OPserver: interactive online-computations of opacities and radiative accelerations

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ABSTRACT
Codes to compute mean opacities and radiative accelerations for arbitrary chemical mixtures using the Opacity Project recently revised data have been restructured in a client–server architecture and transcribed as a subroutine library. This implementation increases efficiency in stellar modelling where element stratification due to diffusion processes is depth dependent, and thus requires repeated fast opacity reestimates. Three user modes are provided to fit different computing environments, namely a web browser, a local workstation and a distributed grid.

Key words: atomic processes – radiative transfer – stars: interior.

1 INTRODUCTION
Astrophysical opacities from the Opacity Project (OP) have been updated by Badnell et al. (2005) to include inner-shell contributions and an improved frequency mesh. The complete data set of monochromatic opacities and a suite of codes to compute mean opacities and radiative accelerations (OPCD2.1)1 have also been publicly released by Seaton (2005) to make in-house calculations for arbitrary mixtures more versatile and expedient. Regarding data accuracy, there is excellent overall agreement between the OPAL (Iglesias & Rogers 1996) and OP results as discussed by Seaton & Badnell (2004), Badnell et al. (2003) and Delahaye & Pinsonneault (2003).

Rosseland mean opacities are sensitive to both the basic atomic data used and the assumed abundances of the chemical elements. What had been a good agreement between theory and the helioseismological data was found to be less good using revised solar abundances from Asplund et al. (2005). The revised OP opacities have been instrumental in discussions of that problem (Antia & Basu 2005; Bahcall et al. 2005b; Delahaye & Pinsonneault 2006).

The modelling of stellar interiors, on the other hand, is being renewed with the solar experience. Present (WIRE, MOST, CoRoT) and future (Kepler) space probes and the well established solar methods are giving the field of asteroseismology remarkable growth and the guarantee of invaluable data (Metcalfe et al. 2004; Kurtz 2005; Christensen-Dalsgaard 2006). In future work on stellar models it may be desirable to take account of revisions in abundances similar to those performed for the Sun.

For some types of stars, models must take into account microscopic diffusion processes, e.g. radiative levitation, gravitational settling and thermal diffusion, as they can affect the internal and thermal structures, the depth of the convection zone, pulsations and give rise to surface abundance anomalies (Seaton 1999; Delahaye & Pinsonneault 2006).
We highlight here some of the key features of the codes in OPCD, thus the use of codes more efficient than those in OPCD of the model and at each time step of the evolution, and radiative accelerations must be repeated at each depth point depends on stellar depth, calculations of mean opacities and validity of this approximation is discussed by Gonzalez et al. (2003).

The OPCD release includes data and codes to compute the radiative accelerations required for studies of diffusion processes. It should be noted that the radiative accelerations are summed over ionization stages and that data for the calculation of diffusion coefficients are calculated assuming that the distribution over ionization stages of the diffusing ions is the same as that in the ambient plasma. The validity of this approximation is discussed by Gonzalez et al. (1995).

In some cases, particularly when element stratification depends on stellar depth, calculations of mean opacities and radiative accelerations must be repeated at each depth point of the model and at each time step of the evolution, and thus the use of codes more efficient than those in OPCD may be necessary. This becomes critical in the new distributed computing grid environments where the network transfer of large volumes of data is a key issue. In the present work we have looked into these problems, and, as a solution, report on the implementation of a general purpose, interactive server for astrophysical opacities referred to as OPserver. It has been installed at the Ohio Supercomputer Center, Columbus, Ohio, USA, from where it can be accessed through a web page or a linkable subroutine library. It can also be downloaded locally to be run on a stand-alone basis but it will demand greater computational facilities. In Section 2 we discuss the computational strategy of the codes in OPCD followed by a description of OPserver in Section 3. In Section 4 we include some tests as an indication of its performance with a final summary in Section 5.

2 OPCD CODES

We highlight here some of the key features of the codes in OPCD. For a chemical mixture specified by abundance fractions \( f_k \), they essentially compute two types of data: Rosseland mean opacities (RMO) and radiative accelerations (RA).

2.1 Rosseland mean opacities

For the frequency variable

\[
u = h\nu/k_B T \quad \text{(1)}
\]

where \( k_B \) is the Boltzmann constant, RMO are given by the harmonic mean of the opacity cross section \( \sigma(u) \) of the mixture

\[
\frac{1}{\sigma_R} = \mu \int_0^{\infty} \frac{1}{\sigma(u)} \, dv \quad \text{(2)}
\]

where \( \mu \) is the mean atomic weight. The \( \sigma(u) \) is a weighted sum of the monochromatic opacity cross sections for each of the chemical constituents

\[
\sigma(u) = \sum_k f_k \sigma_k(u) \quad \text{(3)}
\]

and is conveniently tabulated on the \( v \)-mesh

\[
v(u) = \int_0^u \frac{F(u)}{1 - \exp(-u)} \, du \quad \text{(4)}
\]

where

\[
F(u) = \frac{15u^4 \exp(-u)}{4\pi^4 [1 - \exp(-u)]^2} \quad \text{(5)}
\]

and \( v_\infty = v(u \to \infty) \). The rationale behind the \( v \)-mesh is that it enhances frequency resolution where \( F(u) \) is large (Badnell et al. 2003).

2.2 Radiative accelerations

Similarly, the RA for a selected \( k \) element can be expressed as

\[
g_{\text{rad}} = \frac{\mu k_R \gamma_k}{c \mu_k} \mathcal{F} \quad \text{(6)}
\]

where \( \mu_k \) is its atomic weight and \( c \) the speed of light. The function \( \mathcal{F} \) is given in terms of the effective temperature \( T_{\text{eff}} \) and fractional depth \( r/R_* \) of the star by

\[
\mathcal{F} = \pi B(T_{\text{eff}})(R_*/r)^2 \quad \text{(7)}
\]

with

\[
B(T) = \frac{2(\pi k_B T)^4}{15\pi^2 h^3} \quad \text{(8)}
\]

The dimensionless parameter

\[
\gamma_k = \int \frac{\sigma_k^{\text{nl}}}{\sigma} \, dv \quad \text{(9)}
\]

depends on the cross section for momentum transfer to the \( k \) element

\[
\sigma_k^{\text{nl}} = \sigma_k(u)[1 - \exp(-u)] - a_k(u) \quad \text{(10)}
\]

where \( a_k(u) \) is a correction to remove the contributions of electron scattering and momentum transfer to the electrons. Both \( \sigma_k(u) \) and \( a_k(u) \), which are hereafter referred to as the mono data set (\( \sim 1 \) GB), are tabulated in equally spaced \( v \) intervals to facilitate accurate interpolation schemes.

2.3 Computational strategy

The computational strategy adopted in the OPCD release is depicted in the flowcharts of Figure 1 where it may be seen that calculations of RMO and RA are carried in two stages. In a time consuming Stage 1, RMO and RA are computed with the mixv and accv codes, respectively, on a representative tabulation of the complete temperature-electron-density \( (T, N_e) \) plane. In mixv the chemical mixture is specified in the input file mixv.in as

\[
\{X, Z, N, Z_k, f_k\} \quad \text{(11)}
\]
Figure 1. Flowcharts for the computations of Roseland mean opacities (RMO) and radiative accelerations (RA) with the codes in the OPCD2.1 release. They are carried out in two stages: in a time consuming Stage 1, data are computed for the whole \((T,N_e)\) plane followed by fast bicubic interpolations in Stage 2. The intermediate files \textit{mixv.xx} and \textit{acc.xx} enable communication between these two steps.

where \(X\) and \(Z\) are the hydrogen and metal mass-fractions, \(N\) the number of elements, and \(Z_i\) and \(f_k\) are the metal nuclear charges and fractional abundances. In \textit{accv}, the input data (\textit{accv.in}) are

\[
\{N, Z, f_k, Z_i, N_k, \chi_j\}
\]

(12)

where now \(k\) runs over the \(N\) elements of the mixture, and \(Z_i\) and \(\chi_j\) are respectively the nuclear charge and \(N_k\) abundance multipliers of the test \(i\) element. Input data formats in either \textit{mixv.in} or \textit{accv.in} give the user flexible control over chemical mixture specifications.

As shown in Figure 1, the intermediate output files \textit{mixv.xx} (~85 KB) containing

\[
\{\rho, \kappa_R\}(T, N_e),
\]

(13)

where \(\rho\) is the mass-density, and \textit{acc.xx} (~470 KB) with

\[
\left\{\kappa_R, \frac{\partial \kappa_R}{\partial X}, \gamma, \frac{\partial \gamma}{\partial X}\right\}(T, N_e, \chi_j)
\]

(14)

are written to disk. They are then respectively read by the codes \textit{opfit} and \textit{accfit} in Stage 2 for fast bicubic interpolations of RMO and RA on stellar depth profiles \(\{T, \rho, \tau/R\}\) specified by the user in the \textit{opfit.in} and \textit{accfit.in} input files. The final output files are \textit{opfit.xx} containing

\[
\left\{\log \kappa_R, \frac{\partial \log \kappa_R}{\partial \log T}, \frac{\partial \log \kappa_R}{\partial \log \rho}\right\}(i)
\]

(15)

and \textit{accfit.xx} with

\[
\{\log \kappa_R, \log \gamma, \log g_{\text{rad}}\}(i, \chi_j).
\]

(16)

In this computational approach, performance is mainly limited by the summation in equation (3) which implies disk reading the \textit{mono} data set; for instance, in \textit{mixv} it takes up to \(\sim 90\%\) of the total elapsed time. OPCD2.1 also includes other codes such as \textit{mx} and \textit{ax} which respectively compute RMO and RA for a star depth profile. The chemical mixture can be fully varied at each depth point using the specifications in equations (i)–(ii), the RMO and RA being obtained in a one-step process using bicubic interpolations without splines. These methods are thus suitable for cases with multi-mixture depth profiles \cite{seaton2003}. Further details of all the OPCD codes are contained in the reference manual\cite{http://opalities.osc.edu/publi/OPCD.pdf}.

3 OPserver

In OPserver the computational capabilities of the codes in OPCD2.1 are greatly enhanced by the following innovative adaptations.

(i) The codes are restructured within a client–server network architecture whereby the time consuming Stage 1 is performed on a powerful processor while the fast Stage 2 is moved to the client, e.g. a web server or a user workstation. In this arrangement performance could be affected by the client–server transfer of the \textit{mixv.xx} and \textit{acc.xx} intermediate files, but since they are never larger than 0.5 MB, it is not expected to be a deterrent with present-day bandwidths. In a local installation where both the client and server reside on the same machine, communication is managed through shared buffers in main memory; i.e. the corresponding data in \textit{mixv.xx} and \textit{acc.xx} are not written to disk.

(ii) The codes are transcribed as a subroutine library—to be referred to hereafter as the OPlibrary—which can be linked by the user stellar modelling code for recurrent subroutine calls that avoid data writing on disk. That is, the input data in the \textit{mixv.in}, \textit{accv.in}, \textit{opfit.in} and \textit{accfit.in} files and the output tables in the \textit{opfit.xx} and \textit{accfit.xx} files (see Figure 1) are now handled as subroutine parameters while the intermediate \textit{mixv.xx} and \textit{acc.xx} files are passed via shared main-memory buffers. Chemical mixtures are again specified with the formats of equations (11–12) which allow full variation at each depth point in a single subroutine call.

(iii) RMO/RA are computed with the complete \textit{mono} data set always loaded in main memory thus avoiding lengthy and repeated disk readings. This is achieved by implementing OPserver on a dedicated server where \textit{mono} is permanently resident in RAM, or in the case of a local installation, by disk-reading it once at the outset of a modelling calculation.

(iv) When accessing the remote server, client data requests are addressed through the HTTP protocol, i.e. in terms of a Uniform Resource Locator (URL). This allows data fetching from the central facility through an interactive web page or a network access subroutine, the latter being particularly suitable for a stellar model code that is to be run in a distributed grid environment.

(v) The \textit{do-loop} that computes the summation of equation (3) has been parallelized in OpenMP which provides a simple, scalable and portable scheme for shared-memory platforms.

As shown in Figure 2, the current OPserver enterprise is implemented as a client–server model at the Ohio Supercomputer Center (OSC). The web server communicates with the supercomputer via a socket interface. Earlier versions were developed on an SGI Origin2000 server with the PowerFortran parallelizing compiler. The current version runs on a Linux system with Fortran OpenMP directives. OPserver offers three user modes with full functionality except when otherwise indicated in the following description.

Mode A In this mode OPserver is set up locally on a stand-alone basis (see Figure 2). The facilities of the OSC are
The OPlibrary and monochromatic opacities (mono) are downloaded locally and linked to the user modelling code such that RMO/RA are computed locally. (B) The OPlibrary is downloaded locally and linked to the modelling code but RMO/RA are computed remotely at the OSC. (C) RMO/RA computations at the OSC through a web client.

4 TESTS

OPserver benchmarks were initially carried out on an SGI Origin2000 multiprocessor at the OSC with an earlier release of OPCD. For the standard S92 mixture (Seaton et al. 1994), the mixv code took up to 140 s to compute the mixv.xx file, of which 126 s were dedicated to disk-reading and 14 s to the actual computing of the mean opacities. OPserver took on average 12.0 ± 0.5 s to compute mixv.xx which was not written to disk unless requested. In Figure 3 we show the acceleration obtained on the Origin2000 through parallelization where the computation of mean opacities is reduced to 2 s with 8 processors. Further significant acceleration is prevented by data transfer overheads.

On more recent workstations, the local performances of the codes in OPCD allow both Stage 1 and Stage 2 to be carried out remotely or, alternatively, Stage 2 locally by downloading the mixv.xx/accv.xx intermediate files (see Figure 1) with the browser for further processing with local opfit/accfit executables.

5 SUMMARY

Rosseland mean opacities and radiative accelerations can be computed from OP data in any one of the following ways.

(i) Download the original OPCD_2.1 package as described by Seaton (2005) and perform all calculations locally.

(ii) Mode A, download the upgraded OPCD_3.3 package, install OPserver and perform all calculations locally by linking the subroutines in the OPlibrary. Calculations with OPserver are more efficient but require large local computer memory.

(iii) Mode B, as Mode A but with Stage 1 performed remotely at the OSC. Mode B is convenient if fast calculations are required but local computer memory is limited or when stellar modelling is to be carried out in a grid environment.

(iv) Mode C, perform all calculations remotely at the OSC through an interactive web page whereby files are downloaded locally with the browser.

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Figure 3. Average elapsed time for the computation of RMO (Stage 1) in OPserver as a function of the number of processors on a SGI Origin2000 showing the acceleration obtained through parallelism. The corresponding time taken by the mixv code for this calculation is 140 s where 126 s are taken by data reading from disk.

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