MODEL ATMOSPHERES FOR POPULATION SYNTHESIS

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ABSTRACT. I have used my newly calculated iron group line list together with my earlier atomic and molecular line data, 58,000,000 lines total, to compute new opacities for the temperature range 2000K to 200000K. Calculations have been completed at the San Diego Supercomputer Center for 56 temperatures, for 21 pressures, for microturbulent velocities 0, 1, 2, 4, and 8 km/s, for 3,500,000 wavelength points divided into 1221 intervals from 10 to 10000 nm, for scaled solar abundances [+1.0], [+0.5], [+0.3], [+0.2], [+0.1], [+0.0], [-0.1], [-0.2], [-0.3], [-0.5], [-1.0], [-1.5], [-2.0], [-2.5], [-3.0], [-3.5], [-4.0], [-4.5], and [-5.0]. I have rewritten my model atmosphere program to use the new line opacities, additional continuous opacities, and an approximate treatment of convective overshooting. The opacity calculation was checked by computing a new theoretical solar model that matches the observed irradiance. Thus far I have completed a grid of 7000 model atmospheres at 2 km/s for all the abundances, for the temperature range 3500K to 50000K, and for log g from 0.0 to 5.0. This grid will allow a consistent theoretical treatment of photometry from K stars to B stars. Fluxes are tabulated from .09 to 160 micrometers. Preliminary results are reported for many photometric systems. Work is underway on grids for other microturbulent velocities. Microturbulent velocity strongly affects the interpretation of Cepheid and RR Lyrae photometry. The models, fluxes, and colors are available on magnetic tape and will also be distributed on CD-ROMs.

1. Old models

I start by listing the shortcomings in my old models as I did at an earlier meeting (Kurucz 1987) but this time I can report that I have corrected most of them.

My old models (Kurucz 1979a,b) were produced as long as 18 years ago on computers that are primitive by today's standards. The number of optical depth layers was limited by small memories and slow processors. Now I can compute with many more layers and go to shallower optical depths. This greatly improves the numerical accuracy of the calculated radiation field at wavelengths that have very high or rapidly varying opacity. Fortunately, such wavelengths do not very much affect the structure of a model. There was also a limit to the number of frequencies that I could afford to compute. Now I use up to 1221 wavelength intervals from 9 to 160,000 nm. I can now use 1 nm resolution in the ultraviolet for better comparison to satellite observations.

My old models for F and G stars are systematically in error and predict color indices that are off by as much as 0.05 mag. I assumed that the error was caused by problems in the mixing length treatment of convection and by the omission of molecular line opacity in the coolest models. My theoretical model for the solar photosphere has several per cent error in the flux in the red and, of course, cannot reproduce the molecular features in the ultraviolet. Improvements in my treatment of convection, even going so far as having hot and cold streams, have reduced the error somewhat for the hotter convective models. I have

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also added approximate overshooting and have tried various increases in the mixing-length to scale-height ratio. I now use 1.25. However, I am now convinced that most of the error comes from missing line opacity, including missing atomic line opacity, which turns out to be significant at all effective temperatures. I hope that Nordlund and others will be able to produce models with realistic convection cells to take care of the convection physics, so now I am concentrating on the opacity. I discuss molecular and atomic opacity in the next section.

We do not know much about microturbulent velocity. It has been decreasing as a function of time as the models have improved. In the sun it is depth-dependent varying from about 0.5 to 1.8 km/s. The models assume a constant value. Twenty five years ago, I arbitrarily chose 2 km/s as a nice round number. In some stars it can be much larger or much smaller. Opacity, radiative acceleration, and model structure vary considerably with the microturbulent velocity. It may be that 1 or 1.5 km/s is a good choice for high gravity models. George Michaud tells me that the existence of some types of diffusion implies microturbulent velocities less than 100 m/s. Microturbulent velocity may vary strongly with phase and with depth in pulsating stars, thereby strongly affecting the atmospheric structure and colors. I plan to investigate this through spectrum synthesis. My new grids of models have microturbulent velocity as a parameter, so it must be specified when choosing a model.

The helium abundance is another arbitrary number. I chose 10% by number. Others use a 10% He/H ratio. I have switched to a smaller value because I think it more probable. Small errors in the helium abundance produce errors in the density, electron number, and opacity and consequently produce systematic errors in the derived stellar parameters. The "solar" metal abundances have also changed with time and are not yet final. I now use Anders and Grevesse (1989) abundances.

My old low gravity models have systematic errors because of non-LTE and sphericity effects. So do my new models.

2. New lines and new opacities

I reported on my line and opacity calculations at a NATO workshop in Trieste (Kurucz 1991). The details of my line lists and the opacities can be found in that paper. Here I will give only a brief outline.

My earlier model calculations used the distribution-function line opacity computed by Kurucz (1979ab) from the line data of Kurucz and Peytremann (1975). We had computed gf values for 1.7 million atomic lines for sequences up through nickel using scaled-Thomas-Fermi-Dirac wavefunctions and eigenvectors determined from least squares Slater parameter fits to the observed energy levels. That line list has provided the basic data and has since been combined with a list of additional lines, corrections, and deletions with the help of Barbara Bell and Terry Varner at the Center for Astrophysics. The line data are being continually, but slowly, improved. We collect all published data on gf values and include them in the line list whenever they appear to be more reliable than the current data. I have also completely recomputed Fe II (Kurucz 1981).

After the Kurucz-Peytremann calculations were published, I started work on line lists for diatomic molecules beginning with H_2, CO (Kurucz 1977), and SiO (Kurucz 1980). Next, Lucio Rossi of the Istituto Astrofisica Spaziale in Frascati, John Dragon of Los Alamos, and I computed line lists for electronic transitions of CH, NH, OH, MgH, SiH, CN, C_2, and TiO. In addition to lines between known levels, these lists include lines whose wavelengths are predicted and are not good enough for detailed spectrum comparisons but are quite adequate for statistical opacities. Work is continuing on other molecules and molecular ions, and on the vibration-rotation spectra. I also have data for terrestrial atmospheric molecules.

In 1983 I recomputed the opacities using the additional atomic and molecular data described above which totalled 17,000,000 lines. These opacities were used to produce improved empirical solar models (Avrett, Kurucz, and Loeser 1984), but were found to still not have enough lines. For example, there were several regions between 200 and 350 nm where the predicted solar intensities are several times higher than observed, say, 85% blocking instead of the 95% observed. The integrated flux error of these regions is several per cent of the total. In a flux constant theoretical model this error is balanced by a flux error in the red. The model thus predicts the wrong colors. In detailed ultraviolet spectrum calculations, half the intermediate strength and weak lines are missing. After many experiments, I determined that this discrepancy is caused by missing iron group atomic lines that go to excited configurations that have not been observed in the laboratory. Most laboratory work has been done with emission sources that cannot strongly populate these configurations. Stars, however, show these lines in absorption without difficulty. Including these additional lines produces a dramatic increase in opacity, both in the sun and in hotter stars. A stars have the same lines as the sun but more flux in the ultraviolet to block. In B stars and in O stars there are large effects from third and higher iron group ions. Envelope opacities that are used in interior and pulsation models are also strongly affected.

I was granted a large amount of computer time at the San Diego Supercomputer Center by NSF to carry out new calculations. To compute the iron group line lists I determined eigenvectors by combining least squares fits for levels that have been observed with computed Hartree-Fock integrals (scaled) for higher configurations including as many configurations as I can fit into a Cray. All configuration interactions are included. My computer programs have evolved from Cowan's (1968) programs. Transition integrals are computed with scaled-Thomas-Fermi-Dirac wavefunctions and the whole transition array is produced for each ion. The forbidden transitions can be computed as well. Radiative, Stark, and van der Waals damping constants and Lande g values are automatically produced for each line. The first nine ions of Ca through Ni produced 42,000,000 lines. I will recompute the energy levels and line lists when new analyses become available and I will make the predictions available to laboratory spectroscopists. I plan to do the heavier and lighter elements as a background project.

The models I can compute now are not valid for M stars. I eventually need line lists for the triatomic molecules, but I hope that other people will do the work before I have to learn the physics. I am working on the low temperature bands now, however, for atmospheric transmission.

In late 1988 I used the line data described above to compute new solar abundance opacity tables for use in my modelling. The calculations involved 58,000,000 lines, 3,500,000 wavelength points, 56 temperatures from 2000K to 200000K, 21 log pressures from -2 to +8, and 5 microturbulent velocities 0, 1, 2, 4, 8 km/s, and took a large amount of computer time. The opacity is tabulated both as 12-step distribution functions for intervals on the order of 1 to 10 nm, and as opacity sampling where, simply, every hundredth wavelength point in the calculation was saved. There are actually two sets of distribution functions, a higher resolution version with 1212 "little" intervals, and a lower resolution version with 328 "big" intervals. The "little" wavelength intervals are nominally 1 nm in the ultraviolet and 2 nm in the visible. The opacities were tested by computing a solar model as described below.

Since the beginning of 1990 I have been able to take tremendous advantage of the new Cray YMP at the San Diego Supercomputer Center. In a few months I finished more than I had expected to do in two years. I computed opacities ranging from 0.00001 solar to 10 times solar, enough to compute model atmospheres ranging from the oldest Population II stars to high abundance Am and Ap stars. The hardest part was transmitting the results (200 tapes) back to Cambridge over Internet, but even that usually worked quite well. The exact abundances are [+1.0], [+0.5], [+0.3], [+0.2], [+0.1], [+0.0], [-0.1], [-0.2], [-0.3], [-0.5], [-1.0], [-1.5], [-2.0], [-2.5], [-3.0], [-3.5], [-4.0], [-4.5], [-5.0], and [+0.0, no He]. The final files for each abundance require two 6250 bpi VAX backup tapes. I distribute copies of the tapes on request. I hope to produce CD-ROMs of these opacities that can be read on any workstation with a CD reader.

I am open to suggestions for computing opacities for other abundance mixes. I plan to compute Population II opacities with [+0.4] enhanced alpha process elements, some Am and Ap mixes, and C/O variations.

3. New models

I have rewritten my model atmosphere program to use the new line opacities, additional continuous opacities, and an approximate treatment of convective overshooting. The opacity calculation was checked by computing a small grid of solar models with various microturbulent velocities and mixing-length-to-scale-height ratios. I adopted a solar model shown in Figure 1 that matches the observed irradiance (Neckel and Labs 1984; Labs et al. 1987) with Vturb = 1.5 km/s and l/H = 1.25. I am confident that I have solved the missing opacity problem. I then computed (on Vaxstations) a grid of 400 solar abundance, 2 km/s models covering the effective temperature range from K stars to O stars. The models are listed in Table I. Models cooler than 9000K are convective with l/H = 1.25. The range of this grid should allow photometric calibrations consistent for both cool and hot stars. Note that since triatomic molecules are not included, the models cannot be used for M stars. I have distributed tapes of the models and the flux predicted from each model at 1221 wavelengths in the range .01 to 160 micrometers. The range is enough to treat ionization in H II regions and to calibrate the infrared.

I have computed preliminary UBV and uvby colors and bolometric corrections for the solar abundance grid described above following Buser and Kurucz (1978) and Relyea and Kurucz (1978) including the typographic correction from Lester et al (1986). The colors were normalized by finding the model in the grid that best interpolates the spectrophotometry of Vega (Hayes and Latham 1975; Tug, White, and Lockwood 1977), Figure 2, and that best matches the Balmer line profiles (Peterson 1969) and then by forcing the computed colors for that model to match the observed colors. That model has Teff = 9400K and log g = 3.95 just as in the earlier grid (Kurucz 1979a). However, remember that the helium abundance, metal abundances, line opacity, and resolution are different. Models with lower microturbulent velocity are not observationally distinguishable in the

Table I. Solar abundance models, 2 km/s microturbulent velocity

	log g											
Teff	0.0	0.5	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0	Teff
3500	X	X	X	X	X	X	X	X	Z	Z	Z	3500
3750	X	X	X	X	X	X	X	X	Z	Z	Z	3750
4000	X	X	X	X	X	X	X	X	X	X	X	4000
4250	X	X	X	X	X	X	X	X	X	X	X	4250
4500	X	X	X	X	X	X	X	X	X	X	X	4500
4750	X	X	X	X	X	X	X	X	X	X	X	4750
5000	X	X	X	X	X	X	X	X	X	X	X	5000
5250	X	X	X	X	X	X	X	X	X	X	X	5250
5500	X	X	X	X	X	X	X	X	X	X	X	5500
5750	X	X	X	X	X	X	X	X	X	X	X	5750
6000	X	X	X	X	X	X	X	X	X	X	X	6000
6250	B	X	X	X	X	X	X	X	X	X	X	6250
6500	B	X	X	X	X	X	X	X	X	X	X	6500
6750	B	X	X	X	X	X	X	X	X	X	X	6750
7000	B	X	X	X	X	X	X	X	X	X	X	7000
7250	B	X	X	X	X	X	X	X	X	X	X	7250
7500	B	X	X	X	X	X	X	X	X	X	X	7500
7750		B	X	X	X	X	X	X	X	X	X	7750
8000		B	X	X	X	X	X	X	X	X	X	8000
8250		B	X	X	X	X	X	X	X	X	X	8250
8500		B	X	X	X	X	X	X	X	X	X	8500
8750			B	X	X	X	X	X	X	X	X	8750
9000			B	X	X	X	X	X	X	X	X	9000
9250				B	X	X	X	X	X	X	X	9250
9500				B	X	X	X	X	X	X	X	9500
9750				B	X	X	X	X	X	X	X	9750
10000				B	X	X	X	X	X	X	X	10000
10500				B	X	X	X	X	X	X	X	10500
11000					B	X	X	X	X	X	X	11000
11500					B	X	X	X	X	X	X	11500
12000					B	X	X	X	X	X	X	12000
12500					B	X	X	X	X	X	X	12500
13000					B	X	X	X	X	X	X	13000
14000				B	X	X	X	X	X	X	X	14000
15000					B	X	X	X	X	X	X	15000
16000					B	X	X	X	X	X	X	16000
17000					B	X	X	X	X	X	X	17000
18000					B	X	X	X	X	X	X	18000
19000					B	X	X	X	X	X	X	19000
20000						B	X	X	X	X	X	20000
21000						B	X	X	X	X	X	21000
22000						B	X	X	X	X	X	22000
23000						B	X	X	X	X	X	23000
24000						B	X	X	X	X	X	24000
25000						B	X	X	X	X	X	25000
26000						B	X	X	X	X	X	26000
27000							B	X	X	X	X	27000
28000							B	X	X	X	X	28000
29000							B	X	X	X	X	29000
30000							B	X	X	X	X	30000
31000							B	X	X	X	X	31000
32000								B	X	X	X	32000
33000								B	X	X	X	33000
34000								B	X	X	X	34000
35000								B	X	X	X	35000
37500									B	X	X	37500
40000									B	X	X	40000
42500										B	X	42500
45000										B	X	45000
47500										B	X	47500
50000										B	X	50000

X = converged
B = blows up from radiative acceleration
Z = converged, not realistic because no water opacity

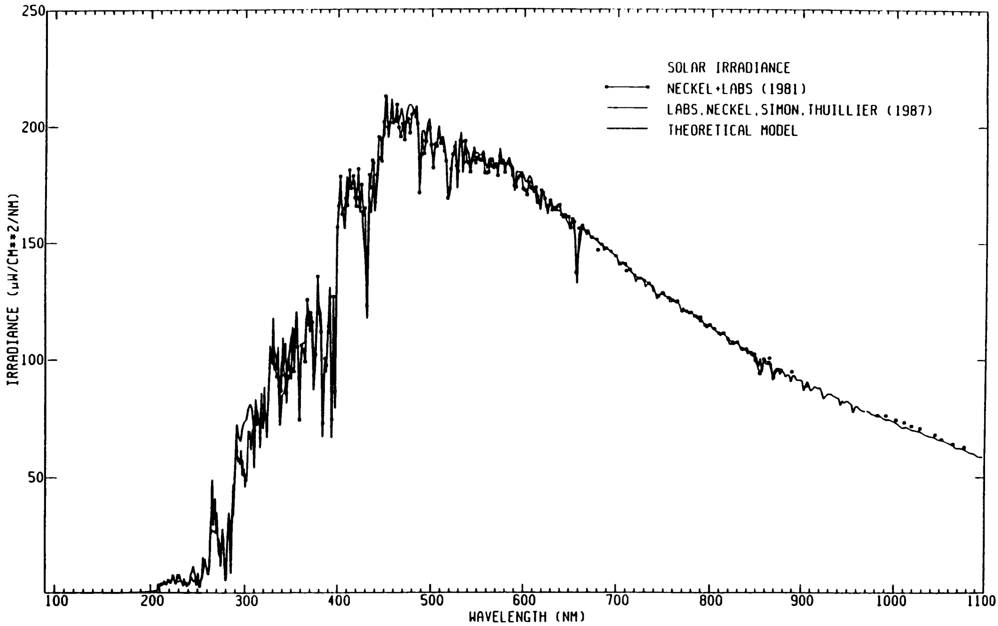

Figure 1. Predicted solar irradiance compared to observed.

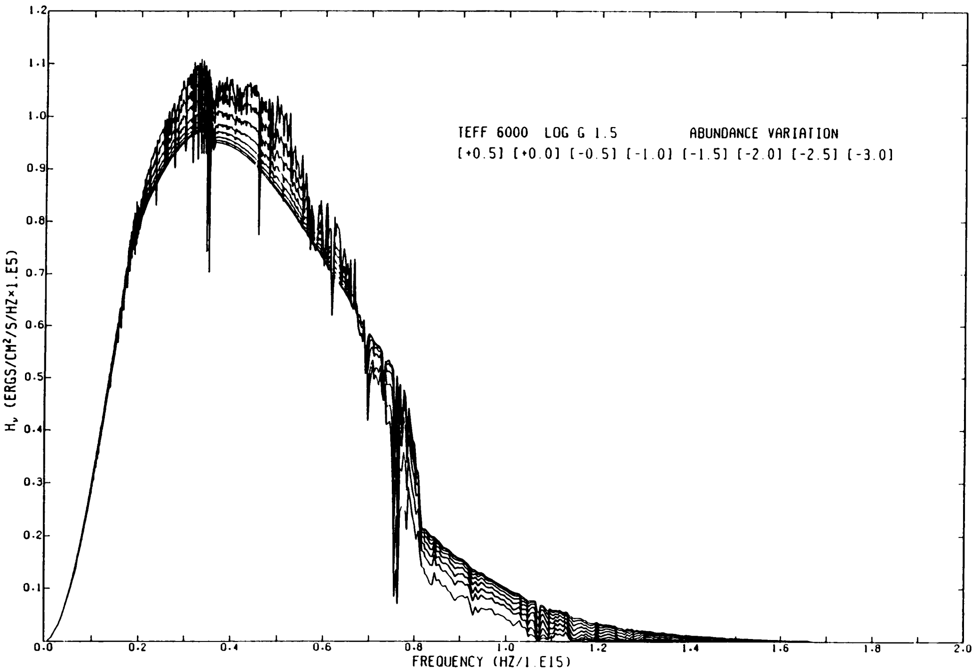

Figure 3. The change in flux distribution for a G giant as the abundance increases from extreme Pop II to extreme Pop I. At the 850 nm maximum the flux increases by 15% (.15 mag). In the Balmer continuum the flux decreases by more than a factor of 2 (1 mag).

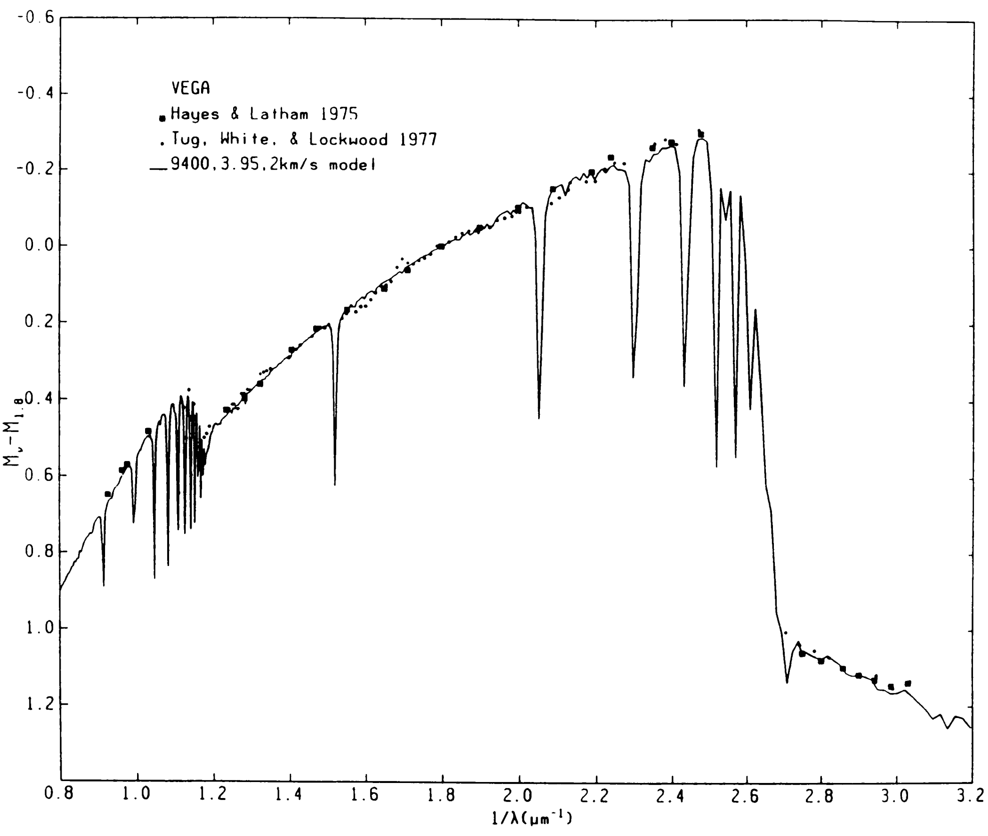

Figure 2. Observed and predicted spectrophotometry relative to 1.8 inverse micrometers (555.6 nm) for Vega. The computed slopes of the Balmer, Paschen, and Brackett continua and the Balmer discontinuity agree with observations.

visible. This model is not a physical model for Vega because Vega does not have solar abundances (for example, see Adelman and Gulliver 1990), but even if the physical parameters are somewhat off, the temperature-pressure structure must be correct in the continuum and Balmer-line-wing-forming layers. A correct model will have a similar structure but perhaps for a somewhat different effective temperature and gravity.

I have begun to compute grids of models on the Cray using the solar abundance, 2 km/s grid for starting models. Thus far I have run approximately 7000 models for all abundances at 2 km/s. Just checking the output is a tremendous amount of work for me. I have to individually rerun mistakes and failures. I will compute the fluxes, predicted photometry, Balmer line profiles, and limb-darkening for each model. At the present time I can supply magnetic tapes with the models for the various abundances. I will also publish the data on CD-ROMs. Most users will be able to find what they need by simple interpolation. For any model I expect to be able to compute a complete, full-resolution spectrum that can be compared to high resolution observations, or degraded to low resolution, say, 0.1 nm.

Figure 3 shows results from these calculations for G giants, a sample of what is now available for population synthesis of galaxies. It is clear that there are strong abundance effects throughout the spectrum. In addition to the variation in the spectral features, there is strong redistribution of energy from the ultraviolet to the red and infrared as the abundance increases. It is clearly impossible to do any type of evolutionary population synthesis based on observed Population I spectra. These models are still in need of improvement, but I hope they allow a significant advance in population synthesis.

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DISCUSSION

ROCCA-VOLMERANGE: For infrared studies it would be necessary to extend your models down to 2000K. Do you think that is possible?

KURUCZ: I do not have line opacity for any triatomic molecules so you would have to ask Gustafsson, or Jorgensen, or Johnson for those models. If the abundances are low so that triatomic opacity is not important, I should be able to compute down to 3000K. At lower effective temperatures the surface temperature is below 2000K which is the lower limit of my tabulated opacities.

GUSTAFSSON: Would you comment on your present recipe for convection and on what effects it has on colours and spectra, as compared with the standard local mixing-length theory?

KURUCZ: There have been several small changes over the years that add up to 0.05 - 0.06 mag in the colors for F and G stars. Lester et al. at Toronto tried several fixes. One I adopted is computing opacities for hot and cold elements and then averaging instead of computing opacity for the average temperature. I recently put in an approximate overshooting by assuming that the center of a bubble stops at the top of the convection zone so that there is convective flux one bubble radius above the convection zone. That flux is found by computing the convective flux in the normal way and then smoothing it over a bubble diameter.