A platform independent, parallel version of Atlas12

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Opacity sampling with Atlas12, the stellar atmosphere code developed by R. L. Kurucz, cannot always be carried out with the desired frequency or depth resolution because of the limited computing power of even the fastest monoprocessors. There are also known problems of portability which make it difficult to run Atlas12 with various compilers on different operating systems.

We have first established a Fortran77 version that can be compiled using the g77 compiler, a useful feature for astronomers having no access to VMS compatible Fortran compilers. In a further step, Atlas12 was successfully ported to Ada95, an object-oriented parallel language. Atlas12 is now platform independent, split up in modules and running in parallel on multi-processor machines. Any limitations as to the maximum number of depth and frequency grid-points and the number of lines that can be treated have been pushed far beyond what is possible with the original version.

We intend to incorporate the continuous opacity routines of Atlas12 in our new CAMAS code for magnetic atmospheres (but also in the existing COSSAM and CARAT codes) in order to be able to compare our results with R.L. Kurucz's de facto stellar atmosphere standard.

Introduction

Atlas12 is a stellar atmosphere code developed by R.L. Kurucz. This opacity sampling code can be used as a (non-magnetic) standard for stars with exotic abundances (Kurucz 1996), albeit without stratification. In its original version the code calculates models with 30.000 points in frequency and a depth-grid with up to 72 points. For some applications (e.g. convective models) a higher resolution in depth would be desirable.

We decided to port the code to the object-oriented parallel language Ada95 because of the need for:

- improved frequency resolution
- improved depth resolution
- ensuing necessity of parallel computation
- modularisation, portability, readability
- compatibility with our Ada95 based spectrum synthesis codes
- solution for the Little / Big Endian problem

One goal was to incorporate the atlas opacities into our existing codes and the new CAMAS code. Thus we needed a modularised version of the code with well defined interfaces.

Resolution

The obvious first step towards better resolution was to get rid of hard coded maximum vector lengths. Fixed array lengths have the big drawback that they usually fill more of the memory than necessary. This problem is easily overcome by the use of dynamic arrays. The maximum required length of all arrays used is evaluated at the beginning of the program by scanning the model file.

But enlarging the number of depth points is not enough to increase the achievable resolution of the model. Originally the Atlas code calculates the mean intensity J, flux H and radiation pressure K by using the matrix method developed by R. L. Kurucz (Kurucz 1969, 1970). This method involves so called "integration matrices" which depend on the optical depth point distribution. Atlas12 uses pretabulated integration matrices and therefore J, H and K can only be derived on a fixed optical depth scale. This requires the interpolation of the source function onto this grid and the interpolation of the results onto the optical depth scale at a given frequency. (see Graph 2) Consequently the maximum number of depth points is also limited by the step width of the fixed optical depth scale of the integration matrices as one will obtain only "empty resolution" by interpolating a large number of points onto a coarse grid.

Obviously there are two methods to overcome this problem:

- Calculate integration matrices with the required step width for J, H and K at the program start.
- Use a Feautrier scheme (Feautrier 1964, Rybicki & Hummer 1991) to calculate J, H and K.

The third possibility, calculating such integration matrices at every frequency point for the given optical depth scale, turned out to be slow and unstable at the same time.

The Feautrier scheme has the advantage that it does not need any pretabulation (see Graph 3). Thus it does not limit the number of depth points. The accuracy (and the CPU-time) of the method depends on both the number of depth points and of angle points.

Parallelisation and Runtime

The calculation of stellar atmospheres is well suited for parallel computation:

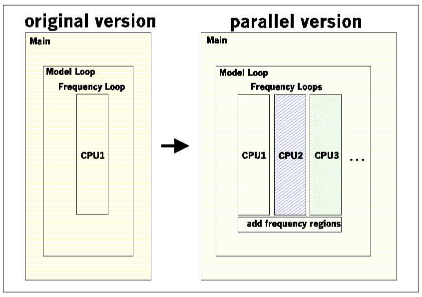
About two thirds of the computing time are spent on the frequency integration part (see Graph 4 and Table 1). We simply need to subdivide the frequency range into subintervals and pass these to different CPUs. The results of these computations are summed up and sent back to the model loop (see Graph 1).

For a comparison of the run-times we have executed 30 iterations on a 12.000K Atlas9 model with 72 depth points and 30.000 frequency points. We also changed some abundances (C,N,O -1dex and Cr, Fe, Ni +1dex) to test the convergence behaviour of our codes.

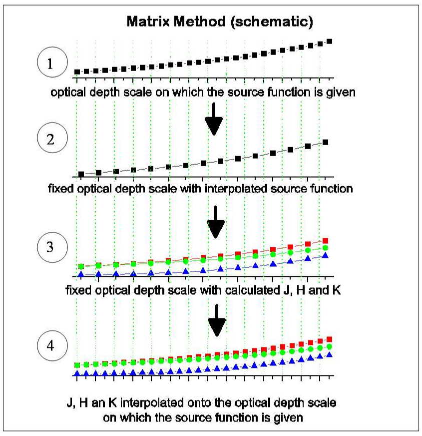
Runtime Table

	total	Main Level	Model Level		Frequency Level	
		total	total	single iteration	total	single iteration
	mm:ss	mm:ss	mm:ss	mm:ss	mm:ss	mm:ss
g77, clone	11:38	0:37	4:00	0:08	7:01	0:14
Ada95, clone	19:34	0:17	7:00	0:14	12:17	0:24
parallel (dual processor)	14:05	0:17	7:00	0:14	6:48	0:14
Ada95, Feautrier, 6 Points	23:11	0:17	7:00	0:14	15:54	0:32
parallel (dual processor)	16:00	0:17	7:00	0:14	8:43	0:17
Ada95, Feautrier, 10 Points	26:52	0:17	7:00	0:14	19:33	0:39
parallel (dual processor)	17:53	0:17	7:00	0:14	10:36	0:21

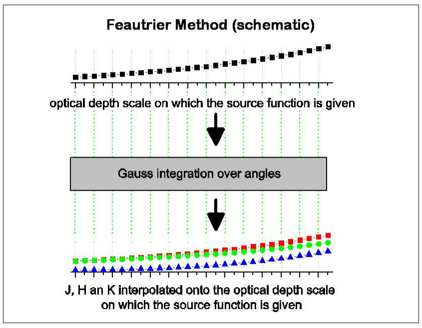
Table 1: The calculations were carried out on an Intel Xeon (2.660 MHz) dual processor machine. We used the compiler switches -O3 for g77 and -O3 -gnatp for the Ada95 compiler, in order to get comparable optimisation.
It can be seen that at the moment the Ada95 code needs more time than the g77 code on the model level because the file handling (in LINOP) takes more time if formatted in/output is used.



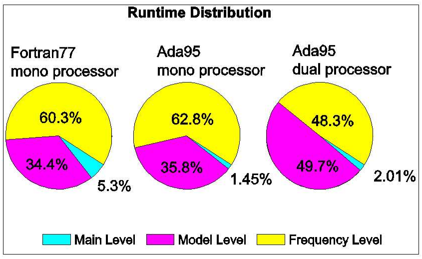
Graph 1: Atlas12 is well suited for parallelisation since the frequency integration can easily be divided into subintervals.



Graph 2: The use of the Matrix Method involves the interpolation of the source function (1) onto the grid on which the integration matrices are pretabulated (2). The resulting J, H and K vectors (3) are interpolated onto the optical depth scale at the frequency (4). Thus the maximum number of depth points that will make sense is limited by the spacing of the pretabulated optical depth scale.



Graph 3: The Feautrier scheme calculates a flux-like and an intensity-like quantity on the given optical depth scale for rays with different angles to the line of sight. A Gauss integration is used to obtain J, H and K. The accuracy of J, H and K can be improved by increasing the number of angles. This method does not carry out any interpolation.



Graph 4: This plot shows that the original code and its Ada95 clone spent about two thirds of the computation time on the frequency integration. The rightmost graph shows how much a second processor can decrease the duration of the frequency integration (see also Table 1).

The code versions compared were:

- a Fortran version which is the original version with some minor changes to make it compilable with the g77 compiler
- an Ada95 version using the matrix method to derive J, H and K
- an Ada95 version using the Feautrier method to derive J, H and K

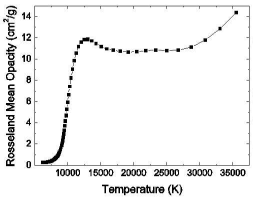
When we compiled the codes we used the -O3 switch for g77 and -O3 -gnatp for the Ada95 compiler to get comparable optimisation. We used a multi-processor machine with two Intel 2.660 MHz CPUs to compare the run-times of the different versions of the code.

At the moment the Ada95 code needs more time than the g77 code in the model level because the file handling in LINOP takes more time if formatted in/output is used.

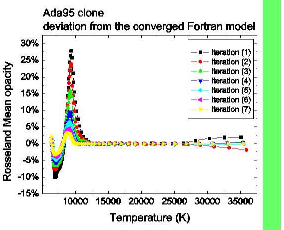
Results and current status

Our calculations showed that our 12000K model converge to the same values with comparable convergence speed. Graph 5 to 8 show the decreasing deviations from the converged model. After 7 iterations all parameters of the models are within 5% relative deviation from the converged model.

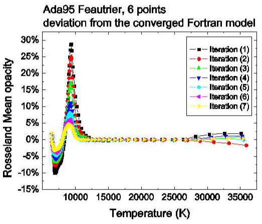
The advantages of the Ada95 code are its suitability for multiprocessor machines and the possibility to calculate more depth points.
The Ada95 code is not yet fully optimised as regards CPU time since so far we have focused on portability and the establishment of well defined interfaces in order to incorporate some parts of the code into our other codes.



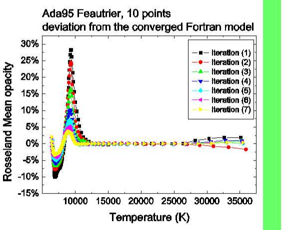
Graph 5: The converged Fortran model for a 12.000K star with 72 depth points, 30.000 frequency points, decreased C,N,O (-1dex) and increased Cr, Fe, Ni (+1dex) abundances.



Graph 6: The Ada95 clone
Deviations from the converged Fortran model



Graph 7: The Feautrier model with 6 points
Deviations from the converged Fortran model



Graph 8: The Feautrier model with 10 points
Deviations from the converged Fortran model

Conclusion

Our version of the code will be useful for the study of phenomena which need improved resolution in depth or frequency.
The new code is parallel and fairly platform-independent. We have tested it with various Linux distributions (Debian, Redhat and Suse) and various processor types (Intel Xeon / AMD Athlon).

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