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Summary/Prognosis of the Workshop

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Abstract. In this talk I will try to: (1) summarize the progress in hardware, software, algorithm, and databases that have made the advances of the last 35 years in stellar atmospheric modeling possible; (2) comment on some of the important papers presented in this meeting; and (3) offer opinions about where fruitful paths for future investigations may lie.

1. Introduction

This has been an exceptionally good workshop. I can remember only two conferences that approach the level of quality of this one: a) the Second Harvard-Smithsonian on Stellar Atmospheres (Gingerich & Whitney 1965) where the first approaches toward computing NLTE line formation were discussed, and b) the radiation hydrodynamics conference held at Systems, Science, & Software, Inc. in 1969, where I learned about Burt Freeman's clever idea of variable Eddington factors (Freeman, et al. 1968) as applied to Laboratory systems.

I am supposed to provide this afternoon's entertainment by giving a summary of the meeting. But I offer two caveats. First, I wrote my last paper on stellar atmospheres about 20 years ago. So I am a fossil, left over from an earlier era. Indeed, my motive in coming to this conference is to *learn from you* about the incredible progress made in this field in the past 20 years. Second, I warn you that it is tempting for an elderly scientist talking about a favorite subject, to reminisce. And those of you who know me can attest that I can resist *anything*, . . . except temptation. So I shall yield to it; I will also give a shamelessly personal view of the history, as I knew it.

I went to graduate school at Caltech in 1959 thinking I might work on stellar interiors and stellar evolution. Two things made me change my mind: (1) I realized that modeling stellar interiors yields only two numbers connected to the real world: a star's "radius" and luminosity. Even then the theoretician's numbers must be converted to *observable* quantities using models of stellar atmospheres. In contrast, the *spectrum* of a star contains a wealth of data about its physical structure and composition, just *pleading* for interpretation. (2) Hoyle was visiting at Caltech in 1960/61. In his lectures, he gave us discouraging blow-by-blow accounts of his fruitless efforts to compute the structure of highly evolved stars by the old method of fitting core and envelope models. It was a complicated process, and it wasn't working. I decided it was hopeless. Ironically, I heard about Henyey's new, two-point boundary-value method for making stellar models at the Berkeley IAU meeting the following summer; it was an adaptation to

astrophysics of methodology from nuclear weapons codes, about which Henyey learned at Lawrence Livermore Laboratory. But the die was already cast for me; I had decided to work on stellar atmospheres.

I started my thesis work on O-star atmospheres in the autumn of 1961. Caltech was then a hotbed of work on both stellar atmospheres, and the significance of the results to broader astrophysical questions. Greenstein's spectroscopic stellar abundance project was in full swing, and the data were of relevance to work on stellar nucleosynthesis by Fowler, Hoyle, and Goett and Margaret Burbidge. We had a constant stream of visitors; luminaries like Unsöld and Payne-Gaposchkin, and brilliant newcomers like Roger and Guisa Cayrel, Sargent, Searle, and Wallerstein. Oke was leading the field of photoelectric spectrophotometry, and had completed a two-channel photoelectric scanner for line-profile work at the 100" coude. At Mount Wilson, Deutsch was working on peculiar A-stars, Merrill on the spectra of evolved giants, and Kraft on the spectra of Cepheids. Also, Christy had begun his monumental computational work on RR Lyr pulsations, using techniques he had mastered at Los Alamos during the Manhattan Project.

2. Computational Tools

Ours is a *computational science*. The equations are nonlinear, with subtle coupling on *multiple scales* which can differ by orders of magnitude. As a result, the radiation field at any one frequency and depth in the medium can depend on the field at *all other* frequencies at *all other* depths. This complicated interlocking results from *scattering*, which allows radiation at some depth and frequency to propagate not only one mean-free-path, for a huge number of mean-free-paths until the scattered photons are finally destroyed in a collisional process while interacting with the material, and their energy is *thermalized*. The earliest work on these problems was analytical, and yielded important insights for highly simplified problems. We began to appreciate the difficulties even better when we began to try to solve the equations computationally.

My first experience with computers was at UCLA in 1957. They had a primitive machine, called SWAC (an acronym for: "National Bureau of Standards Western Automatic Computer"). It was a vacuum tube machine similar to the one made by von Neumann at the Institute for Advanced Study. It occupied an entire old bungalow. It had 64 (!) random-access memory cells (vidicons, each recording 64 bits), a three-address command system, an input/output device (a surplus teletype), and a "rapidly rotating" magnetic drum (with dreadfully long latency and transmission times) for mass storage. Coding it in machine language (overwriting already-used code with data, or vice versa, to minimize accesses to the drum) was torture. By dogged persistence, the applied mathematicians had been able to develop some useful linear algebra routines. It was not unusual to find a large sign posted on the entry, saying "Do not slam door between 2 pm and 4 pm. Large matrix inversion in progress". The machine was slow, and the wiring so fragile that even a mild bump could introduce random bits throughout the memory. The machines of today are to SWAC as an F-16 is to the fragile kite the Wright brothers flew at Kitty Hawk. How did this come about? There are three important elements in the change: hardware, software, and networks.

2.1. Hardware

First, there is hardware. The first commercial machine I worked with, an IBM 704 at Space Technology Laboratories, had a speed of ~ 8 kiloFLOPS, and a memory of 8 - 32 kilowords, each 36 bits long (about 8 - 9 significant figures). These numbers are pathetic by today's standards. When I arrived at Caltech in 1959, we had a Burroughs 220. It had paper-tape input (making corrections was a minor horror), an electrostatic printer that always smudged the output, and required machine-language coding. It was a step backward from the IBM 704. But, in the autumn of 1961, Caltech got access to an IBM 7090 at JPL. We regarded the 7090 as a giant leap forward. Input was from easy-to-correct punched cards. For a big code one had to transport several boxes of 2000 cards apiece to the computer, some miles away (there were *no* networks) by automobile. I used to joke that "computing builds weak minds, but sound bodies". The 7090 was faster than the 704, but I don't remember the numbers; its main advantage was that it was transistorized, hence more reliable. Its mean time to failure was days to weeks; the 704 and its big brother the 709 crashed daily. At the time I thought the 7090 was a wonderful machine; but before I finished my thesis I made a trip to the Scripps Oceanographic Institute in La Jolla, and was surprised by a poster comparing the 7090 to the Control Data Corporation 3600, designed by a young engineer named Seymour Cray. It was faster than the 7090, had a larger memory, and had 60 bit words, hence much better precision. It also had independent peripheral processors to handle I/O. That one man would be the driving force in the industry until his premature death (by auto accident) a few years ago.

Cray's next triumph, the CDC 6600, had multiple add/multiply/logic registers that could operate in parallel, and incorporated his "stunt-box", in which he flagged, in a 10 by 10 matrix, those operations contingent on others, having to wait until the first operation was completed, and those which could simply go ahead, so the results would be ready when finally needed. The 6600 was a very fast machine for its day, and was the workhorse of NCAR for a number of years; NCAR's contribution to its success was to develop smart compilers and highly optimized systems that pushed the hardware to its absolute capacity.

Cray's next step was the CDC 7600, which was pipelined, so that if any register (operating in parallel with others) could be fed a string of data, one would obtain, after a latency, one result per clock cycle at the pipe's output. This machine had the best *balanced* input/output structure of any on which I worked. There was a 65 kiloword fast "small core memory" (SCM), 512 kilowords of slower "large core memory" (LCM), and a huge (much slower) disk farm. Huge block transfers back and forth between SCM and LCM took only a few memory cycles. And transfers between LCM and the disk were double-buffered: a read operation could be started, computations in the SCM continued, and check at a later time to see if it was done; the same for write operations. The parameters of these three memory stages were well matched. Auer and I were able to do some early 2D transport calculations needing about 4 Mwords (in 64 by 64 matrices) on this machine with 100% overlap of the I/O by computations.

And then one day Cray blew us away with his CRAY-1A, a machine with a 200 nanosecond cycle, a megaword (later 4) of fast 64 bit memory, and parallel *vector registers* in which 64 results could be obtained simultaneously. Compu-

tationally, it left the CDC 7600 in its dust. On the other hand, woe to the user who ran out of memory, because once the RAM was used, one had to access the disks, which were slow. Then came the X-MP and Y-MP which had multiple vector processors and, like the 7600, a large additional memory called the SSD (solid state disk) which was mated to the main memory like the LCM had been to the SCM. Then finally the CRAY-2, which had a huge main memory but about the same speed. That's all I remember because by that time I was working mainly on radiation hydrodynamics, and a host of massively-parallel machines, which I do not know how to use properly, came on the market.

An equally important development was the workstation. Today we have workstations with a GB of RAM (the CRAY-1A had only 8 MB!), GHz clock speeds, multiple GB of disk memory, and compilers that support virtual-memory codes, thus managing data- and code-paging automatically. Today for less than \$2000, one can have a machine that vastly exceeds the capacity of a national center like NCAR when the CRAY-1A arrived.

2.2. Software

Equally important, in the mid-1950s a gentleman named John Backus, with a small team at IBM, had developed the first *compiler*, known as FORTRAN I (for FORMula TRANslation) in time for the release of the IBM 704. This result of a small effort *revolutionized* the field. Suddenly it became possible to write code in a form that looked like ordinary mathematical expressions, and let the computer itself translate that language into its own internal machine codes. It speeded up the generation and debugging of a code by orders of magnitude. It was a true breakthrough because it allowed human *creativity* (limited for all of us by an inevitability: death) to be realized in vastly increased *productivity*. FORTRAN has gone through many generations since: e. g. FORTRAN IV, WATFOR, FORTRAN 77, and FORTRAN 90. Many other compiler languages are now available, and one can choose whichever works best for him/her, and the problem at hand.

One notices that I have spoken above mainly about machines built by Mr. Cray. Of course, IBM had not gone out of business. But it *failed* in software. The successor to IBM's 7090/7094 was its System 360/370. Its operating system had been made by several independent groups. It was meant to do everything for everyone; consequently it did nothing well, and was a nightmare to use. It worked, but the human effort required to figure out how to do even the most elementary operations in this unnecessarily complicated system was daunting. In my way of thinking it was like the legendary horse designed by committee, which turned out to be the camel. For me, IBM was totally out of the picture after CDCs and CRAYs became available.

As the industry became more commercialized, its largest profits came from low-end machines having huge numbers of customers. The large scientific/engineering establishments (NCAR, DOE, Boeing, ...) no longer could call the tune. Rather, we have had to accept machines the vendors can make from off-the-shelf components. Today our machines are made of thousands of independent, relatively fast, smaller, processors operating in parallel. The industry paradigm gives each processor its own memory. This *distributed memory* approach causes difficult programming when the physics of the calculation requires essentially all of the memory of all of the processors. Then huge amounts of communication

must occur, and the latency and bandwidth of the internal network becomes critical. For now, their effective programming resides in hands of experts; what is needed are compilers or operating systems that can *automatically* select the most effective communication strategies to eliminate this burden from programmers. A countercurrent in the industry is NEC's Earth Simulator which has 638 nodes, each with 8 *vector* processors (vector length unknown to me) capable of 8 GFLOPS. The total of 5104 processors achieve 35.6-teraFLOPS, and have a total main memory of 10 teraBytes. The data transfer speed is 12 GBytes per second. Time will tell which path the industry follows.

The preferred system software on these machines is now some variant of UNIX, originally developed initially at Bell Laboratories, but now being supplanted by LINUX, which is free.

2.3. Networks

Finally, I must comment on *networks*. The work Auer and I did through the middle 1970's was done without their benefit. For the first conclusive trial of our complete linearization (CL) code for a six-level, three-line ($H\alpha$, $H\beta$, and $P\alpha$), atom on the Goddard IBM 370/95 in New York, we got *one* turnaround per day because we could run only at night. We had to commute daily to New York from New Haven, Connecticut by train. It took a week to find out that the code worked! Later, when I incorporated variable Eddington factors into the code, I had to drive 150 km each way through the dark, frozen, Wisconsin night to get to a machine at Argonne National Lab. I was lucky to get three runs per night. These trips were boring, exhausting, and dangerous. What an *utter waste* of human time and energy! Today, one can sit in one's own office and be connected interactively with a remote computer at the speed of light! The bottom line of the long story above is that computational hardware and software has developed at a breathless rate, and the tools available to us today are to those of 40 years ago, as a surgeon's scalpel is to a meat cleaver.

3. Algorithm and Physical Insight

The other part of the story is *algorithm*. In 1963, Avrett and Krook published their clever temperature correction algorithm, which made possible computation of non-grey LTE model atmospheres in radiative equilibrium (RE). Accurate theories of Hydrogen- and Helium-line (both neutral and ionized) broadening were being published by Griem and his collaborators. Thus, one had the hardware, the software, and the basic physical theories to attempt a large scale computation of stellar atmospheres. Both Strom & Avrett (1965) and I (Mihalas 1965) did that for large grids of continuum-only LTE models. Scattering by electrons in hot stars was handled by lambda iteration; in retrospect, it is likely that for the hottest models the iteration did not converge, but merely stabilized. This problem was overcome by Feautrier (1964, 1967, 1968) with his extremely powerful difference-equation method for solving the second-order differential-equation form of the transfer equation. With it, one can obtain correct solutions even when the thermal part of the source function is extremely small (the limit set only by the machine-word length) compared to the scattering part; it then became possible to make some models allowing for NLTE in continua only, as-

suming the lines were in detailed balance. Such models give qualitatively the correct indication of the direction of departures from LTE in the deeper layers of an atmosphere, because the continua are the most transparent, hence photons respond to the presence of the boundary first at those frequencies.

Starting about 1967, Auer and I tackled the problem of making NLTE models with lines. After some (insufficient) preliminaries (Auer & Mihalas 1968, 1969a, 1969b) we developed the successful CL method (Auer & Mihalas 1969c). We based it on the Feautrier method because differential operators are local, and therefore easily linearized. Shortly after, we put in variable Eddington factors [a special case of the angle- and frequency-integral perturbation methods later developed by Cannon (Cannon 1973a, 1973b)] so we could work with only the moment equations (Auer & Mihalas 1970b). The algorithm was robust and strongly convergent, given reasonable starting models. We were finally able to make multilevel, multiline, NLTE models for O and B stars (Auer & Mihalas 1970a, 1972; Mihalas & Auer 1970) including multiple line transitions of H, He I, and He II. The major fact emerging from this work is that NLTE effects *dominate* the strengths of these spectra in O-stars, and earlier LTE calculations had given seriously erroneous results for T_{eff} , $\log g$, and abundances.

Using these (static) models (Mihalas 1972b, 1972c), we studied the spectra of several light elements: Mg II (Mihalas 1972a); Ca II (Mihalas 1973); N III (Mihalas, Hummer, & Conti 1972; Mihalas & Hummer 1973); a more detailed model of the singlet/triplet lines of He I in B-stars (Auer & Mihalas 1973a); and Ne I in B-stars (Auer & Mihalas 1973b). For Mg II, I found that the LTE work gave an abundance a factor of 10 too large in O-stars. For N III we identified the mechanism that tends to produce emission in $\lambda\lambda 4630\text{--}4634\text{\AA}$, while leaving the $\lambda 4097\text{\AA}$ lines in absorption. Our work is obsolete because stellar winds were not taken into account, hence we could not reproduce the intense emission features in O stars, modeled successfully today by wind models. In the case of He I, we showed that NLTE effects show mainly in the yellow-red lines; we got good agreement with observed equivalent widths of $\lambda 6678$, but our $\lambda 5876$ line strengths are too small, probably because mass motions in the atmosphere were ignored. For Ne I we found that LTE abundances from the strong red lines were spuriously high by a factor of 10, whereas the NLTE results were in agreement with nebular and solar values. It was a great effort to assemble oscillator-strength, photoionization cross-section, and collision-rate data for this calculation; some of it was from mere scaling rules (also known as "a guess"). Someone should certainly do the analysis over again today using OP, OPAL, and Iron Project data (and equivalent widths from modern spectrographs!).

Ultimately I realized that given only the computational techniques we knew, we had reached a dead end. To progress further, we would need to have *line-blanketed* NLTE model atmospheres to get the right UV photoionization rates. Using LTE line-blanketed models would not work because that would force false thermalization in those regions of the spectrum. In short, someone, someday, would have to make blanketed models, allowing for NLTE effects in thousands to millions of lines for many ionic species! And a direct solution of huge numbers of transfer equations using the CL method in its original form (Auer & Mihalas 1969; Auer & Heasley 1976) would be unthinkably expensive. Furthermore, with

the atomic databases available at the time, the data needed for transition rates were simply not there: *We were stymied.*

So I turned to idealized problems of NLTE line formation in extended and expanding atmospheres with Hummer and Kunasz. And what I learned during my first visit to Los Alamos in 1981 led me to change fields, and to begin to study the *dynamics* of radiation interacting with matter in extreme environments. In that connection, let me say that in forty years of teaching, I have told every class of students that "One of the more progressive forces in astrophysics is called *the funeral*. It is when *Old Man* releases his death grip on a field, and new blood comes pouring in with the energy and inventiveness of youth, that there is suddenly rapid, often unimaginable, new progress." Happily, I did not have to test my dictum to its ultimate conclusion to verify its truth. I got out of the way before I got old, and others made the progress.

The impasse just described was broken by two key ideas. The first was Rybicki's (1971) realization that in line formation, core-photons are essentially passive, remaining nearly in detailed balance, whereas photons scattered into the wing can escape freely through the surface. Accounting for core-saturation and wing-diffusion leads to fast approximate methods for solving NLTE line transfer problems. Scharmer (1981), using Rybicki's insights, and extending Cannon's (1973a, 1973b) ideas, developed approximate lambda operators from a rough one-point depth-quadrature. In later papers (Scharmer 1984; Scharmer & Carlsson 1985) the nearly upper-triangular form of the resulting lambda-matrix was exploited, and the process iterated (ALI) to get the *exact* solution. This approach also works well for velocity fields in the medium, and can be generalized to multilevel problems. The breakthrough came when Olson, Auer, & Buchler (1986) showed that if one uses only the *diagonal* of an approximate lambda-matrix, which is trivial to invert, the eigenvalues of the iteration are bounded away from unity, hence it is convergent. This method is easily generalized to multiple dimensions. They further showed that even faster convergence is obtained with standard acceleration schemes (see Ng 1974; Auer 1987, 1991; Klein et al. 1989). Olson & Kunasz (1988) showed how one can write an approximate lambda-matrix by using a short-characteristic method to evaluate its elements, and examined tridiagonal and pentadiagonal representations, which have even smaller eigenvalues, hence faster convergence rates. At that point ALI became the preferred method of solving transfer equations.

The second key idea was Anderson's concept (1985a, 1985b, 1987, 1989, 1990, 1991) of grouping the huge numbers of levels of multielectron atoms into *superlevels*, and representing the transition array between two superlevels as a *superline*. All the levels of a given superlevel have about the same energy relative to the ground state, so that they will be strongly coupled collisionally, and will respond to the same photoionizing radiation, hence can be assumed to have about the same NLTE departure coefficient, and to be distributed in LTE relative to one another. They are also taken to have the same parity, which accounts for dipole transitions between superlevels. With this technique, it is possible to reduce thousands or millions of atomic/molecular energy levels to a much smaller number, and the entire transition array to a few superlines.

These two key ideas in algorithm led to *enormous* increases in the speed of modeling; indeed, they are far more significant than the increases in com-

puter speed. It is now possible to make NLTE models with nonequilibrium line-blanketing by millions of lines from many chemical elements. The barrier of the middle 1970's has been completely demolished!

4. Where we are today

Now I shall try to what I was assigned to do: comment on papers presented at the Workshop. But facing more than 80 papers, I can offer only brief remarks, and only on some of them. I simply urge you *to read them!* And I apologize to any author(s) who feel I have slighted their work; *mea culpa*.

4.1. ALI in static atmospheres

Hubeny's paper giving an overview of Accelerated Lambda Iteration is a pellucid, pedagogical classic, and should be studied carefully by all people who want to understand ALI and how to use it. His §3 tells what ALI is, and how it differs from ordinary lambda-iteration, and §4 gives an excellent discussion of how approximate Λ^* operators are constructed, and what the trade-offs are in selecting one; §5 gives a concise discussion of formal solvers, whose speed are critical in determining the speed of the whole solution. The efficacy of the method in various forms (diagonal or tridiagonal Λ^* , with, or without, acceleration) is shown in figure 1. One sees that even a simple diagonal operator with acceleration is *many* orders of magnitude faster than simple lambda-iteration.

The two papers on "Model photospheres with ALI" by Werner and his colleagues (W) and by Hubeny & Lanz (HL) are identical in name only. They nicely complement each other, fitting together like two pieces of a puzzle; both are classics that *must* be read by anyone who wants to make model atmospheres. HL lay out the basic equations in §2, but (W) give more details about the constraint equations. HL then give a quick outline of the CL method, and its inability to accommodate the frequency-behavior of realistic opacities in their §3. The "main course" of this paper is served in §4. Thus in §4.1 HL put down all the possible ways of improving the speed of raw CL: 1) reducing the number of frequencies, atomic levels, constraints, depth-points, iterations, or 2) finding cheap ways of solving the system without inverting its Jacobian, or 3) using only an approximate iteration method, or 4) simply avoiding linearization at all, if possible. Their discussion of all these possibilities is exhaustive. Of all of them, the one I think is the best is the *hybrid* CL/ALI technique invented by Hubeny & Lanz (1995), which combines the best features of both methods into a single powerful, robust, and efficient code. The basic idea is to linearize all the structural (radiative-, hydrostatic-, and statistical-equilibrium) equations, which contain changes in the mean intensity at each frequency, δJ_ν . Then δJ_ν is eliminated by using the linearized approximate Λ^* -operator in terms of perturbations of the local source function and optical-depth scale, which contain only changes in temperature and level-populations. The discussion of this process by W is especially helpful for the novice, because they describe linearization in the context of ALI, and various approximate methods for solving the resulting equations, in more detail. The consequence is that the size of the grand matrix system to be solved is set mainly by NL , the number of atomic/ionic levels, instead of $NL + NJ$, where NJ is the number of frequencies in the spectrum;

this is a huge advantage because $NJ \gg NL$. One knows that this can be done because one can compute the radiation field if given all level-populations; and the level-populations if given the radiation field. Using both sets of variables is *redundant*. As discussed in HL, in the facile TLUSTY code, one has the option of using anything from pure CL to pure ALI, or any combination between. Adding the concepts of superlevels and superlines (discussed in both papers) to this approach, one is in a position to account for NLTE opacities from thousands to millions of lines, arising from thousands of atomic/ionic levels, with a rigorous, strongly-convergent technique. The summary §7 in W gives a concise history of the development of the basic ideas over the past 30 years.

ALI has become the preferred method of making stellar atmospheres; it also has been generalized beyond its original concept. Thus, Uitenbroek applies ALI to problems with partial redistribution of line photons, and reports the convergence properties comparable to complete-redistribution problems. The method can be extended to multi-dimensional geometry. He displays interesting results for multilevel Ca II and O I resonance-line computations, allowing for interlocking to subordinate levels, and velocity fields. A pointed comparison of ALI with the "standard" lambda-iteration method normally used in planetary atmosphere work is given in the paper by Gusev & Kutepov, who analyze the spectrum of CO₂ in the atmospheres of Mars and Earth. Their figures 1 and 2 show conclusively the greatly superior convergence rates of ALI.

4.2. Moving envelopes

As in static envelopes, ALI plays a major role in computing NLTE spectra from moving envelopes. Again we have two excellent major papers, one by Hamann (WRH) and the other by Höflich (PH).

The work described by WRH is directed mainly toward stars with strong winds, particularly Wolf-Rayet stars. In his code, radiative transfer is done in the comoving frame (because this is the easiest frame to handle line transitions), using moment equations in which the Eddington factors are computed by angle-dependent short-characteristics integrations. These integrations are done using ODEs along the analogs of the Riemann invariants of the hyperbolic system. The moment equations are solved using difference equations. Hamann remarked in the conference that in regions of the flow with steep velocity gradients it is necessary to have enough depth-points to *resolve* the flow so that one does not simply jump totally out of a line in a single cell's integration. This should not be a limiting factor because the calculation is linear in the number of depth-points. (I have always told students that "There is no free lunch at the table of physics! Aside from rare brilliant conceptual breakthroughs, one never gets more out than one pays for.") His code uses diagonal approximate lambda-operators, and allows approximately for clumping of the material (non-unit filling factors). Complex atoms are treated by the superlevel/superline technique, and radiative equilibrium is enforced using the improved Unsöld-Lucy procedure. In clumpy moving media, however, it is not clear that radiative equilibrium is appropriate. Emergent spectra are calculated in the observer's frame, and the results compare very well with observations for the WC5 star WR 111.

The work by PH is directed toward more energetic objects: core-collapse and thermonuclear supernovae, novae, and W-R stars. It is a parallelized code

with physics modules that treat hydrodynamics, an equation of state and opacities from very low to very high densities; a nuclear network, gamma-ray transport using Monte Carlo methods, and radiation transport with 1) a comoving-frame Rybicki scheme, 2) variable Eddington tensor methods, or 3) Monte Carlo. It has adaptive mesh refinement algorithms for the hydro, and ALI (diagonal operators) for the solution of the coupled radiation transport and statistical equilibrium equations. This is a very complex and general code! The payoff is shown in figures 4 and 5: one gets good fits to the B and V light-curves as a function of time, and the spectrum at day 11 after the explosion.

In shorter papers, Lentz, Baron, & Hauschildt discuss a method of solving time-dependent moment equations for supernova lightcurves valid when the structure of the object changes slowly relative to the radiation field. It uses a time-dependent Unsöld-Lucy procedure with work and energy-deposition (e.g. gamma-ray) terms. Thomas, Baron, & Branch describe a code for computing synthetic spectra from 3D (no spherical symmetry) supernova models. It uses Monte Carlo methods to estimate the escape probability of photon in the 3D medium, and treats transport in the expanding envelope by means of the Sobolev approximation. The code offers hope for evaluating the realism of computed 3D explosion models from a comparison of their synthetic spectra with real spectra. The paper by Aufdenberg, Hauschildt, & Baron shows that the interferometric visibility functions predicted from hydrostatic and expanding models can be quite different, and calls attention to the prospect of measuring the relative angular size of M-giants at frequencies inside and outside the strong TiO bands as a test of models.

4.3. Applications to individual objects

What have we done with all this modeling capability?

Static hot stars: Lanz & Hubeny describe their grid of hot-star models (available on the web) on the range $30,000\text{K} \leq T_{\text{eff}} \leq 55,000\text{K}$, $3.00 \leq \log g \leq 4.75$, and seven different sets of compositions they have made using TLUSTY. The UV emergent spectrum from a fully-blanketed model for $T_{\text{eff}} = 30,000\text{K}$ and $\log g = 4.0$ in their figure 1 shows dramatically the errors made in estimating UV fluxes using old LTE and/or unblanketed models. Morisset, Bouret, Schaerer, & Martins discuss the effects of variations in predicted UV fluxes on nebular spectra. García-Gil, Prieto, López & Hubeny discuss the observed and computed visible and near-UV spectra of Vega to evaluate the importance of different sources of opacity in different spectral regions. Ramspeck, Haas, Napiwotzki, & Heber address the HST spectra of one of my favorite stars, the very hot O subdwarf BD+28°4211 using NLTE models with detailed treatment of line-blanketing by iron-group elements. They conclude that the abundance of Fe in this star is down by a factor of 5 - 10 relative to solar, while Ni, Mn, and Cr are near solar. And for a touch of instructive nostalgia, Wiersma, Rutten, & Lanz offer the old calculations of Auer & Mihalas (1969a, b, c) as an *exercise* for students to analyze. I can only say that I wish I had had the opportunity to read this paper and do the “homework” *before* Auer and I had done the calculations; I would have learned a great deal more!

Cool stars: Gustafsson, Edvardsson, Eriksson, & Mizuno-Wiedner present a grid of 5000 LTE (which seems to be a pretty good approximation for computing line-blanketed spectra of cool stars) planar and spherical models for late-type stars, including a detailed treatment of atomic and molecular line-blanketing. Their figure 5 shows excellent agreement between observed and computed spectra; clearly the modern physical databases have had a big impact! Richter, Wood, Bolick, Wötke, & Sedlmayr discuss the lines of FeII and [FeII] in shocked regions of Mira variables. This is a difficult subject, requiring both good hydrodynamics and good NLTE spectral modeling, complicated by the formation of dust in the atmosphere. They show convincingly that the [FeII] lines originate in hot post-shock zones, and are emitted close to the star's photosphere.

Moving Envelopes: Martins & Schaerer examine line-blanketing effects in expanding, NLTE, O-star atmospheres. They show that enhanced blanketing lowers previously-estimated effective temperatures for these stars by 1500K - 4000K because of redistribution of the emergent flux to longer wavelengths. Herrero, Najarro, & Puls analyze Cyg OB2 supergiants using "unified" (hydrodynamical) model atmospheres predicted by two codes. They find both codes show that the effective-temperature scale is several thousand K cooler when both line-blanketing and mass-loss are taken into account. Estimated radii and luminosities change such that the "mass discrepancy" is reduced, and lead to a modified wind-momentum/luminosity relationship. Bolick, Richter, & Sedlmayr presents results from atomic and molecular lines calculated from hydrodynamic models of long-period variables. This is a very ambitious program. Their analysis of the computed spectrum of CO bands provide important insights into the hydrodynamic structure of these stars. The detection of possible signatures of stellar winds in the spectra of subdwarf B-stars is discussed by Heber, Maxted, Marsh, Knigge, & Drew. They suggest that mass-loss could explain the peculiar element-abundances of these stars.

Element Diffusion: Schuh & Dreizler discuss models for chemically-stratified atmospheres of hot DA white dwarfs. They are able to achieve better fits to EUV spectroscopic observations with stratified models than with homogeneous models. Unglaub & Bues discuss models allowing for gravitational settling, radiative levitation, and weak winds with mass-loss rates $\dot{M} \leq 10^{-11} M_{\odot}/\text{year}$. They find they can make reasonable fits to most of the observed data by suitable choices of the three parameters mentioned. Theoretical mass-loss rates from adequate hydrodynamical calculations will help resolve ambiguities.

V4334 Sgr as a counterexample to everything: I love this paper by Kimeswenger. There is *nothing* more salubrious for science than to be presented with something it ought to be able to explain but can't! My best friend ever, W. W. Morgan used to teach me by walking into my office at Yerkes Observatory from time to time, and handing me an utterly horrible spectrum of some "stellar" object, asking "What do you make of *that*?". A humbling but instructive experience! Modelers would be wise to take Kimeswenger's questions seriously.

4.4. Hydrodynamics

In the first of my two papers, I point out the similarities and differences between radiating hydrodynamic flows in astrophysics and in Laboratory applications. The similarities occur in the *kinds of phenomena*. The differences arise because of the huge disparities in timescales (Lab phenomena are *fast!*), space scales, energies (even the most awesome Lab phenomena are puny compared to those in astrophysics), and masses. The latter is especially important: astrophysical flow respond to *gravity*. In Lab problems, gravity enters only as an afterthought. In the second, I give a survey of work on Cepheid atmospheres. At present it is just getting started. The work by Fokin is a good example; he makes NLTE snapshots of important line transitions using LTE dynamical models. The need for further consistency is clear, but difficult to achieve. These issues are addressed well in the short note by Schweitzer and Hauschildt; we should stay tuned.

To me, the two most interesting and important papers in this meeting are by Stein and Nordlund on radiative transfer in 3D models of solar convection, and by Carlsson and Stein on 3D NLTE magneto-radiation-hydrodynamics (!). The methods described by Stein and Nordlund are astute and insightful; they make an exceptionally difficult problem tractable. The high point of their paper for me is their discussion of atmospheric diagnostics, culminating in the single item I will remember best from this meeting: their figure 8, which shows conclusively that in the analysis of line profiles, all effects modeled by “microturbulence” and “macroturbulence” in 1D models, are, in fact, just the superposition of the ensemble of (very different!) line profiles produced by overshooting convective elements. I have always believed that this must be so, but certainly I could never have proved it. This work must be extended to other spectral classes!

Carlsson and Stein address a problem of extreme complexity, which will undoubtedly require much further effort before it is conquered. The challenges laid out in §2 of their paper are awesome. (Surely they should get the Silver Cross with two oak leaf clusters for bravery in the face of the “enemy”.) The code they have produced is of very high quality, using adaptive-grid techniques; they have devised methods to overcome the small convergence radius of the stiff system, and implemented parallelization where possible. Figure 3 in their paper tells the story: the computed results are in qualitative agreement with observation. This is not insignificant, because the flows being modeled are quasistochastic, and only the properties of large ensembles of many realizations will be meaningful.

4.5. Multidimensional media

Radiation transport in multidimensional media is of very great importance in Laboratory, and also in astrophysical contexts: accretion disks; contact or near-contact binary systems, perhaps with intrasystem gas; overshooting convection; unstable winds; novae; supernovae; and others. With the advent of massively-parallel computers, a great deal of effort has been devoted to this problem. From the outset I must point out that all of these phenomena are *dynamical*, and that we are really talking about multidimensional *radiation hydrodynamics*, not just transport. Well-posed, neat academic problems are of little value in this arena, and the methods we develop *must* be robust!

Auer’s paper on getting insight into multidimensional transfer is a didactic jewel. With simple examples, he convincingly makes several key points. 1)

The troublesome part of the problem is to predict the radiation emergent from the material we can actually observe. And that is the part we *want*, because it is there we can make diagnostics! 2) A vital aspect is *scale*: optical depth versus mean-free-path versus thermalization depth; all three critically affect the outcome. 3) Resolution is *key*. Resolution of both boundary layers, and the geometrical distribution of matter in the medium. 4) Gridding can be exceedingly difficult. And at the moment, the most robust method going seems to be local Adaptive Mesh Refinement (AMR), which is, in fact, often employed in Lab codes. And 5) even when “deterministic” methods simply fail, Monte Carlo techniques, now very well developed, can work admirably, and yield insight into very complex problems. Furthermore they are well-adapted to massively-parallel computation. This is a paper all should read.

The paper by Fabiani Bendicho gives a comprehensive review of practically all the problems facing a 2D or 3D modeler. She discusses short characteristics for doing the formal solution, with its related problems of interpolation and boundary conditions. She then describes successful iterative methods (ALI, Gauss-Seidel, successive over-relaxation, nonlinear multigrid), and compares their rates of convergence. The beginner can get much useful guidance here. She is optimistic about the future of these methods, but her own expression “state of the art” says that this work still *is* very much an art, and more work will still be required to deal with all cases.

The short paper by van Noort, Hubeny and Lanz is fascinating. They combine ALI with short characteristics to solve 2D problems in planar, spherical, and cylindrical geometries using a parallelized code. Their figures 1 and 2 show the quick convergence to very well-defined solutions in simple cases. This code may be quite useful in a variety of astrophysical explorations.

Heinzel use ALI and short characteristics to make models of magnetically confined structures on the Sun. Folini, Walder, Psarros, & Desbouefs briefly describe a 3D NLTE code using short characteristics to derive a single system of equations for the angle-integrated mean intensity, which they solve using a modern iterative system-solver. A clever feature of the code is that line-transitions are treated with a Sobolev-type escape probability.

Steinacker describes a code for solving 3D radiative transfer in dust layers and accretion disks around very young stars.

4.6. Methods

In this section I will comment on papers that deal with specific aspects of the atmospheres problem, and use special numerical or physical approaches.

The paper on formal solutions by Auer gives general and insightful answers to the question, “How do we compute the full angle-frequency dependence of radiation, both inside the medium and emergent from it?”. He gives an expert discussion of the *seemingly simple, but actually treacherous*, problem of interpolation of the source function, using the best modern methods. That is followed by clear explanations of how to evaluate the integral of the source function along some path, both in 1D and multi-D media. Finally he addresses the problem of irregular grids encountered in many 3D fluid-dynamical simulations.

Hillier presents a comprehensive discussion of how he solves the statistical equilibrium equations in his moving-atmosphere code CMFGEN. As in ALI, he

uses a linearization of the transfer equation (at a huge number of frequencies) to eliminate the radiation field in terms of changes (as localized in depth as possible) in level populations and temperature. As is known from the celebrated Sobolev approach, expansion of the atmosphere greatly helps localization. He discusses various methods for solving these equations, and for accelerating convergence. Many other important features of his code are also described: atomic data, superlevels, and enforcement of equilibrium constraints. This code has proven to be very effective in practice.

In a short paper Kubát discusses how energy-balance in the material of an atmosphere (static) is best achieved by using three different formulations in three different regimes: 1) in the optically thick regions, the best criterion is to require that the divergence of the frequency-integrated flux be zero; 2) in regions where the atmosphere is becoming optically thin at some frequencies, the best criterion is to require RE via the constraint $\int_0^\infty (\chi_\nu J_\nu - \eta_\nu) d\nu = 0$; 3) in the outermost regions where the continua are extremely optically thin but strong lines are still optically thick, the best criterion is to demand thermal balance between energy input to the electron gas by collisional ionization, photoionization, and free-free absorption of photons, with the energy lost in the inverse processes. This method converges faster and better than using the RE and flux-divergence criteria alone.

Papers by Dreizler and by Hauschildt and his coworkers resurrect the idea of obtaining energy balance in the atmosphere by using a *post-facto* temperature-correction scheme rather than by implicit linearization of the energy equation. Both use improved versions of the Unsöld-Lucy scheme, now including more accurate geometrical information via Eddington factors. More details about performance, which seems satisfactory for the problem considered, are given in Dreizler's paper. The advantage of such an approach, if successful, is that it would eliminate global coupling of all *all* atomic levels in the rate equations, and allow each atom/ion to be solved separately. But I must admit to some skepticism about whether this can be done in a robust way. The problem is scattering. The NLTE problem for, say, the Lyman continuum in RE is *strongly* scattering. My early experience with the Avrett-Krook procedure is that it would fail for such a problem. It was for this reason that Auer and I incorporated RE as a constraint *in* the transfer equation (Auer & Mihalas 1968a). We found that this technique coupled with *analytical* source functions allowed us to solve simple NLTE/RE problems. But the instant we tried to generalize, it failed. We were then driven to CL. My *guess* (perhaps wrong) is that for very difficult problems with a lot of scattering, the improved Unsöld-Lucy method may fail. We have already "cheated" the problem down by orders of magnitude by using ALI; perhaps this last step will be asking too much I can't help but think of a comment we often hear at Los Alamos. As Will Rogers (famous American humorist and folk philosopher) put it: "If it ain't broke, don't fix it". But in the Lab, the motto often seems to be "If it ain't broke, *fix it 'till it is!*" I simply hope that we aren't trying to fix something that "ain't broke" (robust energy balance by CL).

In a more mathematical flavor, Steiner shows that *multigrid* methods, when combined with ALI, can give *extremely* efficient solutions of scattering problems. This may well be the method of the future! And in a very interesting paper, Korčáková and Kubát show how discontinuous finite element methods, a favorite

of both engineers and fluid dynamicists can be employed effectively to solve the 1D comoving-frame transport equation in stellar winds. And finally, some of our bravest colleagues, Höflich, and the trio Baron, Hauschildt, & Lowenthal (BHL) describe the art of parallelization of codes meant to run on massively-parallel machines. I must confess that I fully sympathize with the first line of BHL: "In general, parallelization is a subject to be avoided . . . , however in order to take advantage of the enormous computing power and vast memory sizes of modern parallel supercomputers, we have implemented a parallel version . . . of the code PHOENIX." Now, I *know* that this is "supposed" to be the way of the future, which will yield otherwise unobtainable results in multi-D problems. But the von Neumann paradigm of serial (or only mildly parallel, i.e. having small numbers of processors) machines is *branded* into my cerebral cortex. It may be a case of the old dog who cannot learn new tricks, but I personally think it is not worth spending a fairly large chunk of the limited time I have left in my life to learn the torturous details of coding these hydra-headed machines well. As I remarked above, I will await smart compilers that can do the task for me.

4.7. Data

I have spoken mainly about computers and computation. But all that effort would lead nowhere if we did not have good observations, and good *physical data*. I mentioned above, relative to the work Auer and I did on Ne I, how difficult it was to find the basic atomic data necessary to compute a NLTE spectrum for this ion. Today the situation is vastly better. In the mid-1980s, the Opacity Project team headed by Seaton produced a huge amount of high-quality atomic/ionic cross-section data for calculating stellar envelope opacities. The OP was followed immediately by the Iron Project (IP), which aims at computing collision rates among all levels of atoms/ions up through the iron group, as well as improved optical data. The basic techniques of these calculations are ably summarized by Nahar, who also give references and the URLs of the web sites from which the data can be obtained. One interesting result she describes is a self-consistent treatment of photoionization and unified rates from radiative and dielectronic recombinations; both the upward and downward rates are computed with identical wavefunction expansions. In some cases, the unified recombination rates differ from the sum of the separate rates by factor of 4; these differences are directly attributable to quantum-mechanical interference and coupling effects. This monumental project is a *gigantic* contribution by atomic physicists to astrophysics. It will be of lasting value.

Given the data, how should they be organized for astrophysical purposes? Answers to this question are given by both Lanz & Hubeny, and by Rauch & Deetjen. Lanz and Hubeny are able to include data from tens of thousands of energy levels and millions of lines into their code TLUSTY. They discuss in some detail their implementation of superlevels, and the representation of the collective line opacity by Opacity Distribution Functions (ODF) or the Opacity Sampling (OS) Technique. In the limit of very small sampling-intervals, the two methods are essentially identical; but with wider intervals, ODFs lose details of line blends, which may affect the results. URLs are given for TLUSTY's database and user manual, as well as other primary data sources. Rauch & Deetjen describe carefully the database used by TMAP, the Tübingen Model Atmosphere

Program. They also make extensive use of OP and IP data, and give references. They describe both their methods of forming superlevels and superlines in detail, and the format of their database of ready-to-use model atoms. I strongly endorse their appeal to form a common database so that other workers will not have to repeat the tedious work of assembling all these data and model atoms/ions in the future. I was perplexed (alarmed?) to read that the simple rates for collisional excitation and ionization in H and He that I, and Stone and I had to use in 1967-68 are still cited. Newer experimental results are cited, and surely better theoretical results are now available; considering that H and He are the dominant constituents of stellar atmospheres, the older results should be replaced by modern values as soon as possible!

Data for molecular lines are now in abundant supply compared to 10 years ago. Asensio Ramos & Trujillo Bueno give a good discussion of radiative transfer in molecular lines using quickly-convergent iterative methods. Jørgensen gives a balanced discussion of molecules in cool stellar atmospheres and star-like objects with emphasis on H₂O, CH₄, and C₂. At present, there are significant discrepancies among results obtained from different line lists, and between theoretical versus empirical results. Homeier, Hauschildt, & Allard show that when levels of CH₄ are extrapolated up to $J = 40$, the positions of individual features in the spectrum of T-dwarf model atmospheres remain about the same, but the total band strength fits much better because of the huge numbers of faint lines. Schweitzer, Hauschildt, Baron, and Allard describe how to modify the concepts of superlevels and superlines to apply to molecules. By grouping lines of CO into bins having nearly the same vibrational quantum numbers, and then dividing those bins into sub-bins of nearly the same excitation energy, they obtained 350 superlevels from 3623 original levels. A calculation of the spectrum from these superlevels gives the same results as a direct calculation using all levels. They have similarly reduced the 269,000 energy levels of TiO to 260 superlevels, and expect to achieve a similar level of accuracy in the spectrum.

Recently, considerable attention has been given to opacities in even cooler regimes. Thus Alexander, Ferguson, Tamanai, Bodnarik, Allard, & Hauschildt give a very good general discussion of the opacities of molecules and dust. Tamanai, Alexander, Ferguson, & Sedlmayr discuss the optical constants and extinction efficiency of solids in low-temperature grains. And Semenov, Henning, Ilgner, Helling, and Sedlmayr give Rosseland mean opacities for protoplanetary disks. None of these topics could have been addressed effectively a decade ago.

5. Finis

I personally think that this workshop is an intellectual watershed. In the last 40 years of the 20th century, we have learned how to make physically complete, and computationally accurate, fully line-blanketed NLTE models for static planar and spherical atmospheres and steady flows, as in stellar winds. We truly know what we are doing now! It has been an impressive period of achievement. Originally, we had planned this workshop for September of 2001, the first year of the 21st century; but it was delayed by the tragic events at the World Trade Center. Nevertheless, even a year late, this meeting will be a milestone against which the progress made in the next decades can be measured. My prediction

is that we have only begun... that our modeling capabilities will increase in physical and numerical accuracy (not mere precision!), and that we can attack successfully the spectral analysis of a host of "exotic" (by current standards) objects. And I believe that we are entering the era of the study of the *dynamics* of stellar atmospheres, on all scales, from convection, to pulsation, to explosion. It will give me great satisfaction to keep track of the progress in this field. *Bon voyage!*

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On the personal level, I would like to pay my deep homage to my colleague Dr. Lawrence H. Auer, who has made seminal contributions to not one, but *both*, of the major tools we use today: complete linearization and ALI. He pushed the field forward by decades through his insight. I would also like to acknowledge him and Kathlyn Auer as good friends (and comrade cat-connoisseurs); our interactions, over many years, have made all of us better and stronger people.

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