  for radiative layers
- $\rightarrow$ need to *correct* $T(\tau_{\mathrm{std}})$

repeat until converged . . .

Computation of 3D Model Atmospheres

Solve (time dependent!)

- Continuity equation

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \vec{v})$$

- Navier Stokes equation. E.g. (without viscosity)

$$\frac{\partial \vec{v}}{\partial t} + (\vec{v} \cdot \nabla)\vec{v} = -\frac{1}{\rho}\nabla P + \vec{g}$$

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→ radiative energy transport?

Important Physics

PHOENIX v16 is being used to model

- nova and supernova atmospheres
- main sequence stars, very low mass stars, brown dwarfs & Exoplanet atmospheres
- (red) giants, white dwarfs
- disks (proto-planetary, AGN)

Important Physics

integrated /1D and /3D versions (e.g. same micro physics)

- detailed and stable EOS for huge range of temperatures
- NLTE model atoms with huge number of levels
- dust formation/destruction DRIFT (Helling & Woitke)
- direct opacity sampling of line blanketing
  - atomic line blanketing: $\approx 5 - 30 \times 10^6$ lines dynamically selected from a list of 83×10^6 lines
  - molecular line blanketing: $\approx 15 - 900 \times 10^6$ lines dynamically selected from a list of 2.3×10^9 lines
  - depth dependent line profiles

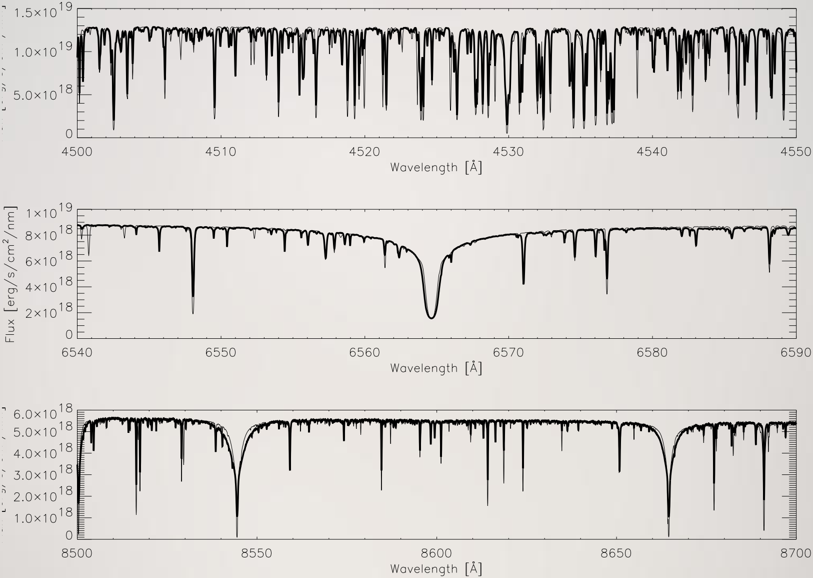
$\Rightarrow$ no ODF or opacity sampling tables (NLTE!).

Important Physics

- radiation transport solved for large optical depths & strong scattering
- static (stars) or allow velocity fields (novae, winds, SNe, turbulence)
- allow irradiation

Example applications

models work well for G2V's



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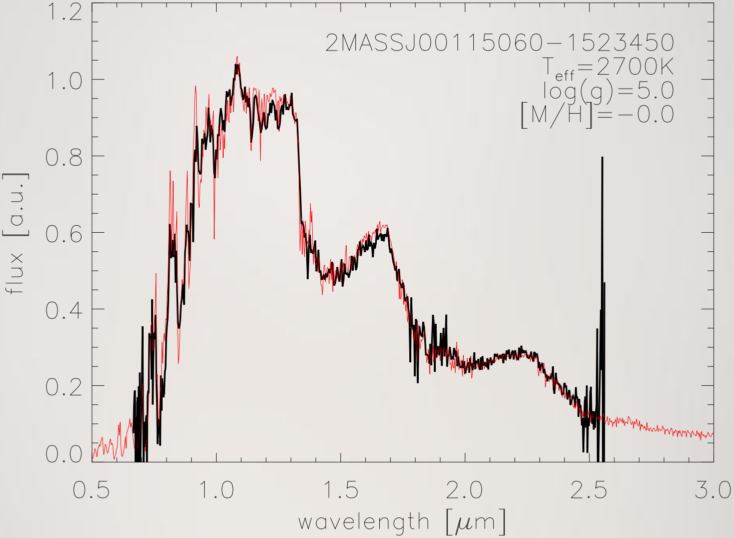

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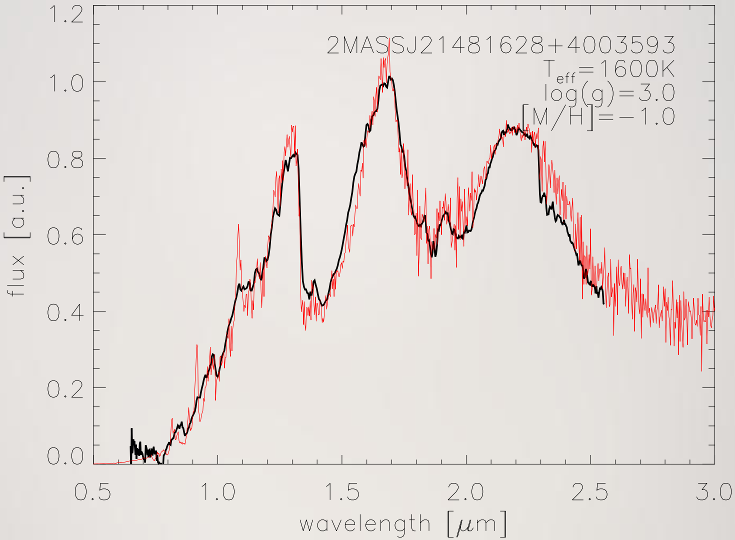
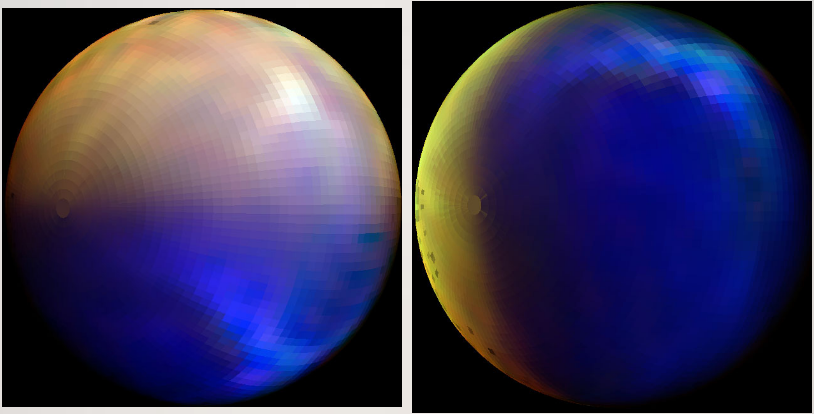


Example applications

3D visualization: GCM Model



PHOENIX/3D

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- no internal hydrodynamics (yet)
- "one shot" radiation, no energy feedback
- atmosphere provided externally (FLASH, PlaSim, . . .)

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Advantages:

- detailed radiation transport (scattering, large τ)
- detailed microphysics (EOS, opacities, NLTE)

PHOENIX/1D

Calculation of atmosphere and spectrum

- same code
- same implementation of physics

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Atmosphere:

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- energy transport by radiation transport for "low" resolution spectrum
- energy conservation by temperature correction (iteration)

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Spectrum:

- different resolution and wavelength range

⇒ Consistent atmosphere and spectrum

Spherical symmetric vs. plane parallel and the role of the Radius

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⇒ for plane parallel objects: R (or M or L) is a scaling factor

Abundance determinations with PHOENIX

Abundances can be changed individually

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But recall:

- designed for consistent atmosphere
- full equation of state
- full opacity

⇒ no quick line profiles

1.5D with PHOENIX/1D

e.g. inhomogenous surfaces:

- specific intensity for each surface area element
- integrate obserable flux yourself

But: non standard output

Irradiation with PHOENIX/1D

- slab for one angle between direction to object center and illumination source
- redistribute energy
- 1.5D

Summary

- 1D: modelling atmosphere and spectrum consistently is possible (and PHOENIX does it)
- 3D: Atmosphere structure and spectrum from it require two calculations (for all codes)