Parallel Supercomputing In Stellar Atmosphere Simulations

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Abstract. In this paper we discuss parallel algorithms for the solution of NLTE stellar atmosphere problems involving static and expanding stellar or planetary atmospheres. We use a scheme of nested iterations that can be used to reduce the high dimension of the problem to a number of problems with smaller dimensions. Although modern iteration schemes are very efficient, parallel algorithms are essential in making large scale calculations feasible, therefore we discuss some parallelization schemes that we have developed.

We also describe two parallel algorithms for line opacity calculations based on a local file and on a global file approach. The performance and scalability of both approaches is discussed for different test cases and very different parallel computing systems. The results show that a global file approach is more efficient on high-performance parallel supercomputers with dedicated parallel I/O subsystems whereas the local file approach is very useful on farms of workstations, e.g., cheap PC clusters.

1. Introduction

Our group has developed the very general non-LTE (NLTE) stellar atmosphere computer code PHOENIX (Hauschildt, 1992, 1993; Hauschildt & Baron, 1999; Hauschildt et al., 1995; Allard & Hauschildt, 1995; Hauschildt et al., 1996;
Baron et al., 1996; Hauschildt, Baron, & Allard, 1997; Baron & Hauschildt, 1998; Hauschildt & Baron, 1999) which can handle extremely large model atoms as well as line blanketing by hundreds of millions of atomic and molecular lines. This code is designed to be both portable and flexible: it is used to compute model atmospheres and synthetic spectra for, e.g., novae, supernovae, M and brown dwarfs, O to M giants, white dwarfs and accretion disks in Active Galactic Nuclei (AGN). The radiative transfer in PHOENIX is solved in spherical geometry and includes the effects of special relativity (including advection and aberration) in the modeling.

The PHOENIX code allows us to include a large number of NLTE and LTE background spectral lines and solves the radiative transfer equation for each of them without using simple approximations like the Sobolev approximation. Therefore, the profiles of spectral lines must be resolved in the co-moving (Lagrangian) frame. This requires many wavelength points (we typically use 150,000 to 300,000 points). Since the CPU time scales linearly with the number of wavelength points, the CPU time requirements of such calculations are large. In addition, (NLTE) radiative rates for both line and continuum transitions must be calculated and stored at every spatial grid point for each transition, which requires large amounts of storage and can cause significant performance degradation if the corresponding routines are not optimally coded.

An important problem in stellar atmosphere calculations is to find a consistent solution of the very diverse equations that describe the various physical processes. We have developed a scheme of nested iterations that enables us to separate many of the variables (e.g., separating the temperature correction procedure from the calculation of the NLTE occupation numbers). This allows us to compute far more detailed stellar atmosphere models than was previously possible, see Hauschildt & Baron (1999); Hauschildt, Baron, & Allard (1997); Baron & Hauschildt (1998); Hauschildt, Lowenthal, & Baron (2001) for details.

In order to take advantage of the enormous computing power and vast aggregate memory sizes of modern parallel supercomputers, both potentially allowing much faster model construction as well as more sophisticated models, we have developed a parallel version of PHOENIX. Since the code uses a modular design, we have implemented different parallelization strategies for different modules (e.g., radiative transfer, NLTE rates, atomic and molecular line opacities) in order to maximize the total parallel speed-up of the code. In addition, our implementation allows us to change the distribution of computational work onto different nodes both via input files and dynamically during a model run, which gives a high degree of flexibility to optimize performance for both a number of different parallel supercomputers (we are currently using IBM SP2s, SGI Origin 2000s, HP/Convex SPP–2000s, and Cray T3Es) and for different model parameters. Since PHOENIX has both large CPU and memory requirements we have developed the parallel version of the code using a MIMD approach. We use the MPI message passing library Message Passing Interface Forum (1995) for portability and simultaneously use both task and data parallelism in order to optimize the parallel speed-up (Hauschildt, Baron, & Allard, 1997; Baron & Hauschildt, 1998).

In our model atmosphere code we have implemented and used direct opacity sampling (dOS) for more than a decade with very good results. During that
time, the size of the combined atomic and molecular line databases that we use has increased from a few MB to \( \approx 10 \text{ GB} \). Whereas the floating point and memory performance of computers has increased dramatically in this time, I/O performance has not kept up with this speed increase. Therefore, I/O performance is today more important that it was 10 years ago and has to be considered a major issue. The availability of large scale parallel supercomputers that have effectively replaced vector machines in the last 5 years, has opened up a number of opportunities for improvements of dOS algorithms. Parallel dOS algorithms with an emphasis on the handling of large molecular line databases are thus an important problem in computational stellar atmospheres. These algorithms have to be portable and should perform well for different types of parallel machines, from cheap PC clusters using Ethernet links to high performance parallel supercomputers. This goal is extremely hard to attain on all these different systems, and we, therefore, consider two different parallel dOS algorithms in this paper and compare their performance on two very different parallel machines. In the next sections we will discuss the direct opacity sampling method, describe the parallel algorithms in detail and then discuss the results of test calculations. We close with a summary and conclusions.

2. Parallel Algorithms

2.1. Global iteration scheme

A simplified flow diagram of PHOENIX is shown in figure 1. As the first step in our outermost iteration loop (the “model iteration”) we use the current best guess of \( \{T, n_i\} \) as function of radius to solve the hydrostatic or hydrodynamic equations to calculate an improved run of \( P_{\text{gas}} \) with radius. Simultaneously, the population numbers are updated to account for changes in \( P_{\text{gas}} \). The next major step is the computation of the radiation field for each wavelength point (the “wavelength loop”), which has the prerequisite of a spectral line selection procedure for LTE background lines (see below). Immediately after the radiation field at any given wavelength is known, the radiative rates and the rate operators are updated so that their calculation is finished after the last wavelength point. In the next steps, the population numbers are updated by solving the rate equations for each NLTE species and new electron densities are computed, this gives improved estimates for \( \{n_i\} \). The last part of the model iteration is the temperature correction scheme outlined above (using opacity averages, etc. that were computed in the wavelength loop) which delivers an improved temperature structure. If the errors in the constraint equations are larger than a prescribed accuracy, the improved \( \{T, n_i\} \) are used in another model iteration. Using this scheme, about 10–20 model iterations are typically required to reach convergence to better than about 1% relative errors, depending on the quality of the initial guess of the independent variables and the complexity of the model. A fully converged solution simultaneously balances the blocks shown in Figure 2. Solving the set of coupled non-linear statistical equations for large numbers of NLTE species requires large amounts of memory to store the rates for each level in all the model atoms at each radial grid point, and large amounts of CPU time because many wavelength points are required in order to resolve the line profiles in the co-moving frame. In order to minimize both CPU and memory
Figure 1. Relation between (some of) the physical and mathematical blocks that describe the physics of a stellar atmosphere. In order to calculate a model atmosphere, a set of value of the physical variables, e.g., temperatures, densities, population densities and the radiation field, must be found that satisfies all constraints simultaneously.
- **RTE**: Radiative Transfer Equation
- **RE**: Radiative Equilibrium
- **EOS**: (generalized) Equation Of State
- **RatEq**: Rate Equations
- **Rates**: radiative & collisional rates

Figure 2. Relations between the main types of variables represented by blocks are indicated. The labels name the equations that relate the block to each other.

requirements we have parallelized the separate Fortran 90 modules which make up the PHOENIX code. Our experience indicates that only the simultaneous use of data and task parallelism can deliver reasonable parallel speedups (Hauschildt, Baron, & Allard, 1997). This involves:

1. The radiative transfer calculation itself, where we divide up the characteristic rays among nodes and use a “reduce” operation to collect and send the $J_\nu$ to all the radiative transfer and NLTE rate computation tasks (data parallelism);

2. The line opacity which requires the calculation of up to 50,000 Voigt profiles per wavelength point at each radial grid point, here we split the work amongst the processors both by radial grid points and by dividing up the individual lines to be calculated among the processors (combined data and task parallelism); and

3. The NLTE calculations. The NLTE calculations involve three separate parts: the calculation of the NLTE opacities, the calculation of the rates at each wavelength point, and the solution of the NLTE rate and statistical equilibrium equations. To prevent communication overhead, each task
computing the NLTE rates is forced to be on the same node with the corresponding task computing NLTE opacities and emissivities, (combined data and task parallelism). The solution of the rate equations parallelizes trivially with the use of a diagonal approximate rate operator.

In addition to the combined data and task parallelism discussed above, PHOENIX also uses simultaneous explicit task parallelism by allocating different tasks (e.g., atomic line opacity, molecular line opacity, radiative transfer) to different nodes. This can result in further speed-up and better scalability but requires a careful analysis of the workload between different tasks (the workload is also a function of wavelength, e.g., the different number of lines that overlap at each wavelength point) to obtain optimal load balancing.

2.2. Wavelength Parallelization

The parallelization of the computational workload outlined in the previous paragraphs requires synchronization between the radiative transfer tasks and the NLTE tasks, since the radiation field and the $\Lambda^*$ (for details see Baron & Hauschildt, 1998) operator must be passed between them. In addition, our standard model calculations use 50 radial grid points and as the number of nodes increases, so too does the communication and loop overhead, therefore, pure data parallelism does not deliver good scalability. We found good speedup up to about 5 nodes for a typical calculation, with the speedup close to the theoretical maximum. However, for 5 nodes the communication and loop overheads begin to become significant and it is not economical to use more than 10 nodes (depending on the machine and the model calculation, it might be necessary to use more nodes to fit the data in the memory available on a single node).

Since the number of wavelength points in a calculation is very large and the CPU time scales linearly with the number of wavelength points, parallelization with respect to the wavelength points can lead to large speedups and to the ability to use very large numbers of nodes available on massively parallel supercomputers. This poses no difficulties for static configuration, but the coupling of the wavelengths points in expanding atmospheres makes the wavelength parallelization much more complex.

We have developed a wavelength parallelization based on a toroidal topology that uses the concept of wavelength “clusters” to distribute a set of wavelength points (for the solution of the wavelength dependent radiative transfer) onto a different set of nodes, see Fig. 3 (Baron & Hauschildt, 1998). In order to achieve optimal load balance and, more importantly, in order to minimize the memory requirements, each cluster (a column of nodes indicated in Fig. 3) works on a single wavelength point at any given time. Each cluster can consist of a number of “worker” nodes where the worker node group uses parallelization methods discussed above (see also Hauschildt, Baron, & Allard, 1997). In order to avoid communication overhead, we use symmetric wavelength clusters: each “row” of worker nodes in Fig. 3 performs identical tasks but on a different set of wavelength points for each cluster. We thus arrange the total number of nodes $N$ in a rectangular matrix with $n$ columns and $m$ rows, where $n$ is the number of clusters and $m$ is the number of workers for each cluster, such that $N = n \times m$. Another way of visualizing this parallelization technique is to consider each wavelength cluster as a single entity (although not a single node or
Figure 3. The basic “torus” design of the wavelength-parallelized version of \texttt{PHOENIX}: groups of processors are divided up into wavelength clusters which will work on individual wavelength points, each wavelength cluster is further divided into a set of worker nodes, where each worker node is assigned a set of specific tasks, e.g., it will work on the LTE background line opacity for a set of radial points. Our design requires that each worker node on all wavelength clusters work on exactly the same set of tasks, although additional inherently serial operations can be assigned to one particular master worker, or master wavelength cluster. This reduces communication between clusters to its absolute minimum and allows the maximum speedup.

CPU) that performs a variety of different tasks at each wavelength point. The entity (cluster) itself is then further subdivided into individual nodes or CPUs each of which perform a given set of tasks \textit{at a particular wavelength point}. This topology can be implemented very efficiently in the context of the \texttt{MPI} library, see Hauschildt, Baron, & Allard (1997) for details.

For a static model atmosphere, all wavelengths and thus wavelength clusters are completely independent and execute in parallel with \textit{no} immediate communication or synchronization along the rows of Fig. 3. Communication is only necessary \textit{after} the calculation is complete for all wavelengths points on all nodes to collect, e.g., the rates and rate operators. Therefore, the speedup is close (80\%) to the theoretical maximum, limited only by to combined IO bandwidth of the machine used.

In order to parallelize the spectrum calculations for a model atmosphere with a \textit{global velocity field}, such as the expanding atmospheres of novae, supernovae or stellar winds, we need to take the mathematical character of the RTE into account. For monotonic velocity fields, the RTE is an initial value problem in wavelength (with the initial condition at the smallest wavelength for expanding atmospheres and at the largest wavelength for contracting atmospheres). This initial value problem must be discretized fully implicitly to ensure stability. In the simplest case of a first order discretization, the solution of the RTE for wavelength point $i$ depends only on the results of the point $i-1$. In order to parallelize the spectrum calculations, the wavelength cluster $n_i$ computing the solution for wavelength point $i$ must know the specific intensities from the cluster $n_{i-1}$ computing the solution for point $i-1$. This suggests a “pipeline” solution to the wavelength parallelization, transforming the “matrix” arrangement of nodes into a “torus” arrangement where data are sent along the torus’ circumference. Note that only the solution of the RTE is affected by this, the calculation of the opacities and rates remains independent between different wavelength clusters. In this case, the wavelength parallelization works as follows: Each cluster can
independently compute the opacities and start the RT calculations (e.g., the $\Lambda^*$ calculations, hereafter called the pre-processing phase), it then waits until it receives the specific intensities for the previous wavelength point, then it finishes the solution of the RTE and immediately sends the results to the wavelength cluster calculating the next wavelength point (to minimize waiting time, this is done with non-blocking send/receives), then proceeds to calculate the rates etc. (hereafter called the post-processing phase) and the new opacities for its next wavelength point and so on.

The important point in this scheme is that each wavelength cluster can execute the post-processing phase of its current wavelength point and pre-processing phase of its next wavelength point independently and in parallel with all other clusters. This means that the majority of the total computational work can be done in parallel, leading to a substantial reduction in wall-clock time per model. Ideal load balancing can be obtained by dynamically allocating wavelength points to wavelength clusters. This requires only primitive logic with no measurable overhead, however it requires also communication and an arbitration/synchronization process to avoid deadlocks. Typically, the number of clusters $n$ (4-64) is much smaller than the number of wavelength points, $n_{wl} \approx 300,000$, so that at any given time the work required for each wavelength point is roughly the same for each cluster (the work changes as the number of overlapping lines changes, for example). Therefore, a simple round robin allocation of wavelength points to clusters (cluster $i$ calculates wavelength points $i$, $n + i$, $2n + i$ and so on) can be used which will result in nearly optimal performance if the condition $n \ll n_{wl}$ is fulfilled. However, once the pipeline is full, adding further wavelength clusters cannot decrease the time required for the calculations, setting a limit for the efficient “radius” of the torus topology. However, this limit can be increased somewhat by increasing the number of worker nodes per wavelength cluster.

Scaling Results For a simple supernova test calculation, we examine both the scaling and performance tradeoff of spatial versus wavelength parallelization in Figure 4. It shows the results of our timing tests for one iteration of a Type Ic supernova model atmosphere, with a model temperature $T_{\text{eff}} = 12,000$ K (the observed luminosity is given by $L = 4\pi R^2 T_{\text{eff}}^4$), characteristic velocity $v_0 = 10000$ km s$^{-1}$, 4666 NLTE levels, 163812 NLTE lines, 211680 LTE lines (for simplicity, all line profile were assumed to be Gaussian), non-homogeneous abundances, and 260630 wavelength points. This is a typical test for production calculations and we have designed this test to have the highest potential for synchronization, I/O waiting, and swapping to reduce performance to simulate a worst case scenario for the parallel performance. It is however, characteristic of the level of detail needed to accurately model supernovae. This calculation has also been designed to barely fit into the memory of a single node. The behavior of the speedup is very similar to the results obtained for test case using a model of a nova explosion Baron & Hauschildt (1998). The “saturation point” at which the wavelength pipeline fills and no further speedup can be obtained if more wavelength clusters are used for the machines used here, occurs at about 5 to 8 clusters. More clusters will not lead to larger speedups, as expected. Larger speedups can be obtained by using more worker nodes per cluster, which also drastically reduces the amount of memory required on each node.
Figure 4. Scalability of the Supernova model atmosphere test run as function of the number of nodes (processing elements or nodes) used. The y-axis gives the speedup obtained relative to the serial run. The different symbols show the results for different numbers of worker tasks for each wavelength cluster.

2.3. Parallel Direct Opacity Sampling

There are a number of methods in use to calculate line opacities. The classical methods are statistical and construct tables that are subsequently used in the calculation. The Opacity Distribution Function (ODF) and its derivative the k-coefficient method have been used successfully in a number of atmosphere and opacity table codes (e.g., Kurucz, 1992). This method works well for opacity table and model construction but cannot be used to calculate detailed synthetic spectra. A second approach is the opacity sampling (OS) method (e.g., Peytremann, 1974). This is a statistical approach in which the line opacity is sampled on a fine grid of wavelength points using detailed line profiles for each individual spectral line. In classical OS implementation, tables of sampling opacities are constructed for given wavelengths grids and for different elements. These OS tables are then used to calculate model atmospheres and, e.g., Rosseland mean opacities. The OS method has the advantage that is more flexible than the ODF approach and it also allows the construction of (typically) low resolution synthetic spectra. The drawback of tables in general is, however, an inherent inflexibility in terms of, e.g., the wavelength grid or the tables’s resolution. For example, to properly account for the pressure broadening of lines an opacity sampling table would have to be a function of temperature and gas pressure,
which leads to very large tables if many wavelength points are tabulated (this is not a problem for ODF tables as the number of wavelength bins in such models is typically very small). In addition, a different code is typically required to calculate high-resolution spectra from the model atmosphere constructed with the ODF or OS tables, which has the potential of introducing systematic errors (e.g., if the atmosphere/table and the synthetic spectrum codes are not synchronized).

In direct opacity sampling (dOS) these problems are avoided by replacing the tables with a direct calculation of the total line opacity at each wavelength point for all layers in a model atmosphere (e.g., Hauschildt & Baron, 1999). In the dOS method the relevant lines (defined by a suitable criterion) are first selected from master spectral line databases which include all available lines. The line selection procedure will typically select more lines than can be stored in memory and thus temporary line database files are created during the line selection phase. The file size of the temporary database can vary, in theory, from zero to the size of the original database or larger, depending on the amount of data stored for the selected lines and their number. For large molecular line databases this can easily lead to temporary databases of several GB in size. This is in part due the storage for the temporary line database: its data are stored for quick retrieval rather than in the compressed space saving format of the master line databases. The number and identity of lines that are selected from the master databases depends on the physical conditions for which the line opacities are required (temperatures, pressures, abundances for a model atmosphere) and thus the line selection has to be repeated if the physical conditions change significantly. As an optimization, it is easily possible to include only lines in the temporary database that can be “seen” by the wavelength grid that will be used in the calculation of the line opacities later on. This is important if, for example, only a narrow range in wavelength is considered at high resolution in order to generate a synthetic spectrum.

The temporary line databases are used in the next phase to calculate the actual line opacity for each wavelength point in a prescribed (arbitrary) wavelength grid. This makes it possible to utilize detailed line profiles for each considered spectral line on arbitrary wavelength grids. For each wavelength grid point, all (selected) lines within prescribed search windows (large enough to include all possibly important lines but small enough to avoid unnecessary calculations) are included in the line opacity calculations for this wavelength point. This procedure is thus very flexible, it can be used to calculate line opacities for both model atmosphere construction (with relatively few wavelength points) and for the generation of high-resolution synthetic spectra. Its main drawback is that the line selection and (in particular) line profile calculations are more costly than table interpolations.

There are currently a large number of significantly different types of parallel machines in use, ranging from clusters of workstations or PCs to teraflop parallel supercomputers. These systems have very different performance characteristics that need to be considered in parallel algorithm design. For the following discussion we assume this abstract picture of a general parallel machine: The parallel system consists of a number of processing elements (PEs), each of which is capable of executing the required parallel codes or sections of parallel code. Each PE has access to (local) memory and is able to communicate data with other PEs.
through a communication device. The PEs have access to both local and global filesystems for data storage. The local filesystem is private to each PE (and inaccessible to other PEs), and the global filesystem can be accessed by any PE. A PE can be a completely independent computer such as a PC or workstation (with single CPU, memory, and disk), or it can be a part of a shared memory multi-processor system. For the purposes of this paper, we assume that the parallel machine has both global and local logical filesystem storage available (possibly on the same physical device). The communication device could be realized, for example, by standard Ethernet, shared memory, or a special-purpose high speed communication network.

In the following description of the 2 algorithms that we consider here we will make use of the following features of the line databases:

- master line databases:
  1. are globally accessible to all PEs
  2. are sorted in wavelength
  3. can be accessed randomly in blocks of prescribed size (number of lines)

- selected line (temporary) databases:
  1. the wavelength grid is known during line selection (not absolutely required but helpful)
  2. have to be sorted in wavelength
  3. can be accessed randomly in blocks of prescribed fixed size (number of lines)
  4. are stored either globally (one database for all PEs) or locally (one for each PE)
  5. are larger than the physical memory of the PEs

**Global Temporary Files (GTF)** The first algorithm we describe relies on global temporary databases for the selected lines. This is the algorithm that was implemented in the versions of PHOENIX discussed in Hauschildt, Baron, & Allard (1997) and Baron & Hauschildt (1998). In the general case of $N$ available PE’s, the parallel line selection algorithm uses one PE dedicated to I/O and $(N-1)$ line selection PEs. The I/O PE receives data for the selected lines from the line selection PEs, assembles them into properly sorted blocks of selected lines, and writes them into the temporary database for later retrieval. The $(N-1)$ line selection PEs each read one block from a set of $(N-1)$ adjacent blocks of line data from the master database, select the relevant lines, and send the necessary data to the I/O PE. Each line selection PE will select a different number of lines, so the I/O PE has to perform administrative work to construct sorted blocks of selected lines that it then writes into the temporary database. The block sizes for the line selection PEs and for the temporary database created by the I/O PE do not have to be equal, but can be chosen for convenience. The blocks of the master line database are distributed to the $(N-1)$ line selection PEs in a round robin fashion. Statistically this results in a balanced load between the line selection PEs due to the physical properties of the line data.
After the line selection phase is completed, the temporary global line database is used in the line opacity calculations. If each of the \( N \) PEs is calculating line opacities (potentially for different sets of wavelengths points or for different sets of physical conditions), they all access the temporary database simultaneously, reading blocks of line data as required. In most cases of practical interest, the same block of line data will be accessed by several (all) PEs at roughly the same time. This can be advantageous or problematic, depending on the structure of the file system on which the database resides. The PEs also cache files locally (both through the operating system and in the code itself through internal buffers) to reduce explicit disk I/O. Note that during the line selection phase the temporary database is a write-only file, whereas during the opacity calculations the temporary database is strictly read-only.

The performance of the GTF algorithm depends strongly on the performance of the global file system used to store the temporary databases and on the characteristics of the individual PEs. This issue is discussed in more detail below.

**Local Temporary Files (LTF)** The second algorithm we consider in this paper uses file systems that are local to each PE; such local file systems exist on many parallel machines, including most clusters of workstations. This local disk space is frequently large enough for the temporary line database and may have high local I/O performance. In addition, I/O on the local disks of a PE does not require any inter-PE communication, whereas globally accessible filesystems often use the same communication channel that explicit inter-PE communication uses. The latter can lead to network congestion if messages are exchanged simultaneously with global I/O operations.

For the line selection, we could use the algorithm described above with the difference that the I/O PE would create a global (or local) database of selected lines. After the line selection is finished, the temporary database could then simply be distributed to all PEs, and stored on their local disk for subsequent use. However, this is likely to be slower in all cases than the GTF algorithm.

Instead, we use a “ring” algorithm that creates the local databases directly. In particular, each of the \( N \) PEs selects lines for one block from the master database (distributed in round robin fashion between the PEs). After the selection for this one block is complete, each PE sends the necessary data to its next neighbor; PE \( i \) sends its results to PE \( i + 1 \mod N \) and, simultaneously, receives data from the previous PE in the ring. Each PE stores the data it receives into a buffer and the process is repeated until all selected lines from the \( N \) blocks are buffered in all \( N \) PEs. The PEs then transfer the buffered line data into their local temporary databases. This cycle is repeated until the line selection phase is complete. The line opacity calculations will then proceed in the same way as outlined above, however, the temporary line databases are now local for each PE.

This approach has the advantage that accessing the temporary databases does not incur any (indirect) Network File System (NFS) communication between the PEs as each of them has its own copy of the database. However, during the line selection phase a much larger amount of data has to be communicated over the network between the PEs because now each of them has to “know” all selected lines, not only the I/O PE used in the first algorithm.
The key insight here is that low-cost parallel computers constructed out of commodity workstations typically have a very fast communication network (100 Mbs to 1 Gbs) but relatively slow NFS performance. This means that trading off the extra communication for fewer NFS disk accesses in the LTF algorithm is likely to give better performance.

2.4. Results

The performance of the GTF and LTF algorithms will depend strongly on the type of parallel machine used. A machine using NFS with fast local disks and communication is likely to perform better with the LTF algorithm. However, a system with fast (parallel) filesystem and fast communication can actually perform better with the GTF algorithm. In the following we will consider test cases run on very different machines:

1. A cluster of Pentium Pro 200MHz PCs with 64MB RAM, SCSI disks, 100Mbs full-duplex Ethernet communication network, running Solaris 2.5.1.

2. An IBM SP system with 200MHz Power3 CPUs, 512MB RAM per CPU, 133 MB/s switched communication network, 16 node IBM General Purpose File System (GPFS) parallel filesystem, running AIX 4.3.

We have run 2 test cases to analyze the behavior of the different algorithms on different machines. The small test case was designed to execute on the PPro system. It uses a small line database (about 550MB) with about 35 million lines of which about 7.5 million lines are selected. The second test uses an about 16 times larger line database (about 9GB) and also selects 16 times more lines. This large test could not be run on the PPro system due to file size limitations and limited available disk space. The line opacity calculations were performed for about 21,000 wavelength points that are representative for typical calculations. The tests were designed for maximum I/O usage and are thus extreme cases. In practical applications the observed scaling is comparable to or better than which found for these tests and appears to follow the results shown here rather well. In the following we will discuss the results for the tests on the different computing systems.

**PPro/Solaris system** The results for the line selection procedure on the PPro/Solaris system are shown in Fig. 5. It is apparent from the figure that the GTF approach delivers higher relative speedups that translate into smaller execution times for more than 2 PEs. For serial (1PE) and 2PE parallel runs the LTF line selection is substantially faster than the GTF algorithm. The reason for this behavior can be explained by noting that the access of the global files is done through NFS mounts that use the same network as the MPI messages. Therefore, \( n - 1 \) PEs request different data blocks from the NFS server (no process was run on the NFS server itself) and send their results to the I/O PE, which writes it out to the NFS server. In the LTF algorithm, each PE reads a different input block from the NFS server and then sends its results (around the ring) to all other PEs. Upon receiving data from its left neighbor, a PE writes it to local disk. This means that the amount of data streaming over the network can be as much as twice as high for the LTF compared to the GTF algorithm.
Figure 5. Results for the line selection process on the PPro/Solaris system. Times are given in wallclock seconds in the upper panel and as relative speedups for the lower panel.
This increases the execution time for the LTF approach if the network utilization is close to the maximum bandwidth. In this argument we have ignored the time required to write the data to local disks, which would make the situation worse for the LTF approach.

The situation is very different for the calculation of the line opacities, c.f., Fig. 6. Now the LTF approach scales well (up to the maximum of 8 available machines) whereas the GTF algorithm hardly scales to more than 2 PEs. The absolute execution times for the LTF approach are up to a factor of 4 smaller (more typical are factors around 2) than the corresponding times for the GTF algorithm (the GTF run with 8 PEs required roughly as much execution time as the LTF run with 1 PE!). The reason for this is clearly the speed advantage of the local disk I/O compared to the NFS based I/O in the GTF code. If more PEs are used in the GTF line opacity approach, the network becomes saturated quickly and the PEs have to wait for their data (the NFS server itself was not the bottleneck). The LTF approach will be limited by the fact that as the number of PEs get larger, the efficiency of disk caching is reduced and more physical I/O operations are required. Eventually this will limit the scaling as the execution time is limited by physical I/O to local disks.

**IBM SP system** We ran the same (small) test on an IBM SP for comparison. The tests were run on a non-dedicated production system and thus timings are representative of standard operation conditions and not optimum values. The global files were stored on IBM’s General Purpose File System (GPFS), which is installed on a number of system-dedicated I/O nodes replacing the NFS fileserver used on the PPro/Solaris system. GPFS access is facilitated through the same “switch” architecture that also carries MPI messages on the IBM SP. The results for the line selection code are shown in Fig. 7. For the small test the results are markedly different from the results for the PPro/Solaris system. The LTF algorithm performs significantly better for all tested configurations, however, scaling is very limited. The GTF code does not scale well at all for this small test on the IBM SP. This is due to the small size, so that the processing is so fast (nearly 100 times faster than on the PPro/Solaris system) so that, e.g., latencies and actual line selection calculations overwhelm the timing. The IBM SP has a very fast switched communications network that can easily handle the higher message traffic created by the LTF code. This explains why the LTF line selection executes faster and scales better for this small test on the IBM compared to the PPro/Solaris system.

The line opacity part of the test shown in Fig. 8 performs distinctively different in the IBM SP compared to the PPro/Solaris system (cf. Fig. 6). In contrast to the latter, the IBM SP delivers better performance for the GTF algorithm compared to the LTF code. The scaling of the GTF code is also significantly better than that of the LTF approach. This surprising result is a consequence of the high I/O bandwidth of the GPFS running on many I/O nodes, the I/O bandwidth available to GPFS is significantly higher than the bandwidth of the local disks (including all filesystem overheads etc). The I/O nodes of the GPFS can also cache blocks in their memory which can eliminate physical I/O to a disk and replace access by data exchange over the IBM “switch”. Note that the test was designed and run with parameters set to maximize actual I/O operations in order to explicitly test this property of the algorithms.
Figure 6. Results for the line opacity calculations on the PPro/Solaris system. Times are given in wallclock seconds in the upper panel and as relative speedups for the lower panel.
Figure 7. Results for the line selection process on the IBM SP system. Times are given in wallclock seconds in the upper panel and as relative speedups for the lower panel.
Figure 8. Results for the line opacity calculations on the IBM SP system. Times are given in wallclock seconds in the upper panel and as relative speedups for the lower panel.
The results of the large test case, for which the input file size is about 16 times bigger, are very different for the line selection, cf. Fig. 9. Now the GTF algorithm executes much faster (factor of 3) than the LTF code. This is probably caused by the larger I/O performance of the GPFS that can easily deliver the data to all nodes and the smaller number of messages that need to be exchanged in the GTF algorithm. The drop of performance at 32PE's in the GTF line selection run could have been caused by a temporary overload of the I/O subsystem (these tests were run on a non-dedicated machine). In contrast to the previous tests, the LTF approach does not scale in this case. This is likely caused by the large number of relatively small messages that are exchanged by the PEs (the line list master database is the same as for the GTF approach, so it is read through the GPFS as in the GTF case). This could be improved, e.g., by choosing larger block sizes for data sent via MPI messages, however, this will have the drawback of more memory usage and larger messages are more likely to block than small messages that can be stored within the communication hardware (or driver) itself.

The situation for the line opacities is shown in Fig. 10. The scaling is somewhat worse due to increased physical I/O (the temporary files are about 16 times larger as in the small test case). This is more problematic for the LTF approach which scales very poorly for larger numbers of PEs as the maximum local I/O bandwidth is reached far earlier than for the GTF approach. This is rather surprising as conventional wisdom would favor local disk I/O over global filesystem I/O on parallel machines. Although this is certainly true for farms of workstations or PCs, this is evidently not true on high-performance parallel computers with parallel I/O subsystems.

3. Discussion and Conclusions

We have presented our approach to the numerical solution to the generalized stellar atmosphere problem in the presence of rapidly expanding flows. We have shown how the use of advanced algorithms may result in the formulation of the problem in such a way that extremely detailed model atoms may be handled in NLTE and the problem can be parallelized in a way that significantly reduces the per processor memory and CPU requirements with modest communication overhead. Parallelization also allows much more complex models to be calculations by giving us access to the large memory sizes that are available on modern parallel supercomputers. Currently, our largest model calculations involve 6000 atomic NLTE level with 65000 primary NLTE lines that are modeled individually, 2-10 million weak atomic secondary NLTE and LTE background lines and, for models of cool stellar winds, 150 million molecular lines. Simulations of this size and level of detail were simply not possible before the development of new radiative transfer algorithms and the availability of parallel supercomputers. We believe that the next step — the computation of moving flows in three spatial dimensions, is becoming tractable on modern parallel supercomputers. There continues to be an urgent need for improvements in the fundamental atomic data which serves as input to these calculations.

In this paper we have discussed two algorithms for parallel spectral line selection and opacity calculations useful for direct opacity sampling models of
Figure 9. Results for the line selection process for the large test on the IBM SP system. Times are given in wallclock seconds in the upper panel and as relative speedups for the lower panel.
Figure 10. Results for the line opacity calculations for the large test on the IBM SP system. Times are given in wallclock seconds in the upper panel and as relative speedups for the lower panel.
stellar atmospheres. The GTF algorithm uses global temporary files to store the list of selected lines, whereas the LTF algorithm stores the scratch files on local disks. These two methods show very different performance characteristics on different parallel systems. On a PC cluster, each processing element (PE) being a PC with its own local disk space and operating system networked with standard IP based Ethernet, the LTF algorithm has disadvantages in the line selection procedure for larger numbers of PEs (≥ 4), probably due to the higher demand put on the communication between nodes using the MPI library, but is slightly faster than the GTF approach if the number of PEs is smaller. However the LTF code produces far faster and better scaling line opacity calculations, which will be the more costly part of a typical atmosphere model run (the line selection is usually required only once at the beginning of a model calculation).

On the common IBM SP parallel supercomputers the situation changes significantly. On this machine, the small test runs so fast that the timing is dominated by side effects. In the large test case, the GTF line selection performs and scales far better than the LTF code. This surprising result is caused by the presence of a parallel filesystem (GPFS) on the IBM that dramatically improves performance of global I/O compared to local disk I/O. The GPFS also boosts the performance for the GTF code for the (in practical applications more important) line opacity calculations, for both the small and the large test cases.

Variations of the algorithms can be constructed, e.g., it is possible to store the master line database on each PE individually and thus totally remove global I/O to a single master line list (this requires enough local disk space to store both the master and temporary databases). Other improvements are possible, e.g., optimization of the I/O blocksize for each type of machine. However, these optimizations are system dependent (and also depend on the load of the machine in general) and thus are not discussed here.

The algorithms and the results show that parallel computing can lead to dramatic speed improvements in stellar atmosphere calculations but also that different algorithms are required for different types and capabilities of parallel machines. The speed improvements can then be used to develop physically more complex and detailed models (e.g., including massive NLTE calculationsconstan and line blanketing, models for M dwarfs with possibly billions of molecular spectra lines or detailed models for stellar winds and for hot stars with radiative levitiation modeling including a large number of elements and ionization stages). This approach sends us one step further to a better physical understanding of stars and their spectra.

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REFERENCES

Hauschildt, P. H. 1992, JQSRT, 47, 433
Hauschildt, P. H. 1993, JQSRT, 50, 301