

Three-dimensional simulations of the upper radiation–convection transition layer in subgiant stars

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ABSTRACT

This paper describes three-dimensional (3D) large eddy simulations of stellar surface convection using realistic model physics. The simulations include the present Sun, a subgiant of one solar mass and a lower-gravity subgiant, also of one solar mass. We examine the thermal structure (superadiabaticity) after modification by 3D turbulence, the overshoot of convective motions into the radiative atmosphere and the range of convection cell sizes. Differences between models based on the mixing length theory (MLT) and the simulations are found to increase significantly in the more evolved stages as the surface gravity decreases. We find that the full width at half maximum (FWHM) of the turbulent vertical velocity correlation provides a good objective measure of the vertical size of the convective cells. Just below the convection surface, the FWHM is close to the mean vertical size of the granules and $2 \times \text{FWHM}$ is close to the mean horizontal diameter of the granules. For the Sun, $2 \times \text{FWHM} = 1200$ km, a value close to the observed mean granule size. For all the simulations, the mean horizontal diameter is close to 10 times the pressure scaleheight at the photospheric surface, in agreement with previous work.

Key words: methods: numerical – stars: atmospheres – stars: interiors.

1 INTRODUCTION

Present-day computers are just about powerful enough to do three-dimensional (3D) simulations of solar convection that employ realistic model physics (Stein & Nordlund 2000). Provided the layer is not too deep (say approximately eight pressure scaleheights in total), the system can be relaxed adequately and an accurate statistical analysis can be performed (Robinson et al. 2003, hereafter denoted ROB3). Although there are two-dimensional (2D) realistic simulations covering a wide range of stellar objects (Freytag, Ludwig & Steffen 1996; Ludwig, Freytag & Steffen 1999), because of the roughly two orders of magnitude increase in the total number of grid points, 3D simulations are still computationally fairly expensive. Consequently, most 3D simulations of realistic convection have been restricted to the Sun (for example, Nordlund 1982; Stein & Nordlund 1998 and references therein) for which we have observations of photospheric granule size and high quality seismic data. As an exception, there is a recent 3D simulation of a late M-dwarf by Ludwig, Allard & Hauschildt (2002). There was also

a series of reasonably realistic 3D simulations of stellar objects in the vicinity of the Sun in the HR diagram by Nordlund & Dravins (1990).

There are many reasons for performing detailed 3D simulations of the outer layers of cool stars with convection zones. The transition from efficient convective transport in the deep envelope into the radiative atmospheric layers takes place in a transition layer of inefficient convection where the temperature gradient is highly superadiabatic, and the poorly known structure of which remains one of the major uncertainties in stellar models. In one-dimensional (1D) stellar models, this region determines the outer boundary condition of the model. This is usually performed using the mixing length theory (MLT) which, given the mixing length, fixes the specific entropy in the deep convection zone, which in turn determines the radius of the model. The model radius thus depends sensitively on the uncertain choice of the mixing length. Physically realistic simulations would remove the mixing length uncertainty.

It is well known that the non-radial p -mode frequencies observed in the Sun and Sun-like stars, are sensitively affected by the speed of sound near the surface. Helioseismology indicates that the mixing length theory is inadequate to model this region (Guenther 1991). The realistic description of convection including the interaction with

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Table 1. Characteristics of the 3D simulations.

Model	Age (Gyr)	$\log T_{\text{eff}}$	$\log g$	Size (Mm)	Grid
S	4.55	3.761	4.44	$5.4^2 \times 2.8$	$114^2 \times 170$
SG1	11.3	3.704	3.75	$13.6^2 \times 9$	$58^2 \times 120$
SG2	11.6	3.698	3.37	$46^2 \times 23$	$58^2 \times 140$

radiative transfer greatly improves the agreement with observation (Rosenthal et al. 1999; ROB3) in the case of the Sun. The recently launched MOST space mission (Matthews et al. 2000) and the missions COROT (Baglin et al. 2002) and Eddington (Favata, Roxburgh & Christensen-Dalsgaard 2000) planned for the next few years, will require convection modelling of the same sophistication for Sun-like stars.

In addition to modifying the p -mode frequencies, the highly superadiabatic layer (SAL) region is responsible for the excitation of the acoustic oscillations. 3D simulations provide the means of calculating the driving of the p -modes due to stochastic excitation (Nordlund & Stein 2001; Stein & Nordlund 2001; Samadi et al. 2003). Radiative hydrodynamic simulations in 3D also yield detailed information concerning the sizes and shapes of convective cells in stars (Kim 1993). These in turn affect the strengths and profiles of absorption lines. Since both the spectral continuum and absorption-line strengths are the result of the density stratification and of the motions in the atmosphere, the determination of abundances and other physical conditions can also be affected (Dravins & Nordlund 1990a,b; Asplund et al. 2000; Steffen & Holweger 2002).

This paper describes physically realistic convection in the Sun and at two points along its future evolutionary track. The three models considered are the present Sun (S), an 11.3-Gyr subgiant (SG1) and an 11.6-Gyr subgiant (SG2). Table 1 shows the position of each model in the $\log g$ – $\log T_{\text{eff}}$ plane. The Sun expands as it evolves off the main sequence into the subgiant region. The surface gravity, which is inversely proportional to the radius squared, drops by a factor of 5 between model S and SG1 and a factor of 2 between SG1 and SG2. The surface flux drops by approximately a factor of 1.7 between S and SG1 and is almost the same in SG1 and SG2. The thickness of the convection zones and the geometric depth of the SAL near the top of the convection zone, are much larger in the subgiants than in the Sun.

This paper concentrates on the following three features of the simulations that cannot be measured in 1D stellar models that use the MLT.

(i) The thermal structure of the outer layers, particularly of the SAL, after modification by 3D turbulence. The entropy jump in the SAL determines the specific entropy in the deep convection zone, which is nearly isentropic. The convection zone specific entropy in turn determines the radius of the stellar model. The thermal structure of this region also strongly affects the frequencies of the non-radial acoustic oscillations (p -modes, Rosenthal et al. 1999).

(ii) The extent of convective overshoot above the formal top boundary of convection. By modifying the atmospheric structure, convective overshoot also affects p -mode frequencies and the continuous and absorption-line spectra (Dravins & Nordlund 1990a,b; Kim & Chan 1998; Demarque, Guenther & Kim 1999; Asplund et al. 2000; Steffen & Holweger 2002).

(iii) The variation of the convection cell sizes in the highly stratified layer. The cell size variation differs from the standard predictions of the MLT.

2 MODELLING REALISTIC SOLAR SURFACE CONVECTION

The governing equations and numerical methods are identical to those used in the simulations of the Sun described in ROB3. Our approach to modelling surface layer convection can be summarized as follows.

(i) Using the stellar evolution code YREC (see, e.g., Guenther et al. 1992), we compute a standard 1D stellar model from which the initial density ρ and internal energy e , required by the 3D simulations, are derived. From an arbitrary initial velocity field $\mathbf{v}$, we then compute ρ , $E (=1/2 \rho v^2 + e)$, ρv_x , ρv_y and ρv_z . These are the dependent variables of the governing equations. The horizontal directions are x and y and z is radially outwards. The 3D simulation is in a Cartesian geometry.

(ii) Using the same tables for the equation of state and the opacities as in the stellar model, we then compute the pressure $P(\rho, e)$, temperature $T(\rho, e)$, Rosseland mean opacity $\kappa(\rho, e)$, specific heat capacity at constant pressure $c_p(\rho, e)$, logarithmic adiabatic gradient $\nabla_{\text{ad}}(\rho, e)$ and some thermodynamic derivatives.

(iii) The radiation flux is then computed using the diffusion approximation in the optically thick regions and the 3D Eddington approximation (Unno & Spiegel 1966) in the optically thin layers. This formulation assumes a grey atmosphere.

(iv) We then integrate the Navier–Stokes equations over one time-step to compute a new set of dependent variables and return to (ii).

Each 3D model can be characterized by its surface gravity, effective temperature and chemical composition. We obtain the surface gravity and stellar flux (which is close to σT_{eff}^4 , where σ is the Stefan–Boltzmann constant) of each star from the 1D stellar evolution model, and then put the values in the 3D code by hand. Full details of the starting model is given in Section 3.1. The equation of state, opacity tables and the Prandtl number (ratio of kinematic viscosity to thermal diffusivity), are the same as used in the simulation of the Sun in ROB3. The initial stratification (run of pressure, temperature, density and internal energy) will depend on the particular model.

2.1 Boundary conditions and thermal relaxation

The convection domain is a box with periodic side walls and impenetrable top and bottom surfaces. A constant energy flux is fed into the base and a conducting top boundary is used. As the stellar flux is computed from the 1D stellar model it is not arbitrary, but is the correct amount of energy flux the computational domain should transport outwards in a particular star.

Although a box with a conducting top boundary condition may take longer to relax than a box with a constant flux at the top, the statistics may be more reliable (Chan 2003). To obtain a thermally relaxed system in a reasonable amount of computer time, we used an implicit numerical scheme, ADISM (alternating direction implicit on a staggered mesh) developed by Chan & Wolff (1982). Our procedure is to compute a model that is deep enough so that there is only a very small feedback of kinetic energy into the system by fluid hitting the base, and shallow enough so that the drop of the vertical velocity at the top is due to convection–radiation losses and the reduction in the buoyancy force in the subadiabatic region, rather than the impenetrable top horizontal boundary itself. The former is confirmed by the smallness of upturn of the horizontal Mach number squared at the base, while the latter is confirmed by running an identical simulation with a slightly damped

horizontal velocity at the top. If the top boundary is far enough out, the ‘damped simulation’ should have almost the same thermal structure and rms vertical velocity as the simulation with an ‘undamped’ stress free top. In other words, if the boundary is far enough up, then the damping should have a minimal effect on the statistics of the flow. The importance of this test was demonstrated in ROB3.

This part of the simulation only requires a small aspect ratio, most often 0.75 and a horizontal grid of 30×30 , with say 140 uniformly spaced vertical grid points. We focused on getting the correct vertical structure before worrying about the domain width. After the narrow column of convecting fluid is relaxed, the layer is periodically extended. To ensure that the box is wide enough, the aspect ratio should be increased until a further increase produces a minimal change in the rms velocities or in the size of the granules. Once a big enough box is found, the convection simulation is run using the ADISM code until it has reached a statistically steady state. One way of checking this is to compare the influx and outflux near the top of the box. They should be within 5 per cent of each other. We also checked that the maximum velocity in the box had reached a statistically steady state.

2.2 Statistical analysis

The relaxed layer is then restarted with a second-order accurate explicit code (Adams–Bashforth time integration). The explicit time-step is approximately five times smaller than the implicit time-step, while an individual integration step takes approximately half the time. Quantities were averaged over a time that was long enough for the averages to be independent of the integration time. Note that prior to statistical averaging, the code is run for a few thousand time-steps. This allows the simulation to adjust to the new time-step and ensure that the influx and outflux are within 1 per cent of each other before computing any statistics. For the Sun model, the statistical convergence took more than an hour of solar surface convection time.

2.3 Statistical definitions

In a turbulent fluid, a quantity q can be split into a mean and a fluctuating part,

$$q = \bar{q}(z) + q'(x, y, z, t). \quad (1)$$

The overbar represents a combined horizontal and temporal average, i.e.

$$\bar{q}(z) = \frac{1}{t_2 - t_1} \int_{t_1}^{t_2} \left(\frac{1}{L_x L_y} \int q \, dx \, dy \right) dt. \quad (2)$$

t_1 is a time after the system has reached a self-consistent thermal equilibrium (the thermal adjustment time). L_x and L_y are the horizontal widths of the box in the x and y direction, respectively. The time required for statistical convergence is $t_2 - t_1$.

The rms value of a quantity q is defined as

$$q'' = \sqrt{\overline{q'^2}}, \quad (3)$$

while the correlation coefficient of two quantities q_1 and q_2 , is defined as

$$C[q'_1 q'_2] = \frac{\overline{q'_1 q'_2} - \bar{q}_1 \bar{q}_2}{q''_1 q''_2}. \quad (4)$$

With periodic side boundaries, isotropy in the large scales means that

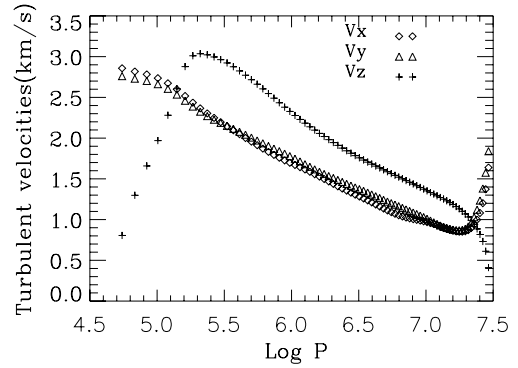


Figure 1. Turbulent velocities in the horizontal and the vertical directions versus depth.

- (i) $C[v'_x v'_y] = 0$,
- (ii) $v''_x = v''_y$.

Generally, second-order quantities such as $C[v'_z v'_z]$ take considerably longer to converge than first-order quantities such as the superadiabaticity, $\nabla - \nabla_{\text{ad}}$. The run of turbulent velocities of a Sun model averaged over 80 min of solar convection time are shown in Fig. 1. By computing the run of both $C[v'_x v'_y]$ and the rms horizontal velocities over different averaging times, we found that $C[v'_x v'_y]$ was close to zero when the rms horizontal velocities (which are also second-order quantities) were almost equal. Even though these two quantities may appear to have converged it does not mean that other second-order quantities have. For each statistical quantity presented in this paper, convergence was thoroughly checked by confirming that averaging over a longer time did not change the result.

3 RESULTS

3.1 Starting models

The 3D simulations described in this paper are for the Sun (S), a subgiant (SG1) of one solar mass and a more evolved subgiant (SG2) also of one solar mass. The 1D solar model used as the initial model for S is a calibrated solar model evolved from the zero-age main sequence (ZAMS). The evolutionary track was then extended beyond the main-sequence turn-off into the subgiant region to obtain initial models for the 3D simulations SG1 and SG2. Some details of the three models are given in Table 1. The surface gravity and effective temperature are in c.g.s. units. Note that between S and SG1 the surface gravity and the effective temperature both change significantly, while between SG1 and SG2 by far the most significant change is in the surface gravity.

The initial 1D solar model for S is a calibrated standard solar model which includes the effects of helium and heavy element diffusion. It is constructed with the semi-empirical Krishna Swamy (1966) $T(\tau)$ relation for the solar atmosphere and uses the MLT in the convective outer layers (Guenther & Demarque 1997; Winnick et al. 2002). Under these assumptions, if the initial solar metallicity $Z_0 = 0.019$ and the age of the Sun is set at 4.55 Gyr, the MLT parameter $\alpha = 1.988$. Note that the radius of a solar model depends sensitively on both the $T(\tau)$ relation in the radiative atmosphere and on the choice of α . The use of the Eddington approximation $T(\tau)$ relation would require $\alpha = 1.678$.

We point out that an evolutionary track for the Sun constructed under the standard assumptions (MLT with constant solar calibrated α), would not pass precisely through the positions in the log g –log

T_{eff} plane adopted for SG1 and SG2. This is because the original models for SG1 and SG2, which were constructed using the standard MLT assumptions, did not provide sufficiently good starting conditions for the 3D simulations, and the simulation failed to evolve towards a statistically stationary state. To overcome this problem, improved 1D starting models for the two subgiant models were then constructed which partially included the effects of turbulence in their outer layers. This was performed using the turbulence parametrization for a 1D stellar model, of the 3D simulation of the Sun by ROB3 due to Li et al. (2002). For a Krishna–Swamy $T(\tau)$ atmosphere, Li et al.’s improved solar models require $\alpha = 2.132$. This value of α was adopted for the SG1 and SG2 starting models. These revisions, due to the effects of turbulent pressure and turbulent kinetic energy, result in a small shift in $\log T_{\text{eff}}$ and $\log g$ for SG1 and SG2 away from the original evolutionary track.

Given the initial solar metallicity Z_0 , the ZAMS hydrogen content X_0 is set by the constraint of the solar calibration described above. We note here that the surface chemical composition changes slightly during evolution. In the Sun (model S), because of diffusion, helium and heavy element abundances are depleted with respect to the ZAMS chemical composition, and $(X, Z) = (0.742\ 39, 0.017\ 069)$. As the evolution proceeds beyond the present Sun, past the main-sequence turn-off and into the subgiant phase, the radius increases and the convection zone deepens, resulting in the dredge-up to the surface of helium and heavy elements that had previously diffused below the convection zone. In the cases of SG1, the chemical composition has changed to $(X, Z) = (0.719\ 338, 0.018\ 38)$. In the more evolved SG2, we have $(X, Z) = (0.713\ 01, 0.018\ 63)$. The effect of these differences in chemical composition are felt on the equation of state (in the H and He ionization zones) and on the opacities (primarily sensitive to Z), but it is relatively minor in the present simulations.

3.2 Box dimensions

The horizontal dimensions of each computational box (column 5 in Table 1) were estimated by assuming that the granule size will scale roughly inversely with g . In ROB3, it was found by trial and error that a width of 2.7 Mm produced nearly the same results as a box of 5.4 Mm in the Sun simulation. As g is approximately five times smaller in the subgiant SG1, the computational box should be at least 13.5 Mm wide. Similarly, model SG2 should be at least 33 Mm wide. The vertical extent of each model is chosen to minimize the effect of the top and bottom boundaries on the interior flow. This test is described in Section 2.1. The final column gives the number of grid points in the two horizontal and vertical directions in the square based box.

Fig. 2 shows contour plots of the instantaneous vertical velocity for the Sun and the 11.3-Gyr subgiant, SG1. The contours are in a horizontal plane near the visible surface. The thick black lines represent the strong downflows which occur at the sides of the granules. The lighter regions denote upflowing fluid or weak downflows. In each case a few granules can be seen to fill the boxes. The boundaries of the granules do not seem influenced much by the sides of the box.

3.3 Superadiabaticity in the simulations and the MLT

Figs 3–5 show the superadiabaticity versus fractional radius for MLT (solid) and simulation (dot-dash), for the present Sun (S), the subgiant (SG1) and the more evolved subgiant (SG2), respectively. The fractional radius is defined as R/R_{model} , where R_{model} is the location

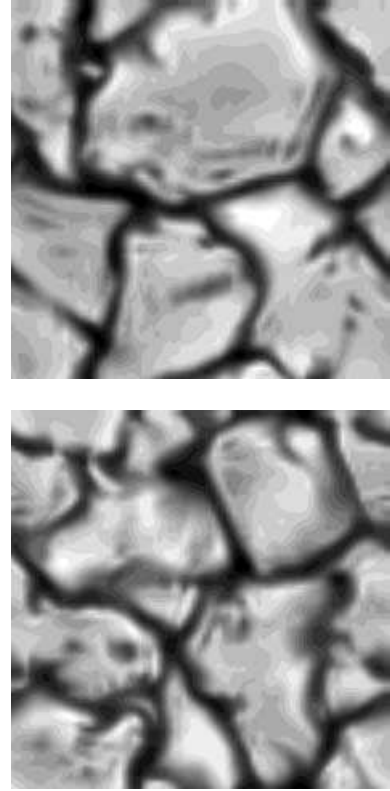


Figure 2. Contours of the vertical velocity near the visible surface for the Sun (upper frame) and the subgiant (lower frame). The dark lines represent strong downflows and the bright regions are upflows. The dimensions of the frames are 3.75×3.75 Mm for the Sun and 13.6×13.6 Mm for the subgiant.

of the visible surface (where $T = T_{\text{eff}}$) in each MLT stellar model. The value of R_{model} is given in terms of $R_{\odot}$ in the second column of Table 2. The individual grid points in the simulations are marked by crosses to show that the SAL is well resolved in each simulation. The vertical lines mark the photospheric (visible) surface in the MLT (solid) and the simulation (dot-dash). The photospheric surface is defined as the point at which the temperature equals the effective temperature. For a 3D simulation this is where the horizontally and temporally averaged temperature equals the effective temperature of the 1D model.

The most obvious effect of turbulence is to push the convection surface outwards from its original position, which had been determined using the MLT. The three figures show that as the Sun evolves, this effect is greatly enhanced. The convective surface, as defined by the Schwarzschild criterion ($\nabla - \nabla_{\text{ad}} = 0$), is moved out from its MLT position by 70, 400 and 1300 km in S, SG1 and SG2, respectively. The photospheric surface is moved out by a similar amount. Rosenthal et al. (1999) found an elevation of the iso-pressure layers in the photosphere of 150 km for the Sun. Their measurement was made by comparing a $100^2 \times 82$ model on a domain of $6 \times 6 \times 3.4$ Mm, with an MLT model. The difference between their result and ours may be due to the different vertical resolutions. For the Sun we also computed the elevation for an 80^3 model on a domain of $4 \times 4 \times 2.5$ Mm. We found that the $\log P = 5$ surface was shifted by approximately 135 km. In that model the SAL peak was slightly higher and the turbulent pressure peak slightly lower, than in our $117^2 \times 170$ model presented in this paper. In fact, the peak values of turbulent pressure and $\nabla - \nabla_{\text{ad}}$ in Rosenthal et al. were

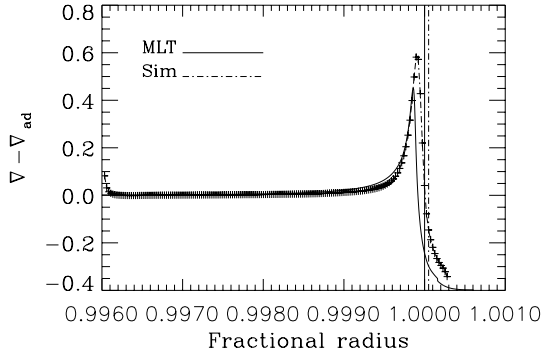


Figure 3. Superadiabaticity versus fractional radius for the Sun (S). For each model, the MLT is denoted by the solid line and the simulation is marked by the dashed line. The vertical grid points in the simulation have been marked individually to show that the SAL was well resolved. The vertical lines show the position of the photospheric surface.

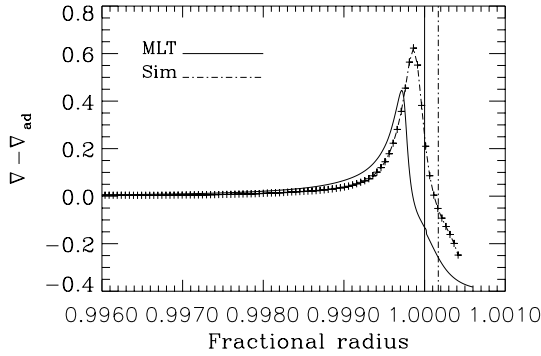


Figure 4. Superadiabaticity versus fractional radius for the subgiant (SG1).

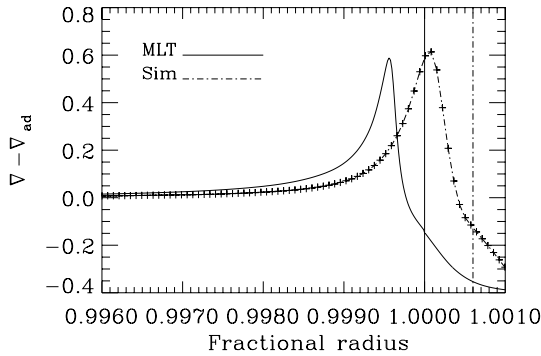


Figure 5. Superadiabaticity versus fractional radius for the more evolved subgiant (SG2).

closer to those found in our 80^3 simulation, rather than our $117^2 \times 170$ simulation. This suggests that the magnitude of the temperature fluctuations (which depend on the peak value of $\nabla - \nabla_{\text{ad}}$) and the turbulent pressure, play an important role in the elevation of the photosphere.

The turbulent pressure $\bar{\rho} v_z'^2$ divided by the gas pressure is plotted for the three models in Fig. 6. Note that the turbulent pressure was also computed as $\bar{\rho} v_z'^2$. We found little difference between the two measurements. The maximum turbulent pressure is approximately 15 per cent in S, 16 per cent in SG1 and over 20 per cent in SG2. The increase in the peak value occurs primarily because the gas

Table 2. The displacement of the convective surface $\delta(\nabla - \nabla_{\text{ad}})$ and the extent of overshoot above the convective surface δ_{OS} . H_p is the pressure scaleheight at the convective boundary.

Model	$R_{\text{model}}/R_{\odot}$	$\delta(\nabla - \nabla_{\text{ad}})$ (km)	δ_{OS} (km)	δ_{OS}/H_p
S	1.0	70	60	0.5
SG1	2.198	400	400	0.75
SG2	6.347	1300	1500	1.0

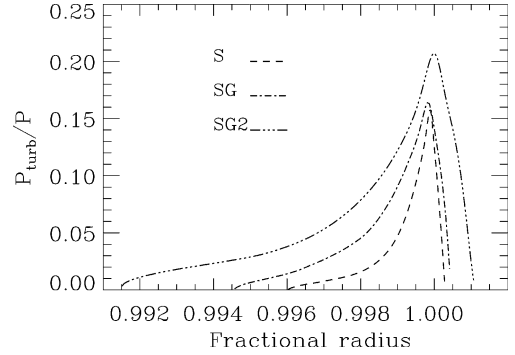


Figure 6. Ratio of turbulent pressure to gas pressure for S, SG1 and SG2, marked by dashes, dot-dashes and triple-dotted-dashes, respectively.

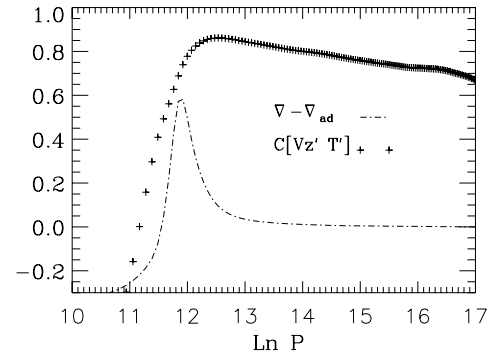


Figure 7. Normalized correlation of the vertical velocity with temperature (see the text) in the Sun. The size of $C[v'_z T']$ is used to estimate the overshoot of turbulent fluid into the stable radiative region. To pinpoint the convection surface (where $\nabla - \nabla_{\text{ad}} = 0$) in the 3D simulation, the superadiabaticity is also plotted. The convectively stable region lies above the depth at which $\nabla - \nabla_{\text{ad}} = 0$. The overshoot is approximately half the local pressure scaleheight.

density in the SAL region is lower in the more evolved models. The convective velocities are actually not much different.

3.4 Overshoot

In the MLT, the convective velocity is set to zero in the subadiabatic (radiative) region. In reality, convective motions overshoot into the stable region. This process is more correctly modelled by 3D simulations.

To estimate the amount of overshoot we plotted $C[v'_z T']$ and $\nabla - \nabla_{\text{ad}}$ versus $\ln P$ for the three models in Figs 7–9. For a mass element, if $C[v'_z T']$ is positive then either v_z and T both exceed their surrounding values or are both less than their surrounding values. In either case it is buoyancy that is accelerating the mass element.

The overshoot distance, defined here as the distance between the depths at which $\nabla - \nabla_{\text{ad}} = 0$ and $C[v'_z T'] = 0$, increases from

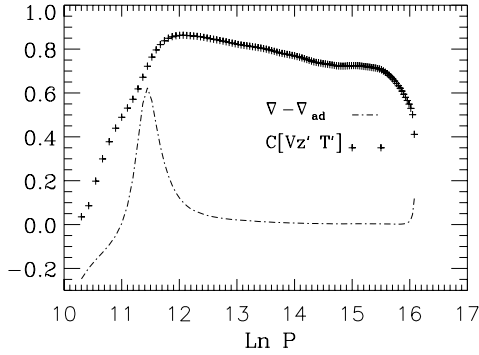


Figure 8. The same quantities as in the previous figure for the subgiant (SG1). The overshoot is approximately 0.75 of the local pressure scaleheight.

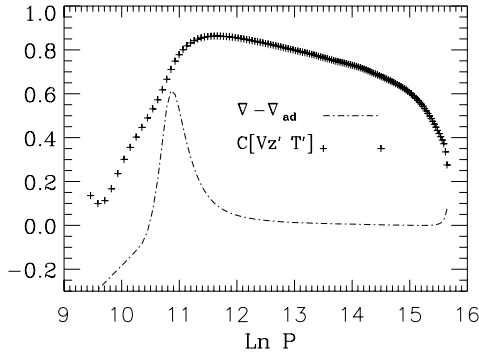


Figure 9. The same quantities as in the previous figure for the more evolved subgiant (SG2). The overshoot is approximately equal to the local pressure scaleheight.

model S to model SG2. For Models S, SG1 and SG2, the distance is 60 km, 400 km and 1500 km, respectively. These distances are very close to the size of the displacement of the SAL from the MLT position by turbulence (as described in the previous section). This is probably because turbulent convective motions (v_z'') are responsible in both cases. This shows that the simulation results are consistent. By comparing the enthalpy flux to the total flux in the subadiabatic region, we find that regardless of how large $C[v_z', T']$ is, in each model the overshooting fluid carries only approximately 1 per cent of the total flux. In the subadiabatic region radiation transports nearly all the energy flux. It seems that the inefficient convective motions carry momentum (via the transport of temperature fluctuations which makes mass elements positively buoyant) rather than heat into the stable (radiative) region. This type of overshoot is similar to that described by Zahn (1991). The overshoot distances represent approximately 0.5, 0.75 and 1.0 local pressure scaleheight for the model S, SG1 and SG2, respectively. The results for overshoot δ_{OS} and the displacement of the SAL δ ($\nabla - \nabla_{ad}$) are summarized in Table 2.

3.5 Vertical size of convective cells

In the convection zones of cool stars, thermodynamical properties can vary over many orders of magnitude. For example the convection zone in the present Sun contains more than 20 pressure scaleheights. It is customary to use the MLT to describe convection in standard stellar structure calculations. The mixing length is then thought of as the distance travelled by a fluid parcel before it mixes with the environment (or equivalently loses its thermal or dynamical identity).

The most common way to evaluate the mixing length is to assume that it is equal to some constant α , of the order of unity, multiplied by the local pressure scaleheight $H_p = P/\rho g$.

In this paper, we will interpret the characteristic vertical length of a convection cell in the 3D simulation as the mixing length. We expect this estimate of the mixing length to vary with depth as in the MLT, but with a different depth dependence.

The 3D simulation provides a natural objective measure of the mixing length. We estimate the characteristic vertical length-scale of a convective cell by measuring the full width at half maximum (FWHM) of the vertical velocity correlation $C[v_z' v_z']$. From that perspective it might seem equally plausible to use the FWHM of entropy or temperature fluctuations. However, as shown for the Sun in fig. 11 of ROB3, the FWHM of entropy is not well defined just below the top of the SAL. Neither is it for temperature. This is because near the convection surface, the upflows lose entropy much faster than the downflows, so that the plot of the FWHM is not symmetric. So while we could use the FWHM of $C[S' S']$ or $C[T' T']$ to estimate the mixing length for deeper convection, it does not give a well-defined vertical length-scale near the top of the SAL.

As $C[v_z' v_z']$ is a second-order turbulent quantity, the statistical convergence is very long. For example, for the Sun at least 100 solar min (20 turnover times) were covered before $C[v_z' v_z']$ had come close to convergence. The plot of the mixing length versus depth (both in Mm) for the Sun, estimated as FWHM, is shown by crosses in Fig. 10. The depth of 0 Mm corresponds to the point at which $R = R_\odot$. In the 1D MLT model this corresponds to the visible surface (photosphere). In the 3D simulation of the Sun, as can be seen in Fig. 3, the convective surface moves out to a point very close to $R_\odot$. This is not true for the other models. The upper convective boundary in the 3D simulation of the Sun is within 0.02 Mm of $R_\odot$. Each cross represents the value of the FWHM at a particular depth. From 0 to 0.75 Mm below the surface, this mixing length is close to 0.6 Mm. This includes the SAL region. Below approximately 0.8 Mm the slope increases sharply and is constant until approximately 1.5 Mm below the surface. The change in the slope near the top (at approximately 0.2 Mm) and near the bottom (at approximately 1.5 Mm) are a consequence of the impenetrable boundaries of the simulations. In the Sun, the cells near the top have a characteristic vertical length of approximately 0.45 Mm (the smallest mixing length in the plot) and thus the effect of the top boundary (which is at -0.25 Mm) is felt at approximately 0.45 Mm below the top of

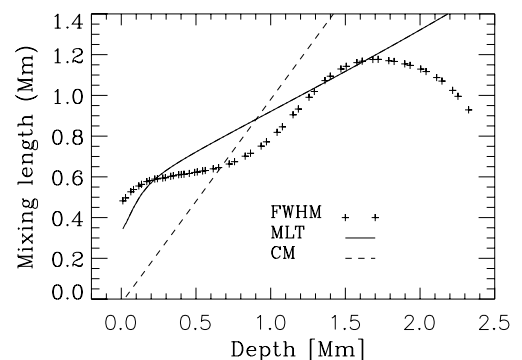


Figure 10. Different prescriptions for the mixing length in a model of the Sun. The value of FWHM from the simulation, $\alpha_\odot \times H_p$ and the distance to the convection surface, are denoted by crosses, solid line and dashed line, respectively. The depth was measured positively inward from the visible stellar surface.

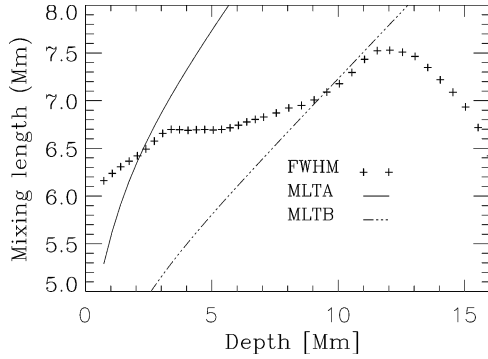


Figure 11. Estimates of the mixing length for the more evolved subgiant. The value of FWHM from the simulation, $\alpha_{\odot} H_p$ (called MLTA) and αH_p (called MLTB, where $\alpha = 1.6$) are denoted by crosses, solid and triple-dotted-dash lines, respectively. The depth was measured positively inward from the visible stellar surface.

the box. Similarly the influence of the bottom of the box on the flow is felt at approximately 1 Mm above the base.

Two alternative prescriptions for the mixing length are commonly used in stellar models. As mentioned above, the most common prescription is to use the product αH_p , where α is the constant mixing length parameter. For the Sun, $\alpha_{\odot} = 2.13$ in the present study. The other prescription is the geometric distance to the convective boundary, as suggested by Canuto & Mazzitelli (1991, hereafter CM), by analogy with laboratory experiments. The convective boundary is defined at the depth of 0.02 Mm in the Sun model. For comparison, these two estimates are given in Fig. 10 as well. The plots show that in the SAL region, the mixing length derived from the FWHM does not generally have the same physical length in stellar models as that based on the MLT or CM values, while outside of the SAL, the FWHM is similar to the MLT prescription.

The departure from the MLT near the surface becomes more pronounced in the subgiant models. Fig. 11 displays the quantities FWHM (crosses) and $\alpha_{\odot} H_p$ (solid line) for the more evolved subgiant SG2. The convective cells show a much more gradual increase with depth in the simulation. In fact, neither MLT prescription works at all. If a smaller α is used (triple-dotted-dash line) in this case $\alpha = 1.6$, the MLT prescription is still very different from the simulation.

In the SG2 case the FWHM values form a plateau between depths of approximately 3 and 6 Mm. The plateau starts further in because the convective cells are much larger in the more evolved subgiant. This means that the effect of the impenetrable boundary on the cell is felt much further in from the top. If we assume that the cells near the top have a characteristic vertical length of approximately 6 Mm, within 6 Mm of the top boundary (which is at -2.6 Mm) the elongation of the cell will be decreased because it impinges with the top impenetrable boundary. This is probably why the curve starts to flatten at a depth of approximately 3 Mm. The value of the FWHM at the plateau is approximately 6.7 Mm.

4 ESTIMATING THE MEAN HORIZONTAL DIAMETER OF GRANULES IN DIFFERENT STARS

The scale of photospheric convection in red giants is generally associated, by analogy with the Sun, with the atmospheric pressure scaleheight or with the thickness of the superadiabatic transition layer (SAL). As pointed out by Schwarzschild (1975), both of these quantities are relatively much larger in terms of the stellar radius in

a red giant than in the Sun. On these grounds, Schwarzschild concluded that only a few tens of cells must be present on the surface of a supergiant down to just a few cells in the most extreme cases such as Betelgeuse, in contrast with 2×10^6 cells observed on the solar surface. Observations of brightness variations in the TiO band on Betelgeuse (Gaustad 1986) and direct imaging of Betelgeuse (Gilliland & Dupree 1996) with the *Hubble Space Telescope (HST)* have yielded results that are compatible with giant cells, although other interpretations (e.g. pulsation) are possible. 3D numerical simulations described in Freytag, Steffen & Dorch (2002), also claim compatibility with the giant cell interpretation, although the smaller cell sizes cannot be resolved in these simulations. On the other hand, Gray (2001) has pointed out that his extensive spectroscopic observations of Betelgeuse are more easily interpreted in terms of hundreds of convective cells per hemisphere.

In this section we will show that our 3D radiative–hydrodynamical simulations suggest granules closer to Gray’s interpretation than to Schwarzschild’s estimate. Rather than use the pressure scaleheight or the thickness of the SAL to estimate the convective cell size, we will use the FWHM of the vertical velocity to estimate a vertical length-scale for the granules. In the preceding section, a plateau in the FWHM graph was pointed out in Figs 10 and 11. By measuring the value of the FWHM at the plateau for the three simulations (S, SG1 and SG2), we found that

$$\text{FWHM} \propto g^{-0.9858}, \quad (5)$$

where the FWHM and g are both in c.g.s. units.

In Gadun et al. (2000), the horizontal diameter of the solar granules was shown to be proportional to the horizontal velocity. Larger granules had bigger horizontal velocities. As the FWHM only tells us about the vertical scale of the convective cells, to find the mean horizontal diameter of a granule we need an estimate of the aspect ratio of a typical granule.

Consider a granule as a cylinder in which fluid rises up along the central axis of the cylinder (representing the centre of a granule) and the down along the outside of the cylinder. Fig. 2 would represent a cross-section of such a cylinder for the Sun or the subgiant. In ROB3, fig. 8 shows a granule with this type of structure. With this picture in mind, the rms horizontal velocity $V_H = \sqrt{v_x'^2 + v_y'^2}$ approximates the velocity across the top of the cylinder and $v_z = v_z'$ approximates the velocity down the sides.

For the Sun, SG1 and SG2, the ratio of V_H to v_z is shown in Fig. 12. Away from the top and bottom, the ratio is approximately unity. The abrupt rise in V_H/v_z shown on the right of the figure is due to the lower impenetrable boundary. At the base the vertical velocity is set to zero, but that boundary is stress free. As v_z' is very small near

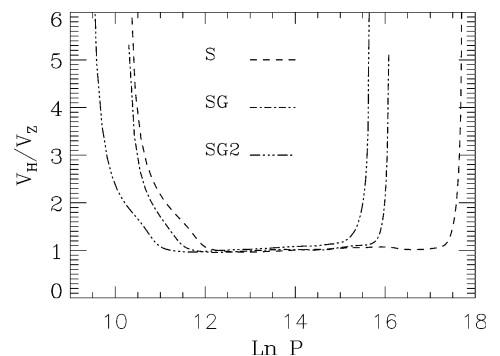


Figure 12. Ratio of the rms horizontal to the rms vertical velocity for each model.

the base, even though the horizontal velocities are small, the ratio must increase significantly as the lower boundary is approached. Moving the lower boundary further down will not eliminate this effect. In the upper regions (the left-hand side of the figure) the vertical velocities decay more gently. The slower decay is because there is a radiation layer in the top part of each simulation. The initial drop in the vertical velocity (and therefore rise in the ratio) is due to radiative losses. The point at which the ratio first starts to increase is close to the location of the maximum superadiabaticity (see Figs 7–9). Above that location, the superadiabaticity decreases. Very close to the top, the ratio shoots up again. This is because the vertical velocity is forced to vanish at the top.

If we assume it takes the fluid a similar amount of time to travel horizontally from the centre of a granule to the outside rim as it does to travel down the outside of the granule, then

$$\frac{r_{\text{gran}}}{\text{FWHM}} \approx \frac{V_H}{V_Z} \approx 1, \quad (6)$$

where r_{gran} is the radius and the FWHM is the length of the hypothetical ‘cylindrical’ granule. This suggests that the average horizontal diameter of granules in each simulation is approximately twice the FWHM.

This is a statistical estimate of the horizontal diameter of a granule. Some granules will be bigger and some smaller. For example, at the instant of time the contours of Fig. 2 were plotted for the Sun, the biggest granule has a diameter of approximately 2 Mm, while the smallest (on the right near the top of the frame) has a diameter of approximately 1 Mm. For the Sun, $2 \times \text{FWHM} = 1.2$ Mm. This is similar to the observed value of approximately 1 Mm, quoted by Allen (Cox 1999).

Schwarzschild (1975) suggested that the aspect ratio of the granules should be approximately 3 and that the vertical size of the granules can be estimated from the width of the SAL. Alternatively, Freytag (2001) points out, on the basis of 2D numerical simulations, that the horizontal diameter is close to 10 times the pressure scaleheight at the photospheric surface. We summarize the horizontal diameters of granules for the different methods in Table 3. The width of the SAL is estimated as the distance between the two points at which the superadiabaticity is 10 per cent of its peak value. The pressure scaleheight H_p at the photospheric surface in the 3D simulation is measured at the point at which $\bar{T} = T_{\text{eff}}$, where T_{eff} is the effective temperature in the corresponding 1D MLT model. The Freytag estimate is very close to ours.

By extrapolating to lower surface gravities, we can very tentatively estimate how big the granules might be for giants, or supergiants. Assuming that $\log g = -0.5$ on Betelgeuse, and that the radius is approximately 800 times the solar radius (Gray 2000), we estimate approximately 600 cells would be needed to cover the whole surface. This extrapolation to Betelgeuse is a very tentative estimate. As well as bridging approximately four orders of magnitude in surface gravity, we have ignored any sphericity effects or variation of g with depth. These would be considerable in a supergiant. Furthermore, Freytag’s relation to the scaleheight allows an a

priori estimate, while our FWHM relation only allows an a posteriori check.

5 CONCLUSION

We have carried out physically realistic 3D simulations for the Sun (S) and two subgiants (SG1 and SG2) representing more evolved stages of the evolution of the Sun. The initial conditions for the simulations were obtained from 1D standard stellar models constructed with the same physical input for the equation of state and opacities as used in the simulations. Convection in the starting model was described using the standard MLT (Böhm-Vitense 1958). The chemical composition and mixing length parameter α were calibrated to the Sun in the standard way (Guenther & Demarque 1997; Winnick et al. 2002).

After relaxation, and given the chemical composition, the 3D simulations reach a steady state which depends only on the input flux at the base of the box and the surface gravity. The memory of any other detail of the 1D initial models, including the uncertainty connected with the value of the parameter α , has been erased.

The rapid expansion of the Sun after leaving the main sequence, has two principal consequences. First, the density/pressure/temperature stratification is spread out over a much bigger geometric distance in the subgiant phase. While the flux in SG1 is approximately half that of the present Sun, the surface gravity is five times smaller. The only significant difference between SG1 and SG2 is in the surface gravity. This means that the transition region from deep convection to the atmosphere (the SAL), of a subgiant occurs in a region of lower gas density compared with the present Sun. As the SAL is a region of highly turbulent dynamics, the effect of turbulent velocities on the local thermal structure will be much more significant in the more evolved models (i.e. the turbulent Mach number v''/c_s is larger). Secondly, as the surface gravity decreases, the convective cells become much larger.

Our 3D simulations shed new light on three important aspects of stellar convection: the effects of turbulence on the thermal structure, the importance of convective overshoot into the radiative atmosphere, and the characteristics of granulation.

(i) Thermal structure and turbulent pressure. The main result is that the thermal structure in the 3D simulations differ increasingly from the predictions of the mixing length theory as the Sun evolves away from the main sequence, and the use of the solar calibrated mixing length ratio becomes progressively worse. As noted by Freytag & Salaris (1999), the structure of the SAL is not adequately reproduced even if a different α is used. Rather, the 3D simulations are the only way to obtain a realistic physical description of the SAL. Note that the SAL is itself a thin transition layer and that for many purposes the details of its structure are of little consequence to stellar evolution. It is the integral properties of the SAL (the entropy jump) that really matter. While the actual SAL thickness has only a very small influence on the stellar radius by itself, the integrated entropy jump determines the specific entropy in the deep convection zone and thus affects the stellar radius sensitively.

A fixed α is inappropriate for modelling the surface layers, because the size of the convective cells is not linearly proportional to any scaleheight (see Fig. 10). This was already apparent in the earlier simulations of Kim et al. (1996). It is also seen in Fig. 10 that using the distance to the surface as the mixing length, as performed by Canuto & Mazzitelli (1991), may also not be quite correct. In the case of deep almost adiabatic convection, Chan & Sofia (1987) found that a fixed α could be used, provided the mixing length was scaled by the pressure scaleheight.

Table 3. Estimates for the average horizontal diameter of granules by three different methods (see the text for details). All values are in Mm.

Model	$2 \times \text{FWHM}$	$3 \times \text{width of the SAL}$	$10 H_p$
S	1.2	0.9	1.4
SG1	5.7	4	5.8
SG2	13.4	11	13.3

The SAL is pushed out further in the more evolved models, partly because the ratio of the turbulent pressure to the gas pressure in the vicinity of the SAL increases as the Sun evolves. Although the turbulent velocities are not significantly different in the subgiant simulations, the gas pressure/density is much lower because of the low surface gravity. It should be noted that in our models opacity is equally important in determining the shape of the SAL. As the convective boundary is located near to where the optical depth is unity, and the optical depth depends on opacity and gas density, both of these quantities will determine the position of the convection boundary.

(ii) Overshoot. The amount of overshoot as a fraction of the pressure scaleheight at the photospheric surface, increases as the Sun evolves away from the main sequence. For the present Sun the overshoot is $0.5 H_p$, for the 11.3-Gyr subgiant it is $0.75 H_p$, while for the 11.6-Gyr subgiant it is approximately H_p . This overshoot is very inefficient at carrying heat and the region is for all practical purposes in radiative equilibrium. Only approximately 1 per cent of the total energy flux is transported into the stable layer by convective overshoot.

(iii) Characteristics of convective cells in surface layer convection. One of the interesting observable features of the outer convection zone is the size of granulation in the atmosphere. Granulation in the Sun is a well studied phenomenon, but as it is such a small-scale feature (approximately 2×10^6 are on the solar surface), it has not been directly observed on any other stars, except through the Doppler broadening of absorption lines. We have attempted to find a characteristic vertical scale for granules as a function of surface gravity. From our simulations we find that over a small depth range just below the surface, the FWHM of the vertical velocity correlation is approximately constant. We choose this length-scale to characterize the vertical extent of the granulation. We have shown that twice this FWHM gives an estimate for the average horizontal diameter of a surface granule. This value is close to Freytag's (2001) previous estimate of 10 times the photospheric pressure scaleheight.

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