Opacities of Molecules and Dust

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As progressively lower temperatures are encountered in a stellar atmosphere, first molecules and finally dust grains become important sources of opacity. The abundance of important molecular and solid absorbers depends upon temperature, pressure, and the chemical composition in complex ways which require detailed equation of state calculations. Molecular spectra, which usually contain thousands or millions of spectral lines, are usually treated statistically in the opacity sampling method. Because of the size of modern line lists and the computation time required to process them, efficient computation of molecular opacity requires careful selection of the wavelengths and the relevant lines. We will discuss these procedures, and the results obtained for important absorbers such as H_2O and TiO.

For temperatures below about 1,800 K, some materials begin to precipitate out of the gas phase as small solid particles. Because these small grains are very efficient absorbers and scatterers of light, they dominate the opacity whenever they exist. The thermodynamic and optical properties of these materials will be explored. Recent results show that even grains with relatively low abundances, such as Al_2O_3 and $CaTiO_3$, can have a dramatic impact on the structure of stellar atmospheres. Most atmospheres with $T_{eff} < 3,000\ K$, both giant and dwarf, have grains in their outer layers in sufficient quantity to affect the emergent spectrum.

Radiative Transfer in Molecular Lines

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Molecular lines are generally very good tracers of the physical conditions in cold regions of the Universe (e.g. molecular clouds, cool stars, etc.), but molecular species are also found in not so cold environments (e.g. the magnetized solar atmosphere). For a reliable interpretation of spectroscopic and spectropolarimetric observations of molecular lines it is often necessary to carry out detailed radiative transfer simulations in molecular lines, both in LTE and NLTE. Here we present a multilevel radiative transfer code for the synthesis of molecular lines in stellar atmospheres, showing some illustrations of calculations in different astrophysical contexts and considering molecules like H_2O, CO and OH. We will discuss our implementation of highly convergent iterative methods and formal solvers with especial emphasis on spherical geometry. We will also present a chemical evolution code which is currently allowing us to check the approximation of instantaneous chemical equilibrium in the calculation of the abundances of a variety of molecular species.

Formal Solution: EXPLICIT Answers

Lawrence Auer

X-3, Applied Physics Division, Los Alamos National Laboratory

Evaluation of the radiation field arising from a specified set of thermodynamic and kinetic material conditions is known as the Formal Solution. The ability to find such solutions efficiently is critical to the iterative solution of the implicit coupled matter plus radiation problem. It is first shown how the exact relativistic radiation transport along a ray may be reduced to a set of easily evaluated integrals. The short characteristic approach is then used to find the formal solution of multi-dimensional radiation problems.

Insight into Multi-Dimensional Transfer

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Although computers are becoming ever more powerful, modelers must be aware of potential computational dangers. Resolution of optical boundaries and interfaces is necessary in order to predict correctly the radiation field. For regular objects this is accomplished simply by using "logarithmic gridding" on the outside edges. For irregular objects, like prominences or loops, resolution of all the interior interfaces is a nearly insurmountable problem. Monte Carlo is a powerful and robust tool for validating deterministic results. It is particularly appropriate in this era of multi-processor computing. It automatically resolves all boundaries, avoids the "ray effects" inherent in the use of distinct rays, can easily treat even fractal structures, and should become a first-look tool for the investigation of the effect of geometrical structure on the radiation field.

Spherical and Expanding Model Atmosphere Predictions for Interferometry

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Direct interferometric measurement of stellar limb-darkening, unambiguously revealed by the shape of the visibility curve a beyond the first null, is presently available for a only a few stars. The vast majority of present day stellar diameter measurements require a theoretical limb-darkening correction to recover the "true" diameter and to interpret multi-wavelength uniform disk results. Compilations of theoretical, wavelength dependent, center-to-limb intensity profiles needed for such corrections are almost exclusively derived from plane-parallel model atmospheres and are therefore generally inappropriate for modeling the atmospheres of giant and supergiant stars. In our theoretical studies of the angular sizes of both hot and cool supergiant stars with the general-purpose stellar atmosphere code `PHOENIX`, we have found significant and testable differences between spherical and plane-parallel model predictions. We show examples of these differences in our studies of 1) the interferometric diameter of the A-type supergiant α Cygni and 2) interferometric diameter ratios at wavelengths inside and adjacent to the 712 nm TiO band for normal M-type giants and supergiants.

Influence of Mass Flows on the Energy Balance and Structure of the Solar Transition Region

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We have extended our previous modeling of energy balance in the chromosphere-corona transition region to include the effects of particle and mass flows. We consider quasi-steady cases satisfying the momentum and energy balance equations throughout the transition region and low corona. We include particle diffusion as well as flows in the non-LTE equations for H, HeI, and HeII. Mass flows substantially affect the ionization and radiative losses of H and He, thereby affecting the structure and extent of the transition region. We find that the H and He line profiles are greatly affected by flows, and that line shifts are much less important than the changes in line intensity and central reversal due to the effects of flows on atmospheric structure. The profiles we compute can generally explain the range of observed high spectral and spatial resolution Lyman alpha profies from the quiet Sun. A full account of this work appears in a paper by Fontenla, Avrett, and Loeser submitted to The Astrophysical Journal.

Parallelization Strategies for ALI Radiative Transfer in Moving Media

E. Baron, P. H. Hauschildt, and D. Lowenthal

University of Oklahoma and University of Georgia

We describe the method we have used to parallelize our spherically symmetric special relativistic short characteristics general radiative transfer code PHOENIX. We describe some possible parallelization strategies and show why they would be inefficient. We discuss the multiple parallelization strategy techniques that we have adopted. We briefly discuss generalizing these strategies to full 3-D (spatial) radiation transfer codes.

NLTE modeling of lines in expanding shells of LPVs

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The dynamics of the cool, shock penetrated, expanding atmospheres of Long Period Variables (LPVs) can be studied by spectral lines of various atoms or molecules. Especially the infrared molecular line profiles of the CO molecule are excellent diagnostic tools appropriate for the overall structure of the inner, expanding circumstellar layers. Due to the high abundance of CO as well as its formation and stability at high temperatures it is dominant in the circumstellar shells of LPVs. If one focuses on the detailed shock structures in atmospheric layers close to the photosphere for example, various optical atomic lines of neutral and ionized metals (e.g. Mg I, Fe I, Fe II) are suitable diagnostic tools (see Richter & Wood 2001, A&A 369, 1027).

To model the various atomic and molecular lines of interest, a radiative transfer code (static, spherical symmetric, co-moving frame, accelerated lambda iteration) has been developed to handle the especially awkward conditions of cool LPV's atmospheres. Here we present and discuss in detail results of the infrared CO-line calculations and give a brief outlook on work in progress for optical metal line calculations.

Simulation of hot methane spectra

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Methane is known to play a crucial role for the structure and spectrum of the coolest stars – T-type dwarfs and carbon-type dwarfs – as well as in hot-Jupiter exoplanets, brown dwarfs, and the proto-solar nebula.

Laboratory data represent well the room temperature monochromatic absorption coefficient of methane, while even the most extensive laboratory data only account for less than 1% of the complete methane absorption coefficient at 3000 K.

We present here the first line-by-line computation of the absorption coefficient of methane aimed at describing the high temperature opacities of the gas-phase. Our preliminary data include 5 million lines with an accuracy in the line position of 1 cm^{-1} for all vibrations and rotational values up to J=65, and with an accuracy of approximately 10% in the intensity. The preliminary data have a fair degree of completeness for temperatures up to 2500 K, but cover for the moment only the limited spectral region from 800 to 4000 cm^{-1}.

Density Functional Calculations for Atoms in very Strong Magnetic Fields

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In this contribution the results of density functional calculations for multi electron atoms such as helium , carbon and neon in extremely strong magnetic fields of the order of $10^9 \to 10^{13}$ Tesla , such as they exist on neutron stars, are presented. We show the results obtained for eigenergies using three different functionals. By comparing the energies for helium with those obtained using the Hartree Fock method we establish which functional is most suitable for calculating atomic data via this method. We also present preliminary results for matrix elements of dipole transition in helium and carbon. Some ideas for improving the accuracy of these calculations are also discussed.

Cool helium-rich white dwarfs: molecular opacities

I. Bues

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For helium-rich white dwarf model atmospheres with effective temperatures below 5000 K, molecular transitions of polyatomic molecules of carbon, hydrogen and even pressure-induced helium compounds become important for the opacity and thus for the pressure stratification. We investigate infrared pressure broadened features and their role in shifting the flux to the blue region of the spectrum. For $T_{eff} = 4500$ K and 4300 K, $\log g = 8$, results will be shown and compared to observed fluxes. The importance of grains in the outermost layers will be discussed.

Numerical Multi-D Radiation (Magneto-) Hydrodynamics

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The problem of 3D Radiation Magneto-Hydrodynamics is too complex to solve numerically in the general case; approximations are needed to bring the numerical complexity to tractable levels. These approximations are problem dependent. We will use the case of the Solar chromosphere to illustrate these issues. The implementation of a 1D Radiation Hydrodynamics code with a rather detailed and realistic treatment of the coupling between radiation and matter is described. Scaling properties and parallelization issues are discussed. Various strategies and on-going work for the implementation of a 3D Radiation Magneto-Hydrodynamics code are described.

Polarized radiation transfer – practical experience with the accelerated lambda iteration method

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Neutron stars and some of the white dwarfs have magnetic fields. The light emitted by these stars is polarized and can be characterized by the four Stokes components I, Q, U, and V. Therefore the polarized radiation transport equation differs significantly from the non-magnetic case. It is a system of linear differential equations coupled in I, Q, U, and V with depth dependent opacities and magneto-optical parameters. The most potential method, the accelerated lambda iteration, is presented in detail and practical experiences calculating neutron star atmospheres are reported.

Temperature Correction Schemes

Stefan Dreizler

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The pro and contra for using temperature correction are discussed on the basis of our linearization scheme and our implementation of an Unsöld-Lucy temperature correction. I will show the improvements which partly overcome the typical weakness of the UL-scheme as well as our generalization to non-LTE.

Basics Multidimensional Radiative Transfer

P. Fabiani Bendicho

THEMIS

In the last years, the improvement in the observations and the increasing spatial resolution obtained open a wide range of questions related to the diagnostic and simulation of multidimensional plasmas. This contribution focuses on the development and implementation of efficient 2D and 3D radiative transfer (RT) methods that allow Non-LTE effects in inhomogeneous astrophysical plasmas to be rigorously investigated. We discuss the optimal way to solve the multidimensional RT problem with emphasis on the numerical difficulties arising from interpolation and boundary questions. We present some 3D formal solvers that are suitable for both, unpolarized and polarized RT. Finally we show the power of current multidimensional codes with some illustrative and realistic Non-LTE multilevel calculations in 2D and 3D schematic models of stellar atmospheres.

The Ionizing Continuum from Theta 1 Ori C, the ionizing star in the Orion Nebula

Gary J. Ferland

Physics, University of Kentucky

The talk will discuss what is known about the stellar continuum produced by the central star in the Orion Nebula. Nebular spectroscopy and related analysis results in an accurate determination of the continuum between 900A and 200A. Of the stellar atmospheres available today, the Mihalas (1972) come the closest to reproducing the inferred continuum. This star could serve as a benchmark in understanding future atmosphere calculations.

Some Aspects of Modelling of Pulsating Atmospheres

Andrew B. Fokin

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Nonlinear modelling of pulsating stars have two special aspects. Firstly, a self-consistent time-dependent model must include not only the optically thin atmospheric region, but also the large sub-photospheric envelope, which generates the auto-exited oscillations. The physical conditions and spatial scales of these regions are very different, while the accuracy of calculations should be as high as possible, especially of the calculation of periodic radiative shock waves. As show numerical experiments, loss of accuracy in the description of the atmospheric dynamics can strongly affect the motions on the inner matter, and vice versa, to say nothing of the sintetic line spectrum which is one of the main goals of the atmosphere modelling. Secondly, to obtain the attractor (normally the limit cycle) we must run our hydrodynamic model from $\approx 10^2$ to $\approx 10^4$ pulsational cycles, with normally thousands of intermediate models (time steps) per cycle. It is thus clear that one should reasonably simplify the problem of the radiative hydrodynamics if we wish to see the results. In the same time the accuracy must be high enough to obtain physically plausible results. In the present talk I shall describe one of possible approaches to this problem. The talk consists of three parts: Radiative Hydrodynamics of Pulsating Models; Line Profile Modelling; Radiative Shocks in Pulsating Atmosphere.

A new method for 3D radiative transfer with adaptive grids

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We present a new method for 3D NLTE radiative transfer in moving media, including an adaptive grid, along with some test examples and first applications. The central features of our approach we briefly outline in the following.

For the solution of the radiative transfer equation, we make use of a generalized mean intensity approach. In this approach, the transfer eqation is solved directly, instead of using the moments of the transfer equation, thus avoiding the associated closure problem. In a first step, a system of equations for the transfer of each directed intensity is set up, using short characteristics. Next, the entity of systems of equations for each directed intensity is re-formulated in the form of one system of equations for the angle-integrated mean intensity. This system then is solved by a modern, fast BiCGStab iterative solver. An additional advantage of this procedure is that convergence rates barely depend on the spatial discretization.

For the solution of the rate equations we use Housholder transformations. Lines are treated by a 3D generalization of the well-known Sobolev-approximation. The two parts, solution of the transfer equation and solution of the rate equations, are iteratively coupled.

We recently have implemented an adaptive grid, which allows for recursive refinement on a cell-by-cell basis. The spatial resolution, which is always a problematic issue in 3D simulations, we can thus locally reduce or augment, depending on the problem to be solved.

Comparisons between Observed and Computed Visible and Near-UV Spectra of Vega

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By using the Synspec program with different LTE and NLTE atmospheric models of Alpha Lyrae (Vega, spectral type A0V), we obtain different emitted fluxes. Taking into account the distance from Hipparcos, it is obtained the spectrum that would be observed from Earth for each model. This spectrum is compared with UV calibrations from the IUE and UARS satellites and visible ground-based observations. Absolute fluxes from the SOLSTICE experiment onboard UARS provide an independent source to assess the quality of the available data. The main goal of this work is to better understand and solve the controversy about the missing opacity problem in the UV. This is just the first step in that direction.

2D NLTE code

Leonid Georgiev and John Hillier

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We are developing a new code capable of treating multidimensional problems. The rate equations are solved using a preconditioning technique using a local ALO. A formal solver, based on the mothod of short characteristics, is used for the continuum and the bound-bound transitions are treated using Sobolev approximation. The temperature corrections are done using a linearization of the electron termal balance equation. In this poster we present the code techniques and its performans in some test cases. The results are compared with CMFGEN.

Hydrodynamic model atmospheres for hot stars

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Recent non-LTE models for expanding atmospheres, accounting for iron group line-blanketing and clumping, show a radiative acceleration which supplies a large part of the driving force of hot star winds. Aiming at the calculation of hydrodynamically consistent atmosphere models, we developed a method for the solution of the hydrodynamic equations, taking into account the radiation pressure from the comoving-frame radiation transport. In this work we describe our approach for the solution of the hydrodynamics and present first examples of consistent wind models for hot stars.

Infrared radiative cooling / heating of the terrestrial mesosphere / lower thermosphere: Non-LTE analysis of the CRISTA limb radiance data

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The new model of radiative cooling/heating of the mesosphere and lower thermosphere (MLT) in the ro-vibrational bands of atmospheric gases (CO_2, O_3, H_2O, CO, NO, N_2O and others) accounts for vibrational and rotational non-LTE, line-overlapping, and absorption and transformation of the near-infrared solar radiation. The model utilizes ALI technique for the solution of the system of kinetic equations and the DFE radiative transfer algorithm. The contributions of various band to the total cooling/heating are analyzed. The model is applied to the calculation of the MLT cooling/heating for atmospheric data retrieved from the CRISTA limb radiance measurements. Implications for modeling of the MLT region are discussed.

A Grid of Model Atmospheres for Cool Stars

Bengt Gustafsson[1],
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An extensive grid of spherically symmetric model atmospheres of stars with

- 2500 K $\leq T_{\text{eff}} \leq$ 8000 K,
- $-1.0 \leq \log g \;\; (= \log GM/R^2) \leq 5.0$ (cgs units),
- different combinations of M and R,
- $-5 \leq [A/H] \leq 1$, and
- a number of CNO abundance combinations

is being constructed with an updated version of the MARCS program.

Special efforts are made to reach accuracy and completeness in opacity data. Opacity sampling is used with 10,000 and (for a minority of models) 90,000 wavelength points. Synthetic spectra are also provided.

We shall show how these classical models may be used to illustrate important physical properties of cool star atmospheres.

Dominating solar opacity sources in the near UV

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Rozanov et al. (2002) have determined that the influence of the solar irradiance variability on the chemical composition in the stratosphere is dominated by two narrow bands in the UV centered around 215 nm and 265 nm. We have evaluated the dominant opacity sources at these wavelengths and find it necessary to include the complex continuum absorption cross sections from the lower levels of neutral metals. We present our straightforward solution how to describe these opacities. There is the obvious need to treat the line blanketing which mainly depends on the completeness of the line list. We base our calculations on a combination of the spherically symmetric non-LTE 'Kiel-code' and the spectral synthesis by the SYNSPEC code. In order to evaluate the quality of our computations we compare our predictions with the UV spectrum observed by SUSIM.

Line-profile variations in eclipsing binaries

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The Fourier method of spectra disentangling generalized to the case of variable strength of lines (cf. Hadrava 1995, A&AS 114, 393 and 1997, A&AS 122, 581) applied to the spectra obtained during eclipses of a binary proved to be sensitive to the variations of limb-darkening across line-profiles. These variations reflect the vertical structure of the eclipsed atmosphere and, consequently, they yield, in addition to the frequency distribution of the radiative flux usually computed from the model atmospheres, another tool for the observational diagnostics of stellar atmospheres. Here we present the first examples of line-profile variations during an eclipse, which are calculated from the intensity distribution on the surface of model atmospheres (cf. Kubát 2001, A&A 366, 210). Consequences for the correct calculation of rotational broadening are also mentioned.

Basic ALI in Moving Atmospheres

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The non-LTE radiative transfer problem requieres the consistent solution of two sets of equations: the radiative transfer equations, which couple the spatial points, and the equations of the statistical equilibrium, which couple the frequencies. The ALI method allows for an iterative scheme, in which both sets of equations are solved in turn.

For moving atmospheres, the radiative transfer is preferably formulated in the comoving frame and thereby becomes a partial differential equation. "Clasical" numerical solution methods are based on differencing schemes. For better numerical stability, we prefer "short characteristics" integration methods. For angle-dependent "ray-by-ray" integration the formulation is straightforward, while for the angle-integrated "moment equations" a more sophisticated formalism based on "Riemann invariants" is being developed.

Iron line blanketing is accounted for by means of the "superlevel" concept. In contrast to static atmospheres, the frequencies can not be re-ordered in the moving case because of the frequency coupling from Doppler shifts.

One of our future aims is the coupling of elaborated radiative transfer calculations with the hydrodynamical equations in order to understand the driving of strong stellar winds, especially from Wolf-Rayet stars.

Temperature Correction Schemes

Peter Hauschildt

University of Georgia, Athens, USA

Parallelization

Peter Hauschildt

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Stellar wind signatures in sdB stars?

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SdB stars are extreme horizontal branch stars which are sufficiently hot and numerous to be the main contributors to the UV excess in early type galaxies. Most of the sdB stars are formed by close binary evolution. Their atmospheric abundance patterns are highly peculiar. Due to diffusion processes, some elements can be strongly depleted (e.g. helium) while others are enriched even with respect to solar composition. Standard diffusion theory fails to explain the observed abundances (even for the rather simple atom helium) by orders of magnitude. Mass loss has frequently been envoked to explain the observed abundances. Such attempts have met with limited success. Since no indications for stellar winds have been found mass loss rates are free parameters for the diffusion models. Recently, we have discovered anomalous Hα profiles in four out of a sample of 43 sdB stars and argue that these profiles are distorted by stellar winds.

2D Radiative Transfer in Magnetically-Confined Structures

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Magnetically confined structures in the solar atmosphere exhibit a large complexity in their shapes and physical conditions. As an example, we show the case of so-called magnetic dips in prominences which are in magnetohydrostatic equilibria. For such models we solve 2D non-LTE multilevel problem for hydrogen with PRD in Lyman resonance lines. The iterative technique used is based on the MALI approach with simple diagonal ALO and SC formal solver. To compute the hydrogen ionization balance, the preconditioned MALI equations are linearized with respect to atomic level populations and electron density and solved iteratively using the Newton-Raphson scheme. Two additional problems are addressed: (i) an adequate iteration method for cases when the column-mass scale is used in one of the two dimensions but varies along the other dimension (which has a geometrical scaling); and (ii) a possibility of using AMR (Adaptive Mesh Refinement) algorithms to account for steep 2D gradients of selected variables (temperature, density, etc.).

Spectroscopic Analysis of Cyg OB2 O supergiants using Unified Model Atmopsheres

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We present first results of an spectroscopic analysis of 7 O supergiants in Cyg OB2 using two different model atmosphere codes (Santolaya-Rey, Puls, Herrero, 1997, A&A 323, 488; and Hillier & Miller, 1998, ApJ 496, 407). The first code has been improved including an estimation of metal line blocking effects (Puls, in prep.). The second one has been improved including a photospheric density structure (Najarro et al., in prep.). The results from both codes compare well within the observational uncertainties.

The main result of these analyses is a lower temperature scale for O supergiants as compared with previous analyses using either plane-parallel, hydrostatic or spherical, mass-lossing models (see Herrero, Puls, Villamariz, A&A 2000, 354, 193). The lower temperatures are thus an effect of the additional metal line opacity and the large mass-loss rates. In some cases, the new derived effective temperature is reduced up to 10 000 K.

As a consequence, radii and luminosities are also changed, reducing the mass discrepancy and modifying the Wind Momentum- Luminosity Relationship.

On the Solution of the Rate Equations.

D. John Hillier

University of Pittsburgh

To construct non-LTE model atmospheres it is necessary to solve the radiative transfer equation at hundreds of thousands of frequencies, and to solve thousands of rate equations at each depth while simultaneously satisfying the constraint of radiative equilibrium. Ideally we would like a stable code that converges rapidly to the desired solution with minimal assumptions. Unfortunately stability and speed are often mutually exclusive.

We examine the approach taken in CMFGEN, a non-LTE code used for modeling the spectra of hot stars with stellar winds, and compare the techniques used with those used in other codes. An honest appraisal of CMFGEN's convergence properties are given, and we discuss when difficulties occur.

We examine the solution of the rate equations in detail, and highlight the coupling between the radiative equilibrium equation, and the rate equation. Procedures for ensuring stability and accelerating convergence are discussed. We also examine the tradeoff between local and non-local operators.

Atmospheres and Spectra of Magnetic Neutron Stars

Wynn C.G. Ho and Dong Lai

Cornell University

We construct atmosphere models for strongly magnetized neutron stars with surface fields $B \sim 10^{12} - 10^{15}$ G and effective temperatures $T_{\rm eff} \sim 10^6 - 10^7$ K. The atmospheres directly determine the characteristics of thermal emission from isolated neutron stars, including radio pulsars, soft gamma-ray repeaters, and anomalous X-ray pulsars. In our models, the atmosphere is composed of pure hydrogen or helium and is assumed to be fully ionized. The radiative opacities include free-free absorption and scattering by both electrons and ions computed for the two photon polarization modes in the magnetized electron-ion plasma. We describe a modified (due to the two photon modes) Unsöld-Lucy temperature correction method to establish radiative equilibrium and the resulting temperature profile. We discuss the effect of vacuum polarization, which modifies the dielectric property of the medium and gives rise to a resonance feature in the opacity; this feature is narrow and occurs at a photon energy that depends on the plasma density. Vacuum polarization can also induce resonant conversion of photon modes via a mechanism analogous to the MSW mechanism for neutrino oscillation. We discuss the subtleties in treating the vacuum polarization effects. We show that vacuum polarization produces a broad depression in the X-ray flux at high energies, which arises from the density dependence of the vacuum resonance feature and the large density gradient present in the atmosphere, and the depression of continuum flux strongly suppresses the equivalent width of the ion cyclotron line.

Parallization

P. Höflich

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Parallel computing has turned out as a enabling technology to solve complex physical systems. However, the transition from shared memory, vector computers to massively parallel, distributed memory systems and, recently, to hybrid systems poses new challenges to the scientist. We want to present a cook-book (with a very strong, personal bias) based on our experience with parallization of our code. Some of the general tools and communication libraries are discussed. Our approach includes a mixture of algorithm based, grid based and physical module based parallelization. The advantages, scalability and limitations of each are discussed at example calculations for supernovae. We hope to show that effective parallelization becomes easier with increasing complexity of the physical problem making stellar atmosphere beyond the classical assumptions very suitable.

ALI in Rapidly Expanding Envelopes

P. Höflich

Dept. of Astronomy, University of Texas at Austin

We discuss our current implementation of the ALI method into our radiation-hydro code for rapidly expanding, low density envelopes commonly found in core collapse and thermonuclear supernovae (+ novae and WR stars). Due to the low densities, non-thermal excitation by high energy photons (e.g. from radioactive decays) and the time dependence of the problem, significant departures from LTE are common throughout the envelope even at large optical depths.

ALI is instrumental for both the coupling of the statistical equations and the hydrodynamical equations with the radiation transport (RT). We employ several concepts and approximations to improve the stability, and convergence rate/ control including the concept of leading elements, the use of net rates, level locking, reconstruction of global photon redistribution functions, equivalent-2-level approach, and predictive corrector methods. For appropriate conditions, the solution of the time-dependent rate equations can be reduced to the time-independent problem plus the (analytic) solution of an ODE For the 3-D problem, we solve the radiation transport via the moment equations. To construct the Eddington tensor elements, we use a Monte Carlo scheme to determine the deviation of the solution for the RT equation from the diffusion approximation (ALI of second kind).

At the example of a subluminous, thermonuclear supernova (SN 1999by), we show an analysis of the light curves, flux and polarization spectra and discuss the limitations of our approach.

Methane Opacities in T-dwarf Atmospheres

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We present the current status of PHOENIX model atmospheres for dwarfs of spectral type T, typical for older field brown dwarfs and low-mass brown dwarfs. In comparison to warmer L dwarf atmosphers, the spectral features of these objects can largely be reproduced by treating the influence of dust in the limiting case of complete settling, i. e. neglecting the dust opacity (Cond models). One major challenge in modelling cool brown dwarf atmospheres is the correct treatment of the molecular lines of H_2O and CH_4. These are the dominant opacity sources in the IR and responsible for the very blue colours of T dwarfs in the near infrared. Reliable opacity data for these absorbers are thus mandatory for a correct determination of the temperature structure as well as for detailed modelling of the characteristic absorption features in the H and K bands, which are the defining criteria of spectral class T.

Line lists extracted from low temperature atmospheric databases such as HITRAN and GEISA are generally strongly limited to lower-state energies. To overcome these limits, a new list of line-by-line predictions for the methane opacities from the four lowest vibrational states has been computed with the Spherical Top Database System (STDS). Improvements of these line lists have been achieved thanks to recent successes in the experimental calibration of the molecular parameter describing the vibrational and rotational bands in the spherical top model. This allowed extrapolations to higher rotational states than previously possible. As a result our opacity sampling models now allow a much more complete reproduction of the strong features occuring in the temperature regimes of brown dwarf atmospheres. A more diffuse background opacity remains due to the extremely high line density from higher vibrational states, which at this time can be described only partly by statistical models.

Basic ALI in Plane-parallel Atmospheres and Formal Solvers

Ivan Hubeny

NOAO, Tucson, USA

Model Photospheres with ALI

Ivan Hubeny

NOAO, Tucson, USA

AUTOMATED SPECTRAL ANALYSIS

C.S.Jeffery

Armagh Observatory

At Armagh Observatory we continue to make incremental improvements to our core model atmosphere and synthetic spectrum software, STERNE and SPECTRUM. These are employed in the analysis of low-, intermediate and high-dispersion dispersion multi-wavelength data for extreme helium stars and subdwarf B stars, including binaries. In order to make these analyses more objective, we tested a variety of χ^2-minimization procedures. These operate both with precomputed model grids and by recomputing synthetic spectra as required. As a consequence we have been able to analyse large datasets efficiently. Key results have led to the detection of secular contraction and the direct measurement of masses in extreme helium stars. This has been pivotal in identifying extreme helium stars as the product of mergers between CO and He white dwarfs. A time-resolved analysis of the short-period pulsator V652 Her involved the automatic measurement of effective temperatures and surface gravities from over 50 high-dispersion optical spectra. Semi-automatic techniques are even more important for the analysis of binary stars, including the discovery of a new hydrogen-deficient binary, BI Lyn. While our techniques have been developed using LTE models, it is likely that the efficiency gains could be even greater when extended to non-LTE models.

Computational Astrophysics Tools for the GRID

C.S.Jeffery

Armagh Observatory

The newest generation of telescopes and detectors and large scale astronomical databases are delivering vast volumes of astronomical data and creating increasing demands for their analysis and interpretation. Methods for such analyses rely heavily on computer-generated models of growing sophistication and realism. These pose two problems. First, simulations are carried out at increasingly high spatial and temporal resolution and physical dimension. Second, the dimensionality of parameter-search space continues to grow. Major computational problems include ensuring that parameter-space volumes to be searched are physically interesting and match observational data efficiently and without overloading the computational infrastructure.

For the analysis of highly-evolved hot stars, we have developed a toolkit for the modelling of stellar atmospheres and stellar spectra. We can automatically fit observed flux distributions and/or high-resolution spectra and solve for a wide range of atmospheric parameters for both single and binary stars. The software represents a prototype for generic toolkits that could facilitate data analysis within, for example, a Virtual Observatory.

We introduce a proposal to integrate a range of such toolkits within a heterogeneous network so as to facilitate data analysis. For example, data-mining functions will combine new observations with data from established archives. A goal-seeking algorithm will use this data to guide a sequence of theoretical calculations. These simulations may need to retrieve data from other sources, atomic data, pre-computed model atmospheres and so on. Such applications using widely distributed and heterogeneous resources will require the emerging technologies of computational grids.

Four numerical approaches to solve the radiative transfer equations in magnetized white dwarf atmospheres

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The observed spectrum and wavelength dependent polarization of magnetic white dwarfs can be analyzed by simulating the transport of polarized radiation through a magnetized stellar atmosphere.

The four coupled radiative transport equations for the Stokes parameters I, Q, V, and U, can be solved by different numerical approaches. In this talk the numerical results and efficiencies of four different methods are discussed: (a) the method of Wickramasinghe & Martin which assumes that the source function is linear in the optical depth and that between two successive depth points the Stokes parameters can be described by exponential functions; (b) accelerated Λ iterations (see also the talk by J. Deetjen) (c) an approximation for large Faraday rotation, and (d) the matrix exponential solutions.

Molecular opacities and cool star atmospheres

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The rapid development during recent years in observational facilities, has made it possibly to observe cool stars at wavelengths which were never before accessibly, and at fainter absolute magnitudes than ever. These improvements have further increased the demand for extensive and accurate input data of many kinds, in order to make it possible to model and understand the new observations.

Comparison between synthetic spectra and the new high-quality observations has been an extra challenge in modelling the atmospheres of cool objects. It has lead to real progress in the field, but also to new *ad hoc* speculations based on models lacking reliable input data.

I review here recent progress in obtaining the necessary molecular data for the coolest objects, which include the coolest red giants, cool white dwarfs and cool main sequence dwarfs, as well as proto-solar nebulae, brown dwarfs and hot-Jupiter giant planets.

I will, in particular, report on recent calculations of the opacities of water and methane.

Time-dependent flare models with MALI

J. Kašparová, P. Heinzel, M. Varady, M. Karlický

Astronomical Institute of Academy of Sciences of the Czech Republic, Ondřejov

Temporal variations of Hα line profile intensities related to electron beams are presented. We show first results of time dependent simulations of a chromospheric response to a 1 sec monoenergetic electron beam. 1-D hydrodynamic code together with particle representation of the beam have been used to calculate atmospheric evolution. Time dependent radiative transfer problem has been solved for the resulting atmosphere in the MALI approach, using the Crank-Nicholson implicit scheme. Non-thermal collisional rates were included in linearised equations of statistical equilibrium.

V4334 Sgr (Sakurai's Object) - problems or a test for atmosphere modeling ?

S. Kimeswenger

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The central star V4334 Sgr (Sakurai's Object) of the planetary nebula PN G010.4+04.4 underwent in 1995-1996 the rare event of a very late helium flash. It represents only one out of two such events during the era of modern astronomy (the second event was V605 Aql = Nova Aql 1919, see Koller & Kimeswenger, 2001, ApJ, 559). All the other prominent objects of that type originate from events occurring several thousands of years ago (e.g. A30, A78). Hence, only snapshots can be modeled for those objects. These born-again objects, claimed to be possible progenitors for PG1159 class stars in general, all have unusual high carbon abundances. Thus it is of special interest for stellar evolution theory and theory of convection (Herwig, 2001, ApJL, 554, L71) to model the detailed observations obtained during the last four years. Models of the expanding shell depend essentially on basic stellar parameters of the illuminating source (effective temperature, surface gravity and stellar radius). Most of them depend strongly on the assumed distance to the object. Some models may give some constraints on this parameter, but most of them depend on the assumption as input parameter (see Kimeswenger 2001, Ap&SS in press, http://arxiv.org/abs/astro-ph/0105119). V4334 Sgr allows for the first time a dynamic consideration of this type of object from the very beginning.

The object showed us its stellar atmosphere only for about one year before hiding in its shell. I present here a model which is able to describe the complete photometric behavior of the object, including the fine structure dips of the optical light curve during the first two years of the mass loss and the dust formation. Those models depend only weakly on the details of the input from stellar models. Although assuming a distance and the effective temperature and thus the luminosity is needed as start point. This links to a set of questions, concerning the stellar atmosphere models obtained for the first year of its rapid evolution (Asplund et al. 1999, A&A, 343, 507; Pavlenko et al. 2000, 354, 229).

Heating of a White Dwarf atmosphere by irradiation with cyclotron emission

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Universitäts Sternwarte Göttingen, germany

Rate Equations with ALI

Lars Koesterke

NASA Goddard Space Flight Center

One of the kernels of the widely applied Accelerated Lambda Iteration (ALI) for the construction of non-LTE model atmospheres is the solution of the rate equations, i.e. the calculation of level population numbers from a given radiation field. Due to the so-called "acceleration", which is vital for the overall convergence, this set of equations is usually non-linear. In my talk I will discuss the Newton iteration which is the prototype of all fast and reliable methods for the solution of non-linear equations, and its derivatives, namely the Broyden and the Kantorovich method. I will show that the attributes fast and reliable are aligned, which also means that slow methods are virtually of no use. This is demonstrated by means of the slow Unsöld-Lucy temperature correction scheme. I will also show how the non-linear equations can be transformed into linear equations by two techniques named preconditioning and linearization, respectively. At last I will focus on the construction of the Λ-operator, i.e. the "accelerating" term. In static atmospheres the operator can be easily derived from the solution of the radiation transfer while in moving atmospheres life is much more difficult.

DFE Method in Moving Media

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We tested, if it's possible to solve the equation of radiative transfer in moving media effectively using the discontinuous finite element method. We show here a solution of this equation written in the comoving frame for two cases- with aberration and with its omission. We compare these results with a static case and with classical Feautrier method.

Modeling of multicomponent radiatively driven stellar winds using Newton-Raphson method

Jiří Krtička

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We present a simple method for solution of onecomponent and multicomponent hydrodynamic equations based on the Newton-Raphson method. We show that this method can be used for the solution of stationary hydrodynamic equations. This method has been used for the calcuation of the low density stellar wind models for which the multicomponent nature of the wind influences the overall wind structure.

A computer code for calculation of NLTE model atmospheres using ALI

Jiří Kubát

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A code for calculation of NLTE model atmospheres in hydrostatic and radiative equilibrium in either spherically symmetric or plane parallel geometry is described. The method of accelerated lambda iteration is used for the treatment of radiative transfer. Other equations (hydrostatic equilibrium, radiative equilibrium, statistical equilibrium, optical depth) are solved using the Newton-Raphson method (linearization). In addition to the standard output of the model atmosphere (dependence of temperature, density, radius, and population numbers on column mass depth) the code enables optional additional outputs for better understanding of processes in the atmosphere. The code is able to calculate model atmospheres of plane-parallel and spherically symmetric semi-infinite atmospheres as well as models of plane parallel and spherical shells. There is also an option for solution of a restricted problem of a NLTE line formation (solution of radiative transfer and statistical equilibrium for a given model atmosphere). The overall scheme of the code is presented.

Calculation of temperature using a thermal balance of electrons

Jiří Kubát

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Instead of the standard equation of radiative equilibrium the equation of thermal balance of the electron gas is used for the determination of the temperature structure of the stellar atmosphere. The thermal balance method is extremely useful in outer parts of stellar atmospheres with optically thick lines, where sometimes the common method based on radiative equilibrium fails to converge. On the other hand, thermal balance method sometimes fails at the inner parts of the atmosphere where collisions dominate.

A Grid of NLTE Line-Blanketed Model Atmospheres

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We have constructed a grid of over 300 NLTE fully-blanketed model atmospheres covering the parameter range of O-type stars at various metallicities. We have assumed a plane-parallel geometry, hydrostatic and radiative equilibria. The models incorporate about 100,000 NLTE atomic levels of over 40 ions of H , He, C, N, O, Ne, Si, P, S, Fe, and Ni, which are grouped into about 900 superlevels. The models will be made publicly available in the coming months.

Atomic Data in NLTE Model Atmospheres

T. Lanz

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Extensive sources of atomic data are required to calculate NLTE line-blanketed model atmospheres. I will discuss their implementation in our NLTE model atmosphere code, TLUSTY, and in our spectrum synthesis code, SYNSPEC, with a particular attention to the statistical methods required to incorporate the opacity of iron-peak elements. A few typical results and comparisons to other codes will be shown.

Time-Dependent Moment Equation Solution for Supernova Light Curves

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We have developed a time-dependent solution to the moment equations to solve for the temperature structure and radiation field of objects where the temperature and structure of the object change slowly relative to the radiation field, like supernovae. We have restored the time derivative terms to the transport equation and modified our method for the formal solution and approximate lambda operator.

Wanted: Best method for solving the transfer equation in multi-D hydrodynamical model atmospheres

Hans-Günter Ludwig

Lund Observatory, Sweden

My talk is intended to stimulate discussions about methods in radiative transfer for hydrodynamical model atmospheres of late-type stars. I will present a number a number of inherent problems, show how they are presently tackled (if so), and ask for ideas for more efficient approaches. The transperancies of my talk can be found in
http://www.astro.lu.se/~hgl/public_files/tuebingen2001.ps (4.3Mb)

Line blanketing effects in atmospheres of O stars

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We have computed new models of O stars atmospheres with the non-LTE comoving frame code CMFGEN (Hillier & Miller 1998) including the effect of spherical extension due to wind. Line blanketing is taken into account thanks to a method of super-levels. The comparison with pure H-He models show that the wind ionisation and the emergent spectrum are modified when metals are included. This results in a modification of the EUV flux and in a shift of the Teff-scale towards cooler values. We study quantitatively this last effect and its dependence on model parameters (mass loss rate, metallicity, shape of the velocity field, microturbulence). The implications of the change of the effective temperature scale for the ionizing fluxes are also discussed.

Radiation Hydrodynamics in Stellar Atmospheres

Dimitri Mihalas

X-3, Applied Physics Division, Los Alamos National Laboratory

The radiation received from stars provides the diagnostic tool to infer temperatures, densities, hydrodynamic motions, and chemical compositions in their atmospheres. For most stars it appears to be an adequate first approximation to assume that there are no large-scale hydrodynamic motions. However, in the most luminous stars the intense radiation field deposits sufficient photon momentum in the outermost layers to drive them off in a supersonic hydrodynamic flow. Likewise, in exploding stars such as novae and supernovae, the dominant form of energy and momentum content and transfer may reside not in the material flow, but in the radiation field. Further, pulsating stars are driven by an internal "radiation engine" in which the variation of the opacity of the material with temperature and density acts as a thermodynamic valve. In all these objects, and adequate analysis of the physics of the atmosphere requires application of the discipline of Radiation Hydrodynamics, where one considers the dynamics of a two-component (at least!) radiating fluid. This talk will illustrate some aspects of the radiation-material interaction that produce large-scale motions in stellar atmospheres and envelopes, and make some connections between stellar and laboratory radiation-driven phenomena.

Comparison of dissociation equilibrium constants

Michelle Mizuno-Wiedner

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Testing EUV hot stars emission with nebular modelling of IR lines

Morisset, C., Bouret, J.-C., Scharere, D. and Martins, F.

As the bulk of radiation in early type stars is emitted in the Lyman continuum and thus inaccessible to direct observations (except in extremely rare cases) it is crucial to find indirect tests to constrain this part of the spectrum, where the essential atmospheric conditions are settled. Nebular observations combined with detailed photoionisation modeling can in principle provide such strongly needed constraints. Here we present the current status of available constraints on the ionising fluxes of O stars and first results from extensive photoionisation model grids using recent non-LTE line blanketed model atmospheres including stellar winds and plane parallel models for O stars (CoStar: Schaerer & de Koter 1997, WMBASIC: Pauldrach et al. 2001, CMFGEN: Hillier & Miller 1998, TLUSTY: Hubeny & Lanz 2001). The method and its dependence on nebular parameters (geometry etc.) are discussed. Our models are compared to a sample of HII regions observed with ISO providing a measure of the ionisation degree through numerous IR fine structure lines.

AcDc - A new code to calculate the vertical structure of accretion disks

T. Nagel, S. Dreizler, K. Werner

Institut für Astronomie und Astrophysik Tübingen

We present a new code to calculate the vertical structure of accretion disks in cataclysmic variables. The disk is divided into concentric rings, each ring is treated like an independent plane-parallel radiating slab. We first calculate a gray LTE model and then a NLTE model of the ring. Finally we integrate over all ring spectra to get the spectrum of the full disk for a specific inclination angle. The system of hydrostatic and radiative equilibrium, atomic level populations and particle conservation is solved consistently with the radiative transfer. This allows to calculate detailed theoretical spectra of accretion disks. Comparison with observations will allow to derive radial temperature distribution, mass accretion rate, viscosity and chemical composition. We also plan to compare our vertical structures to those of hydrodynamic simulations in order to estimate the influence of a detailed radiation transport on the stratification.

Solutions of polarized line transfer equations

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Recent developments in the NLTE polarized line formation theory in Astrophysics is discussed. Attention is focussed on pure theoretical aspects of the problem.

A conventional method of solving the line transfer equation is described briefly, in order to give a perspective to the modern Polarized Approximate Lambda Iteration (PALI) methods, which are developed only in recent years. Sample results computed using this old finite difference method for the polarized line transfer in planar and spherical media are presented. These examples include polarized resonance scattering in spherical media, polarized line formation in expanding atmospheres, and the role of collisional frequency redistribution in polarized line scattering.

Further, the basic characteristics of a PALI method are described using a prototype resonance polarization problem, keeping the assumption of CRD. Directions are given about the manner in which the presence of an external weak magnetic field can be incorporated in a PALI method. This is basically, the well known problem of Hanle effect in weak magnetic fields. The PALI method for Hanle effect is then described, first with CRD, and then with PRD scattering mechanism. Finally the generalization of PALI to the most difficult problem we have attempted until now, namely the study of partial frequency redistribution in the presence of collisions and an external weak magnetic field, is presented. Once again, sample results are shown to illustrate the essentials of PALI method, and the nature of solutions computed using this method. A comparison of the conventional and the PALI approaches is made, in some cases.

The Iron Project and NLTE stellar modeling

Sultana N. Nahar

The Ohio State University

Non-LTE models of stellar atmospheres require large amount of atomic parameters for collisional and radiative processes specific to many excited atomic levels. The collisional process is primarily electron impact excitation (EIE) of ions, while the radiative processes are: photoionization, electron-ion recombination, and bound-bound transitions. I will describe the latest developments in theoretical computations under the international collaboration the Iron Project (IP), and further extensions, following the Opacity Project (OP). The aims of these projects are to obtain accurate radiative and collisional data for EIE collision strengths, photoionization cross sections, and oscillator strengths of most astrophysically abundant ions for applications to astrophysical opacities and modeling of a variety of objects such as nebulae, AGN, and stellar plasmas.

As an extension of the OP and the IP, a self-consistent and unified theoretical treatment of photoionization and recombination has been developed. Both the radiative and the dielectronic recombination processes are considered in an unified manner, and the photoionization and recombination cross sections are computed using identical wavefunction expansions, thus ensuring self-consistency in an ab initio manner. All calculations for the various atomic parameters are carried out using the accurate and powerful R-matrix method in the close-coupling approximation. Another recent development is the inclusion of relativistic fine structure effects in Breit-Pauli approximation, especially for highly charged and for heavy ions. Atomic data for many ions have been recalculated to higher precision using larger waverfunction expansions. At the prevailing densities and temperatures in stellar atmospheres, the role of metastable states and low-lying fine structure levels in photoionization and recombination of ions bears special emphasis. I will present recent results from the Ohio State atomic-astrophysics group, highlighting the recent benchmarking of the computed photoionization and recombination cross sections with new laboratory experiments using accelerator based light sources for photoionization, and from heavy ion storage rings for electron-ion recombination.

I will also describe the efforts for an electronic web-interactive database, TIPTOPBASE, to enable the Opacity and the Iron Project data to be accessed. TIPTOPBASE will also include electron-ion recombination data and new fine structure transition probabilities. Of particular importance for stellar applications is the recent devlopment of efficient opacity codes by M.J. Seaton. Seaton's codes will enable, for the first time, on-line computations of 'customized opacities', with user-specified mixture of elements. In addition, radiative accelerations may also be obtained to compute radiative forces on elements (particularly iron) to study processes such as 'levitation' in stellar envelopes and environments.

SELF-CONSISTENT AB INITIO CALCULATIONS FOR PHOTOIONIZATION AND RECOMBINATION

Sultana N. Nahar

The Ohio State University

Most astrophysical plasmas entail a balance between ionization and recombination. We present new results from a unified method for self-consistent and ab initio calculations for the inverse processes of photoionization and (e + ion) recombination. The treatment for (e + ion) recombination subsumes the non-resonant radiative recombination and the resonant dielectronic recombination processes in a unified scheme (S.N. Nahar and A.K. Pradhan, Phys. Rev. A 49, 1816 (1994);H.L. Zhang, S.N. Nahar, and A.K. Pradhan, J.Phys.B, 32,1459 (1999)). Calculations are carried out using the R-matrix method in the close coupling approximation using an identical wavefunction expansion for both processes to ensure self-consistency.

The results for photoionization and recombination cross sections may also be compared with state-of-the-art experiments on synchrotron radiation sources for photoionization, and on heavy ion storage rings for recombination. The new experiments display heretofore unprecedented detail in terms of resonances and background cross sections and thereby calibrate the theoretical data precisely. We find a level of agreement between theory and experiment at about 10 % for not only the ground state but also the metastable states. The recent experiments therefore verify the estimated accuracy of the vast amount of photoionization data computed under the OP, IP and related works. features. Present work also reports photoionization cross sections including relativistic effects in the Breit-Pauli R-matrix (BPRM) approximation. Detailed features in the calculated cross sections exhibit the missing resonances due to fine structure.

Self-consistent datasets for photoionization and recombination have so far been computed for approximately 45 atoms and ions. These are being reported in a continuing series of publications in Astrophysical J. Supplements (e.g. references below). These data will also be available from the electronic database TIPTOPBASE (http://heasarc.gsfc.nasa.gov)

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NLTE Spectral analysis of iron group elements in the hot subluminous O-star BD+28°4211

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An analysis of UV spectra of BD+28°4211 obtained with the STIS spectrograph onboard the HST is presented. The spectral analysis is based on NLTE model calculation, which deal with the lineblanketing of iron group elements in great detail. Improved model atoms for iron group elements were set up and new interband cross sections were calculated. Comparison with observation allowed, Mn and Cr lines to be identified for the first time. The abundances of Fe, Ni, Cr and Mn are determined and point to the presence of diffusion processes in the atmosphere of BD+28°4211.

Handling of Atomic Data

Thomas Rauch

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State-of-the-art NLTE model atmosphere codes have arrived at a high level of "numerical" sophistication and are an adequate tool to analyze the available high-quality spectra from the infrared to the X-ray wavelength range. The computational capacities allow the calculation which include all elements from hydrogen up to the iron group and the lack of reliable atomic data has become a crucial problem for further progress.

We summarize briefly the available sources of atomic data and how these are implemented in the Tübingen Model Atmosphere Package (TMAP).

NLTE Modeling of Fe II and [Fe II] lines in the shocked atmospheres of M Miras

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Our observations of cool, shock penetrated, expanding atmospheres of M-type Mira stars (see Richter & Wood 2001, A&A 369, 1027) showed that in particular the emission lines of Fe II and [Fe II] are good diagnostic tools to study the physical conditions in the shocked region close to the photosphere of these stars. The erratic appearance of these particular emission lines in stars which had just had a bright light maximum suggests that they require an exceptionally bright maximum for excitation. Presumably, these are associated with stronger shock waves. According to the phase of their appearance it can be estimated, that the Fe II as well as the [Fe II] emission lines must originate close to the star at $\sim 1 - 3R_*$.

To model the Fe II and [Fe II] emission lines and to analyze the hydodynamical conditions which lead to their formation, detailed NLTE radiative transfer calculations in spherical symmetry, applying a co-moving frame formalism and using accelerated lambda iteration have been carried out on a series of specific hydrodynamical shock structures. Our basic parameter studies reveal that the lines from ionized iron originate right from the shock front and that they are in fact emitted close to the stars photosphere.

Work in progress will provide detailed line profiles to fit the observed line shapes in order to extract the full information given by the emission lines of ionized iron in M Miras. Dust formation takes place approximately in the same regions were the Fe II and [Fe II] emission lines originate. Hence a detailed study of these lines will offer the unique possibility to determine the physical conditions in the dust formation zone and thereby will shed some light on the basic mechanism of dust formation in M-type Mira stars.

Utrecht Radiative Transfer Courses

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The Utrecht course *"The Generation and Transport of Radiation"* teaches basic radiative transfer to second-year students. It is a much-expanded version of the first chapter of Rybicki & Lightman's *"Radiative Processes in Astrophysics"*. After this course, students understand why intensity is measured per steradian, have an Eddington-Barbier feel for optically thick line formation, and know that scattering upsets LTE. The text is a computer-aided translation by Ruth Peterson of my 1992 Dutch-language course. My aim is to rewrite this course in non-computer English and make it web-available at some time. In the meantime, copies of the Peterson translation are made yearly at Uppsala – ask them, not me. Eventually it should become a textbook.

The Utrecht course *"Radiative Transfer in Stellar Atmospheres"* is a 30-hour course for third-year students. It treats NLTE line formation in plane-parallel stellar atmospheres at a level intermediate between the books by Novotny and Boehm-Vitense, and Mihalas' *"Stellar Atmospheres"*. After this course, students appreciate that epsilon is small, that radiation can heat or cool, and that computers have changed the field. This course is web-available since 1995 and is regularly improved – but remains incomplete. Eventually it should become a textbook.

The three Utrecht exercise sets *"Stellar Spectra A: Basic Line Formation"*, *"Stellar Spectra B: LTE Line Formation"*, and *"Stellar Spectra C: NLTE Line Formation"* are IDL-based computer exercises for first-year, second-year, and third-year students, respectively. They treat spectral classification, Saha-Boltzmann population statistics, the curve of growth, the FAL-C solar atmosphere model, the role of H-minus in the solar continuum, LTE formation of Fraunhofer lines, inversion tactics, the Feautrier method, classical lambda iteration, and ALI computation. The first two sets are web-available since 1998; the third will follow.

Acknowledgement. Both courses owe much to previous Utrecht courses taught by the late Kees Zwaan. The third exercise set was developed by Phil Judge, Mandy Hagenaar, and Thijs Krijger.

Reverse acknowledgement. If you are a user of this free material you might refer to this summary and so boost my citation standing. Corrections are also welcome.

Compact and Handy FORTRAN Code SMART for Physics of Stellar Atmospheres

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A new computer code SMART (**S**pectra from **M**odel **A**tmospheres by **R**adiative **T**ransfer) for computing the stellar spectra, forming in plane-parallel atmospheres, has been compiled by us and A. Aret. To guarantee wide compatibility of the code with shell environment, we chose FORTRAN-77 as programming language and tried to confine ourselves to common part of its numerous versions both in WINDOWS and LINUX. SMART can be used for studies of several processes in stellar atmospheres. The current version of the programme is undergoing rapid changes due to our goal to elaborate a simple, handy and compact code.

Instead of linearisation (being a mathematical method of recurrent approximations) we propose to use the physical evolutionary changes or in other words relaxation of quantum state populations rates from LTE to NLTE has been studied using small number of NLTE states. This computational scheme is essentially simpler and more compact than the linearisation. This relaxation scheme enables using instead of the Λ-iteration procedure a physically changing emissivity (or the source function) which incorporates in itself changing Menzel coefficients for NLTE quantum state populations. However, the light scattering on free electrons is in the terms of Feynman graphs a real second-order quantum process and cannot be reduced to consequent processes of absorption and emission as in the case of radiative transfer in spectral lines.

With duly chosen input parameters the code SMART enables computing radiative acceleration to the matter of stellar atmosphere in turbulence clumps. This also enables to connect the model atmosphere in more detail with the problem of the stellar wind triggering.

Another problem, which has been incorporated into the computer code SMART, is diffusion of chemical elements and their isotopes in the atmospheres of chemically peculiar (CP) stars due to usual radiative acceleration and the essential additional acceleration generated by the light-induced drift.

As a special case, using duly chosen pixels on the stellar disk, the spectrum of rotating star can be computed. No instrumental broadening has been incorporated in the code of SMART.

To facilitate study of stellar spectra, a GUI (Graphical User Interface) with selection of labels by ions has been compiled to study the spectral lines of different elements and ions in the computed emergent flux.

An amazing feature of SMART is that its code is very short: it occupies only 4 two-sided two-column A4 sheets in landscape format. In addition, if well commented, it is quite easily readable and understandable. We have used the tactics of writing the comments on the right-side margin (columns starting from 73).

Such short code has been composed widely using the unified input physics (for example the ionisation cross-sections for bound-free transitions and the electron and ion collision rates). As current restriction to the application area of the present version of the SMART is that molecules are since ignored. Thus, it can be used only for luke and hot stellar atmospheres.

In the computer code we have tried to avoid bulky often over-optimised methods, primarily meant to spare the time of computations. For instance, we compute the continuous absorption coefficient at every wavelength. Nevertheless, during an hour by the personal computer in our disposal AMD Athlon XP 1700+, 512MB DDRAM) a stellar spectrum with spectral step resolution $\lambda/d\lambda = 3D100\ 000$ for spectral interval $700 - 30\ 000$ Å is computed.

The model input data and the line data used by us are both the ones computed and compiled by R. Kurucz. In order to follow presence and representability of quantum states and to enumerate them for NLTE studies a C^{++} code, transforming the needed data to the LATEX version, has been compiled. Thus we have composed a quantum state list for all neutrals and ions in the Kurucz file 'gfhyperall.dat'. The list enables more adequately to compose the concept of super-states, including partly correlating super-states.

We are grateful to R. Kurucz for making available by CD-ROMs and Internet his computer codes ATLAS and SYNTHE used by us as a starting point in composing of the new computer code. We are also grateful to Estonian Science Foundation for grant ESF-4701.

Model Atmospheres of Massive Post-AGB Stars

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Computation of element diffusion in non-LTE stellar atmosphere models

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The Tübingen model atmosphere program PRO2 in its standard form approximates stellar atmospheres as plane parallel, chemically homogeneous atmospheres in radiative and hydrostatic equilibrium. Together with the solution of rate equations in full non-LTE for sophisticated atomic data this makes PRO2 especially suitable for application to hot compact stars. Several extensions to this concept have recently been or are currently being implemented (see talks and posters by Werner, Nagel, Dreizler, Deetjen.) This poster presents the modifications made to correctly describe the chemically stratified atmospheres of hot white dwarfs and possibly sdB stars. In these stars, a large fraction of all heavy elements has disappeared from the outer layers due to gravitational sedimentation (Schatzman 1949). Traces of metals may however be sustained by radiative levitation provided the radiation field is intense enough to supply substantial momentum transfer. The radiative acceleration is excerted on trace elements by a non-LTE radiation field through the element's local opactity and therefore can vary strongly with depth. Balancing the radiative acceleration and the effective gravitational acceleration (including the effects of the electrical field that builds up through diffusion of electrons) yields an equilibrium condition for each atomic species (see e.g. Chayer et al. 1995). Its solutions yields equilibrium abundances, but as these also determine the opacity there exist s a intimate coupling to the radiative acceleration. Therefore the whole system has to be solved self-consistently, which is done here by iteration (Dreizler 1999). Presented below are some results of such calculations which have been sucessfully used to reproduce the observed EUV spectra of a sample of hot DA white dwarfs (Dreizler & Wolff 1999; Schuh 2000; Schuh et al. 2001a,b,c).

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Using Superlevels to Calculate Molecular NLTE

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We present the method we use in the atmosphere code PHOENIX to calculate molecular NLTE. It is based on the concept of superlevels. Superlevels consist of many similar levels added together which are assumed to be populated by a relative LTE distribution. This reduces the size of the system of rate equations to be solved tremendously. However, we modified the classical superlevel method and combined it with our dynamical opacity sampling technique which allows us to treat millions of lines. Therefore, we can calculate the transitions with maximum accuracy. We demonstrate the qualities of this method with the examples of CO and TiO.

Putting Radiation Hydrodynamics into a Detailed Model Atmosphere Calculation

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Non-grey hydrodynamics is still clearly not practicle. However, it is possible to combine a grey radiation hydrodynamics code and a non-grey model atmosphere code to obtain more realistic results. In this presentation we describe our current work in combining the atmosphere code PHOENIX and the radiation hydrodynaimcs code TITAN. We use PHOENIX to tabulate the material functions like the equation of state and the mean opacities. For example, TITAN can then calculate a shock propagating through an atmosphere for which the initial structure is provided by PHOENIX. The resulting atmospheric structures will then be fed back into PHOENIX to calculate high resolution spectra including NLTE treatment. Our goal is to apply this method to obtain high quality spectra of Mira variables as a function of phase.

Opacities for protoplanetary disks

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The increase of computer power and the growing knowledge about dust and gas species in different astrophysical environments during the last decade allows the consideration of more complicated opacity models in a variety of hydrodynamical calculations. Unfortunately, there is a lack of studies which focus on calculations of the opacity due to both dust grains and gas species for temperatures between few and few thousands K, typical of protoplanetary disks, based on the best estimates on the dust composition and recent improvements in molecular line lists.

Our aim is to introduce such a model using the unification of dust– and gas–dominated opacities. Additionally, we investigate the influence of the Rosseland mean values derived with two different opacity models on the thermal structure of an active steady-state accretion disk.

Reflection Effect in Close Binaries

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The theoretical modeling of binary systems can be performed by considering realistic models which take into account the radiative transfer, hydrodynamics, reflection effect, temperature structure etc. Since the problem is complex, we have studied some of idealized models which will help us in understanding the important physical processes in close binaries. A method has been developed for obtaining radiation field along the spherical surface irradiated by an external point source, extended source of radiation as first step to understand the reflection effect in close binary systems. The method has been extended to the case of atmospheres distorted due to self rotation of the component and tidal effects due to the presence of its companion. We have computed the effects of irradiation on the line formation in the expanding atmospheres of the components of close binary systems.

We notice that the expansion of the medium produces P Cygni type profiles and the irradiation enhances the emission in the lines although the equivalent widths reduce considerably. In the case of distorted atmospheres, the self radiation produces the absorption line and the combination of self radiation andirradiation from the secondary component produces the emission profile.

Radiation Transfer in 3D Numerical Simulations

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We simulate convection near the solar surface, where the continuum optical depth is of order unity. Hence, to determine the radiative heating and cooling in the energy conservation equation, we must solve the radiative transfer equation (instead of using the diffusion or optically thin cooling approximations). A method efficient enough to calculate the radiation for thousands of time steps is needed. We explicitly solve the Feautrier equation along a vertical and four straight, slanted, rays (at four azimuthal angles which are rotated every time step) assuming LTE and using a 4 bin opacity distribution function. We will discuss details of our approach. We also present some results showing comparison of simulated and observed line profiles in the Sun, the importance of 3D transfer, stokes profiles for intergranule magnetic fields and micropores, and the effect of radiation on p-mode asymmetries.

3D radiative transfer for young stellar objects

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The general problem of performing 3D continuum radiative transfer in dust layers and accretion disks around young stellar objects is briefly reviewed. With emphasis on the technical aspects of the solution algorithm, we present direction grid nodes equally distributed on the unit sphere, obtained by applying a Metropolis algorithm. The influence of numerical diffusion on the solution using first-order finite differencing is discussed and a solution appropriate for 3D radiative transfer is given. A generator for grids used to solve the 3D radiative transfer equation with the finite differencing method is given. The grid is adaptive and optimized to minimize the first order discretization error. We show that for the calculated grid, the optical depth throughout every grid cell is below a given threshold and allows global error control for solutions of radiative transfer problems on the grid. The proposed grid generation algorithm is easy to implement and allows pre-calculation of the grids. Moreover, the grids can be stored in integer arrays making a fast solution of the radiative transfer equation possible. We suggest to use individual grids for each frequency to use the global error control of the grid generation method. It is shown that the use of one single grid for all frequencies can lead to large discretization errors. A first comparison to Monte-Carlo code results for a simple rotational symmetric accretion disk configuration is shown.

Multi-Grid Radiation Transfer Revisited

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Multi-grid radiation transfer is an efficient method for solving a variety of radiation transfer problems, in particular problems of multiple spatial dimensions on scalar computers. This advantage is lost on massively parallel machines in which the computational grid can be directly mapped onto the processor array. Contrary to operator splitting methods, the convergence rate of the multi-grid method does not deteriorate with increasing spatial resolution of the computational grid. It is therefore well suited for high resolution problems, while performance at low resolution is not better than the best operator splitting methods.

There exists a considerable variety of basic multi-grid algorithms, which leave ample room for improvements of the few multi-grid radiation-transfer calculations that have been carried out so far. This poster is available under http://www.kis.uni-freiburg.de/~steiner/#sec6

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Optical Constants and Extinction Efficiency of Solid Materials

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The emergent spectrum of star is determined by the transfer of radiation through the matter in the outer layers of the star. Scattering and absorption of radiation by grains is very efficient. Calculation of extinction efficiency is very important application to the study of the formation and evolution of small stars and large planets, including Jupiter and Saturn in our solar system, the formation and structure of stellar winds, and the properties of the interstellar medium. Especially, when we consider about interstellar grains, extinction efficiency provides essential clues to understanding astrophysical phenomena.

We focused on the low temperature ($T_{\rm eff} \approx 2000\,K$) extinction efficiency condensed absorbers over a wide range of temperatures, we searched the literature to obtain optical constants for as many materials as possible. As a result of the search, we compute the extinction efficiency of 27 different kinds of species with 37 different data sets. Likewise, the values of the optical constnats change with how scientsists measure (parallel or perpendicular), temperature, or a particle size. We examined how different values of the optical constants affect to the extinction efficiency calculation.

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Synthetic spectra from 3D models of supernovae

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Supernova explosion modelers are generating new 3D models while polarization data indicate that some supernovae may not be spherically symmetric. In order to reconcile new models with real supernova explosions, synthetic spectra will be necessary. We outline our efforts to build a 3D radiative transfer code called Brute, built on the parameterized SYNOW direct analysis paradigm. Radiative transfer in Brute is performed by the Monte Carlo method, in particular based on the methods described by Lucy and Mazzali in various papers. The current purpose of our code is to investigate the likelihood of detecting interesting geometrical phenomena in supernovae. Future work will concentrate on enhancing the code to improve both resolution and the radiative transfer treatment.

The Non-LTE Problem of the Second Kind: the generation and transfer of polarized radiation

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The standard Non-LTE problem consists in calculating the atomic level *populations* that are consistent with the *intensity* of the radiation field generated within any given stellar atmospheric model. In contrast, the Non-LTE problem of the second kind is, indeed, like an "algebraic Annapurna": it requires to calculate the diagonal and non-diagonal elements of the *atomic density matrix* (associated to each level i of total angular momentum J_i) that are consistent with the *intensity* and *polarization* of the radiation field generated within the (generally magnetized) stellar atmospheric model under consideration. After arguing why this problem is of real astrophysical interest, I will introduce the relevant equations and the basic anisotropic radiation pumping processes. Finally, I will show how to solve efficiently Non-LTE problems of the second kind via the development and application of fast iterative methods and accurate formal solvers of the Stokes vector transfer equation.

Multi-level Accelerated Lambda Iteration with PRD

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When parts of a spectral line form (i.e., have optical depth near unity) in a region of a stellar atmosphere where radiative excitation in the line dominates over collisional excitation, effects of coherent scattering have to be taken into account. In this paper we will discuss the problem coherent scattering poses for multi-level radiative transfer solutions and how this problem can be solved efficiently. Several examples will be discussed. Among them are a comparison of radiative cooling rates due to the calcium H and K lines computed with angle-dependent and angle-averaged redistribution, and complete redistribution, and a demonstration of the importance of cross-redistribution for the formation of the oxygen resonance triplet at 130 nm.

Diffusion calculations with mass loss in hot white dwarfs and subdwarfs

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The combined effects of diffusion processes and weak winds have been investigated for hot white dwarfs on the upper cooling sequence with effective temperatures $T_{\rm eff} > 50000$K and for subdwarf B stars in the range 25000K $\leq$ $\mathrm{T_{eff}}$ $\leq$ 40000K. Within the outer stellar envelope characterized by mass depths $< 10^{-2} M_*$ for the elements H, He, C, N and O the equations of continuity and the momentum equations are solved simultaneously. So from a given initial composition the time evolution of the various abundances is predicted. Detailed opacity calculations allow to take into account the effect of the changing composition on the temperature structure. The winds are assumed to be chemically homogeneous and the mass loss rate $\dot{M}$ is considered as a free parameter.The results show that for subdwarf B stars weak winds with $10^{-14} \leq \dot{M} \leq 10^{12} M_\odot$/yr may explain the typical helium deficiencies and lead to abundance anomalies of heavy elements. In addition, according to the location of these stars in the $T_{\rm eff} - \log g$ diagram the existence of weak winds is plausible. For hot white dwarfs we expect the onset of gravitational settling when during the cooling process the mass loss rate decreases below about $10^{-11} M_\odot$/yr. For a final clarification of the chemical evolution of hot white dwarfs theoretical mass loss rates from hydrodynamical model atmospheres are required.

Analysis of B Supergiants revised: plane-parallel vs Unified models

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We compare B supergiants stellar parameters derived from analyses using plane-parallel and unified model astmospheres. Both codes are stationary, NLTE and un-blanketed, and the atomic data set is also the same for both of them. Plane-parallel model atmospheres are calculated with ALI using DETAIL/SURFACE for silicon level populations and for the emergent spectra. Unified models are calculated using the code by Santolaya-Rey, Puls and Herrero (1997).

Instabilities in radiation driven stellar winds

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Although basic properties of radiatively driven stellar winds of hot stars are successfully described with the theory of stationary wind, some observations like strong X-Ray emission, extended absorption throughs in P-Cygni profiles can not fit this theory exactly.
Including of the radiation driven instabilities seems to be necessary for the description of these effects. Focusing on Rayleigh-Taylor type instabilities, determinating of their growth rate and the influence of the Kelvin-Helmholtz instability, we summarize importance of this type instabilities on the radiatively driven stellar wind of hot stars.

Model Photospheres with Accelerated Lambda Iteration

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We review the computational procedure to construct classical line-blanketed NLTE model atmospheres with the ALI method. In detail we discuss: Approximate Lambda Operators, fast solution techniques for non-linear rate equations, pre-conditioning of rate equations, super-level approach for heavy metal line-blanketing. Most recent successes and failures in applications are shortly presented.

NLTE in a hot hydrogen star: the Auer & Mihalas 1969 papers revisited

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We pay tribute to two landmark papers published by Auer & Mihalas in 1969. They modeled hot-star NLTE-RE hydrogen-only atmospheres, using two simplified hydrogen atoms:

- ApJ 156, 157: H I levels 1, 2 and c, Lyman α the only line
- ApJ 156, 681: H I levels 1, 2, 3 and c, Balmer α the only line

and computed LTE and NLTE models with the single line turned on and off. The results were extensively analyzed in the two papers.

Any student of stellar line formation should take these beautiful papers to heart. The final exercise in Rutten's lecture notes *"Radiative Transfer in Stellar Atmospheres"* asks the student to work through five pages of questions concerning diagrams from the first paper alone! That exercise led to the present work in which we recompute the Auer-Mihalas hot-hydrogen-star models with TLUSTY, adding results from a complete hydrogen atom for comparison.

Our motivation for this Auer-Mihalas re-visitation is twofold:

- to add diagnostic diagrams to the ones published by Auer & Mihalas, in particular B_ν, J_ν, S_ν graphs to illustrate the role of the radiation field, and radiative heating & cooling graphs to illustrate the radiative energy budget,
- to see the effect of adding the rest of the hydrogen atom.

2-dimensional non-LTE Radiative Transfer in Cartesian, cylindrical and spherical coordinates

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A new Radiative Transfer code that can calculate the non-LTE line transfer problem in a two-level atom formulation in Cartesian, cylindrical and spherical coordinate systems is presented. The transfer equation is solved using the ALI and the short characteristics methods, while allowing for an arbitrary 3-dimensional velocity field.

The code is modularised so that changing geometry can be accomplished by simply setting a switch, and parallelised for use on a networked PC cluster to increase computational speed. The spatial parallelization method is employed. It is found to be robust and efficient, while not relying heavily on fast communication.

The internal accuracy of the code is tested extensively in all three geometries and is shown to be in good agreement with appropriate 1-D solutions.