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COMMENTS ON THE USE OF PANDORA

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ABSTRACT One of the most versatile NLTE radiative transfer codes available to the public is the PANDORA code created by E.H. Avrett and R. Loeser of the Harvard–Smithsonian Center for Astrophysics. A description of the advantages and disadvantages of using the code is presented here.

Keywords: Radiative transfer; NLTE; computer codes; PANDORA

INTRODUCTION

I describe the advantages and disadvantages of using the non–local thermodynamic equilibrium (NLTE) radiative transfer code PANDORA created by E.H. Avrett and R. Loeser (see their paper in this conference series). Under development since 1966, it is a very large and sophisticated computer program which contains over 3500 subroutines. PANDORA solves the coupled equations of radiative transfer and statistical equilibrium in a self consistent manner using the *equivalent two–level atom* approach. This is one of the major two techniques for solving these equations — the other being the *complete linearization* method. See sections 12–1 and 12–3 in Mihalas (1978) for further comments on these two competing techniques.

I first began to use PANDORA in 1986 while working on my dissertation research of cool carbon star chromospheres (Luttermoser *et al.* 1989). I have successfully operated PANDORA on VAX mainframes, a microVAX II, and on VAXstations. The bulk of my current calculations are now done on a VAXstation 3100. I will first present what I consider to be the major disadvantages of PANDORA, followed by advantages. Although users of other large NLTE codes may claim to have encountered no disadvantages in using these codes, I remind the reader that no computer code is perfect. One must balance disadvantages and advantages with respect to the goals of the research in question.

THE DISADVANTAGES

PANDORA checks the machine on which it is operating for various attributes as a safeguard against overloading the machine. As a result of these safeguards, PANDORA is operating system dependent. There is a VMS version and a Unix version. Since I only have experience with the VMS version, the comments here pertain to VAXes. PANDORA requires an extremely large virtual memory allocation to operate — 50,000 pages (1000 pages equals 0.512 megabytes (Mb) of virtual memory) are required for the page file quota on a PANDORA user account. It is often difficult to get a system manager to give this large of a quota on a multi–user machine. This of course can be circumvented by having your own workstation. Once PANDORA fills internal memory, it dumps data to disk during a run (over and above the virtual memory page swapping) to a temporary file. For example, on a VAXstation 3100 with 12 Mb of RAM, a run utilizing the background Kurucz bound–bound opacities requires 106,000 blocks of free disk space (note that 1000 blocks equals 0.512 Mb of disk space). A 5–level hydrogen model atom in spherical geometry, including a macroscopic velocity field and Lyman–α in partial redistribution requires approximately 200,000 free blocks!

The equivalent two–level approach to the solution of the transfer equation can be slow, particularly in a cool, low density medium (*i.e.,* M–type and N–type giant star atmospheric models). It is fairly quick in warmer (K type and earlier) giant models and in main sequence models. The main difficulty in the cooler, low density models results from the net radiative rate ($A_{ji}\rho_{ji}$) of a transition being negative and much greater than the collisional and other rates (Z_{ji}) associated with the transition. This can lead to negative departure coefficients and source functions, which can lead to inconsistencies in the solution (see Avrett and Loeser (1987) for a detailed description of this problem).

To operate PANDORA in its most basic form requires about a two week learning period. PANDORA can generate a tremendous amount of output regarding information of the run. Fortunately this output is well commented, so only a few extra months are usually required to fully understand it. Although PANDORA has a user's manual describing the various input parameters and switches, there is no manual that describes the physics. One must consult the various published papers by Dr. Avrett to understand the physics and mathematical techniques used in the code (see Avrett and Loeser in this workshop proceedings for a list).

THE ADVANTAGES

Perhaps the main advantage of PANDORA is the tremendous amount of physics it contains. One can perform calculations in either plane–parallel or spherical geometries; include macroscopic velocity fields in the rate, source function, and line profile calculations; assume a semi–infinite atmosphere or finite slab model; and irradiate the atmosphere with an external radiation field. Many types of opacities are included in the code, from bound–free transitions of 11 different species to various free-free opacities and scattering events, to name just a few. Atomic models are read in as external data files, so one can construct any type of arbitrary atomic model or modify older atomic models as updated cross–sections are published.

PANDORA contains many self–correcting mechanisms to overcome difficulties in convergence. Self–consistency checks are made for each iteration to confirm whether a solution is converged. The ability exists to print out as much information on a run as one may require for detailed analyses. This leads to tremendous insight on the physical mechanisms involved in the radiative transfer. Apart from the long output file, one can generate additional output files which contain a variety of information from net radiative cooling rates to the emergent spectrum. Such output files are handy when using PANDORA calculations in supplementary research. For instance, I am currently calculating NLTE net radiative cooling rates from PANDORA in a *snapshot* approximation of the Bowen (1988) hydrodynamic models of Mira–type variables. These cooling rates are then mapped back into the Bowen code to refine the models. At the same, the synthetic spectra generated by PANDORA can be compared to observations (see Luttermoser and Bowen in this conference series). In essence, the main disadvantages of the code results directly from its enormous size, which also gives rise to the primary advantage of the code.

CONCLUSION

I have outlined the advantages and disadvantages of using the NLTE radiative transfer code PANDORA. The majority of both the advantages and disadvantages arise from the large size of the code. Although the equivalent two–level approach is often criticized, it is very useful in gaining physical insight on the mechanisms controlling the excitation, ionization, and line broadening in a stellar atmosphere.

As an example, Luttermoser and Johnson (1992) have used PANDORA to investigate the ionization and excitation in late–type giant star atmospheres. Some of the interesting discoveries of this paper include: (1) The assumption of detailed balance, especially in the Lyman lines, can lead to severe over/under–excitations and ionizations in the chromospheric/photospheric regions of these models. (2) Carbon abundance plays a distinct role in the ionization and excitation of hydrogen through the carbon bound–free opacity under the Lyman lines. (3) *Backflowing* chromospheric (or shock) radiation has a major influence on the excitation and ionization of hydrogen and the neutral metals at photospheric depths. Without the detailed printout and the equivalent two–level atom approach of PANDORA, it would have been virtually impossible to extract all the complications in the transfer of radiation in these models.

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