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ACCURACY AND PERFORMANCE OF A NUMERICAL CODE FOR THE SOLUTION OF THE KOMPANEETS EQUATION IN COSMOLOGICAL CONTEXT

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SUMMARY – In this report we present some of the tests we carried out to verify the accuracy, reliability, and performance of a recent update to recent NAG versions of a numerical code, KYPRIX, specifically written for the solution of the Kompaneets equation in cosmological context, first implemented in the years 1989-1991, aimed to the very accurate computation of the cosmic microwave background (CMB) spectral distortions under quite general assumptions. After a brief introduction on general aspects concerning the global computational time and the impact of the various aspects of the code on it and on the accuracy of the numerical integration, we focus on some dedicated tests. First we compare the results of the update version of the code with those obtained with the original one, for some representative cases. Then we discuss to specific quantitative tests: the energy conservation and the time behaviour of the electron temperature. Finally we focus on some properties of the free-free distortions relevant for the long wavelength region of the CMB spectrum. All the tests support the very good accuracy and reliability of the new code version.

1 Introduction

After a brief discussion on theoretical aspects of the evolution of the cosmic microwave background (CMB) spectrum, in Procopio & Burigana (2005) we described the implementation (Burigana et al. 1991) and the updating (Procopio 2005) of a numerical code, KYPRIX, dedicated to the numerical integration of the Kompaneets equation (Kompaneets 1956). Once termined the updating of the numeric integration code, we have carried out many accuracy and performance tests. A good code quality requires at least: high numerical precision compared to the knowledge, both theoretical and observational, of the considered problem and physical meaning of the results obtained from the numerical integration based on a specific NAG routine (D03PCF for the update version – D03PGF for the original version) for partial differential equations. Moreover, for several specific computations some other routines, mainly from the NAG package albeit also from the Numerical Recipes (Press et al. 1992) package, are used in the code. Since different routines can solve the same mathematical problems using different numerical methods and/or implementations, typically with different settings and different input parameters, we have also verified that the adopted routines allow an appropriate efficiency and accuracy.

In order to evaluate the global CPU time of the code, we performed many runs with very different settings. The global CPU time interval ranges from few minutes for cases in which the integration starts at low redshifts to about 5 hours for cases starting at very high redshifts ($y(z) \simeq 5$). There are many factors that take role in determining the global CPU time. The complete Kompaneets equation (Burigana et al. 1995) is in fact composed by several terms. In the KYPRIX code we can select the physical processes to be considered in the numerical integration and the global CPU time increases with the number of activated processes.

Of course, the global CPU time depends on the parameters related to the numerical integration characteristics. The number of points adopted for the x grid has a great influence on the global CPU time. The integration interval starts from a point, A, and ends to a point, B, and it is discretized in a number of spatial steps given by the parameter $NPTS$. Clearly, the integration accuracy improves with $NPTS$ because of the incresing of the density of the adopted mesh point grid. In most of the cases $NPTS$ is set up to a very large value. We find that the global CPU time is approximately proportional to $NPTS$ ($t_{CPU} \propto NPTS$).

The parameter that plays the most relevant role in determining the global CPU time is the accuracy required for the time integration. The final solution precision depends on the value of the corresponding parameter ACC. Only for very high accuracy (ACC $\sim 10^{-12} - 10^{-14}$) the CPU time reaches the duration of some hours while keeping ACC $\gtrsim 10^{-5}$ the integration is carried out in few minutes. Anyway, the limits imposed by CMB spectrum observations drive us to investigate in particular on small distortions. It is then necessary to work with low values of ACC (in general, $\lesssim 10^{-4}$).

Once termined the better choice of the various numerical routines and fixed the characteristics of the time integration, we have carried out several tests in order to verify the physical validity of the results given by the code KYPRIX.

2 Comparative tests

The first kinds of tests consisted simply in comparing the results obtained with the update version of KYPRIX with those obtained with the original version for the same sets of input parameters (compare Fig. 1 with Fig. 2). To this purpose, we have considered some interesting cases carried out in the past. In particular we used the input parameters adopted in Burigana et al. (1995) where also semianalytical descriptions of the numeri-

cal solutions of the Kompaneets equation were reported. Relatively small distortions have been assumed in these tests: the amount of exchanged fractional energy is $\Delta\epsilon_r/\epsilon_i = 10^{-4}$ and we started the integration from a redshift corresponding to $y_h(z) \simeq 0.25$ in one of the two cases and $y_h(z) \simeq 1$ for the other case. The input cosmological parameters are: $H_0 = 50,\ \widehat{\Omega}_b = 0.03,\ k = 1.68,\ T_0 = 2.726$ K where k gives the contribution of relativistic neutrinos to the dynamics of the universe. Clearly, the results given by the update version of KYPRIX are fully consistent with the those reported in Burigana et al. (1995). Moreover, since in that paper a seminalytical description of the solution of the Kompaneets equation is given, it is clear that a good agreement of the numerical results obtained with the original and update code represents a further confirmation of the analytic solution validity.

3 Energy conservation test

In the code output file DATIP we store values of several parameters of interest. Two of them provide very useful information on the goodness of the numerical integration. The first one is the ratio, ϵ_r/ϵ_i, between the radiation energy density today and the energy density corresponding to the unperturbed distribution function before the distortion footnoteFor example, for a Bose-Einstein distorted spectrum $\epsilon_r/\epsilon_i = \phi^4 f(\mu)/[\phi_0^4 \varphi_0^{4/3}(\mu)]$ (see, e.g., Sunyaev & Zeldovich 1970, Danese & De Zotti 1977).. In absence of dissipation processes, the perfect energy consevation is represented by the constance of this ratio at all the times during the integration. To determinate the accuracy supplied by KYPRIX, the values of ϵ_r/ϵ_i are stored at the starting of the integration and at many following times. In order to estimate the precision of the energy consevation, we define the quantity:

$$\frac{|(\epsilon_r/\epsilon_i)_{t=t_{start}} - (\epsilon_r/\epsilon_i)_{t>t_{start}}|}{(\epsilon_r/\epsilon_i)_{t=t_{start}} - 1},$$

that gives the relative induced error in the energy conservation with respect to the initial value of $\Delta\epsilon_r/\epsilon_i$, or more formally, the relative error induced by numerical uncertainty on the amount of fractional injected energy.

A typical result is reported in Fig. 3.

Since the same absolute numerical integration error corresponds to a larger relative error for a smaller distortion, i.e. for smaller $\Delta\epsilon_r/\epsilon_i$ in these models, we could in principle expect a degradation of the energy conservation for decreasing distortions. Our tests indicate in fact that the maximum induced error shows an increasing of the degradation of the energy conservation for decreasing distortions adopting the same accuracy parameters. On the other hand, one can select them according the specific problem. We find that for suitable choices of the integration accuracy parameters, the above relative error can be kept always below $\simeq 0.05\%$ without requiring a too large computational time. Finally, we note that in some circumstances the scheme for the electron temperature evolution in the new version of KYPRIX (backward differences), different from that used in the original one (implicit scheme), could imply some small discontinuities in the evolution of the electron temperature and of $\Delta\epsilon_r/\epsilon_i$. On the other hand, we have verified that this effect does not affect the very good accuracy of the solution, because of the very small amplitude of these discontinuities and of the corresponding energy conservation violation.

4 Comparing the analytical behaviour of ϕ with the numerical one

While the energy exchange between matter and radiation is leaded by Compton scattering (in the absence of external energy dissipation processes), electrons reach the equilibrium Compton temperature (Peyraud 1968, Zeldovich & Levich 1968), $T_{e,eq}$, in a time shorter than the expansion time. For $y_h \ll 1$, (non primordial heating processes) Compton scattering is no longer able to significantly modify the shape of the perturbed spectrum and the final electronic temperature ϕ_f (remember that $\phi = T_e/T_r$), immediately after the decoupling, is very close to $\phi_{eq} = T_{e,eq}/T_r$. On the other hand, we know that for energy injections at redshifts corresponding to $y_h \gtrsim 5$ Compton scattering can estabilish kinetic equilibrium between matter and radiation. This corresponds to a Bose-Einstein spectrum, with a final electron temperature given by (Sunyaev & Zeldovich 1970, Danese & De Zotti 1977):

$$\phi_f(y_h \gtrsim 5) = \phi_{BE} \simeq (1 - 1.11\mu_0)^{-1/4}\,,$$

where $\mu_0(\ll 1)$ is the dimensioneless (initial) chemical potential. Moreover, in this case the evolution of the chemical potential, $\mu(z)$, and the relation between it and the amount of fractional energy injected, $\Delta\epsilon/\epsilon_i$, depends on the energy injection epoch.
For the intermediate energy injection epochs, corresponding to $y_h \lesssim 5$, the final value of ϕ (a function depending on y_h) is between the values of ϕ_{BE} and ϕ_{eq}, because the Compton scattering works to produce a Bose-Einstein like spectrum anyway (Burigana et al. 1991). At these epochs the relation between the chemical potential and the amount of fractional injected energy injected is simply given by (Sunyaev & Zeldovich 1970, Danese & De Zotti 1977):

$$\mu_0 \simeq 1.4\,\frac{\Delta\epsilon}{\epsilon_i}\,.$$

By exploiting the numerical results, Burigana et al. (1995) found a simple formula for ϕ:

$$\phi_f(y_h) = \frac{k}{5}\frac{5 - y_h}{k + y_h}(\phi_{eq} - \phi_{BE}) + \phi_{BE}\,, \qquad (1)$$

where $k = 0.146$. Moreover, this expression represents an accurate description of the evolution of ϕ for any value of y_h. In facts, for a value of y ($y < y_h$) we have:

$$\phi(y, y_h) = \phi_f(y_h - y)\,. \qquad (2)$$

In the considered cases, as in many situations of interest, the perturbed spectrum of the radiation (immediately after the heating process) could be described by a superposition of blackbodies and the equilibrium temperature is given by (Zeldovich & Sunyaev 1969, Zeldovich et al. 1972, Burigana et al. 1995):

$$\phi_{eq} \simeq (1 + 5.4\,y^*)\phi_i\,,$$

where $\phi_i = T_i/T_r = (1 + \Delta\epsilon/\epsilon_i)^{-1/4} \simeq 1 - y^*$ and the Comptonization parameter y^* could be related to the amount of fractional energy exchanged by (Zeldovich & Sunyaev 1969, Zeldovich et al. 1972, Burigana et al. 1995):

$$y^* \simeq (1/4)\Delta\epsilon/\epsilon_i\,.$$

Through Eqs. (1) and (2) we can test the behaviour of the electron temperature during the numerical integration of the Kompaneets equation carried out with the new code version. With the increasing of the time variable, the values of ϕ are saved into the file DATIP, from

the initial time step to the final one. Fig. 4 shows the two behaviours of ϕ (the numerical one and the analytical expression given by Eqs. (1) and (2)) while Fig. 5 displays their difference.

This test is of particular importance for the check of the validity of the results. In fact, the numerical computation of ϕ during time evolution of the system is of crucial relevance because of the role of ϕ in the Kompaneets equation. As remembered in the previous section, in the new version of the code a different scheme is used with respect to that implemented in the original version. The verification of the very good agreement of the above behaviours of ϕ further supports the substantial equivalence of the two code versions, their reliability, and, in particular, the negligible impact of the new adopted numerical scheme for the evolution of ϕ (in principle less stable than the implicit scheme) with respect to the old one.

5 The analytical behaviour of y_B

As already discussed by Sunyaev & Zeldovich (1970), accurate measures of the CMB spectrum in the Rayleigh-Jeans region could provide quantitative informations about the thermal history of the universe at primordial cosmic epochs. On the other hand, photon production processes (mainly radiative Compton at earlier epochs and bremsstrahlung at later epochs) work to reduce the CMB spectrum depression at long wavelengths (see Danese & De Zotti 1980) since they try to estabilish a true (Planckian) equilibrium. For $z < z_p$ (Danese & De Zotti 1980; Burigana et al. 1991) with

$$z_p \simeq 2.14 \times 10^4 \left(\frac{T_0}{2.7\,K}\right)^{1/2} \left(\frac{k}{1.68}\right)^{1/4} \widehat{\Omega}_b^{-1/2}\,,$$

low frequency photons are absorbed before Compton scattering brings them to higher frequencies.
In case of small and late distortions ($z_h \lesssim z_p$), a good approximation of the whole spectrum is given by (Burigana et al. 1995)

$$\eta(x,\tau) = \eta_i e^{-(\tau-\tau_h)} e^{-(\tau-\tau_h)} \int_{\tau_h}^{\tau} e^{(\tau'-\tau_h)} \frac{1}{e^{x/\phi(\tau')}-1} \mathrm{d}\tau'$$

$$+u \frac{x/\phi_i e^{x/\phi_i}}{(e^{x/\phi_i}-1)^2} \left(\frac{x/\phi_i}{\tanh(x/2\phi_i)} - 4\right),$$

where the index i denotes the initial value of the corresponding quantity and u is the Comptonization parameter. This expression provides also an exhaustive description of continuum spectral distortions generated in various scenarios of (standard or late) recombination or associated to the cosmological reionization. For an initial blackbody spectrum, at dimensionless frequencies $x_B \ll x \ll 1$ the above equation can be simplified and reduces to (Burigana et al. 1995)

$$\eta \simeq \eta_{BB,i} + \frac{y_B}{x^3} - u\frac{2}{x/\phi_i}\,;$$

here y_B, an optical depth of the universe for bremsstrahlung absorption (radiative Compton can be neglected at late epochs), is analogous to the Comptonization parameter and it is given by

$$y_B = \int_{t_h}^{t} (\phi-\phi_i)\phi^{-3/2} g_B(x,\phi) K_{0B} \mathrm{d}t = \int_{1+z}^{1+z_h} (\phi-\phi_i)\phi^{-3/2} g_B(x,\phi) K_{0B} t_{exp} \frac{\mathrm{d}(1+z)}{1+z}\,;$$

x_B is the frequency at which $y_{abs,B} = 1$ (Zeldovich et al. 1972; De Zotti 1986). The dependence of the Gaunt factor (Karsaz & Latter 1961, Rybicki & Lightman 1979, Burigana et al. 1991) on x and ϕ at very long wavelengths is weak: $g_B \propto \ln(x/\phi)$.

In terms of brightness temperature, the distortions at low frequencies (at any redshift) could be write as

$$\frac{T_{br} - T_r\phi_i}{T_r} \simeq \frac{y_B}{x^2} - 2u\phi_i \,,$$

where $T_r = T_0(1+z)$.

In order to show that our numerical solution follows the behaviour described by the last equation, we can compute y_B from the brightness temperature derived from the numerical solution:

$$y_B \simeq x^2\left(\frac{T_{br} - T_r\phi_i}{T_r} + 2u\phi_i\right). \tag{3}$$

As shown in Fig. 6, at low frequencies y_B approaches an almost constant value with varying frequency. This is correct only for $\lambda > 200 - 300$cm while at higher frequencies y_B is no longer almost constant (see again Fig. 6) because of the dependence of the Gaunt factor on x and ϕ as expressed in the definition of y_B.
We can write an expression describing the brightness temperature through a constant parameter y_B, derived from Eq. 3 (see Fig. 7) applied to the range at very long frequencies ???, to verify the goodness of the below expression

$$T_{br,y_B} = \left(\frac{y_B}{x^2} - 2u\phi_i + \phi_i\right) \cdot T_r$$

in comparison with the numerical results. Note that when the Gaunt factor dependence on x and ϕ produces a significantly varying y_B (see Fig. 6), the Comptonization decrement is more relevant than the free-free excess in determining the brightness temperature, as evident from the good agreement of the two curves in Fig. 7. Clearly, the brightness temperature derived in this way works only up to frequencies approaching that at which the excess in the brightness temperature produced by the Comptonization begins (see Fig. 7). The reported numerical result refers to a heating process corresponding to a full reionization starting at $z \simeq 20$ with $\phi = 10 \times 10^4$ K.

6 Conclusion

We have presented some of the tests we carried out to verify the accuracy, reliability, and performance of a recent update to recent NAG versions of a numerical code, KYPRIX, specifically written for the solution of the Kompaneets equation in cosmological context, first implemented in the years 1989-1991, aimed to the very accurate computation of the cosmic microwave background (CMB) spectral distortions under quite general assumptions. We have briefly introduced the general aspects concerning the global computational time and the impact of the various aspects of the code on it and on the accuracy of the numerical integration. We have than we focussed on some dedicated tests.

First, we have compared the results of the update version of the code with those obtained with the original one, for some representative cases, finding an excellent agreement.

We have than discuss to specific quantitative tests. The verified a very good energy conservation accuracy: for appropriate choices of the code accuracy parameters, the fractional injected energy is conserved within an accuracy better than 0.05%, or, in other words, possible energy conservation violations are negligible in practice for theoretical predictions and for comparison with current and future data. We have tested the time behaviour of the electron

temperature finding an excellent agreement with the results found with the original code version, in spite of the different schemes adopted to update the evolving electron temperature.

Finally we have focussed on some properties of the free-free, distortions relevant for the long wavelength region of the CMB spectrum, by checking the new code version, as the original one, very accurately recovers the existing analytical approximations in their limit of validity.

All the above tests support the very good accuracy and reliability of the new code version.

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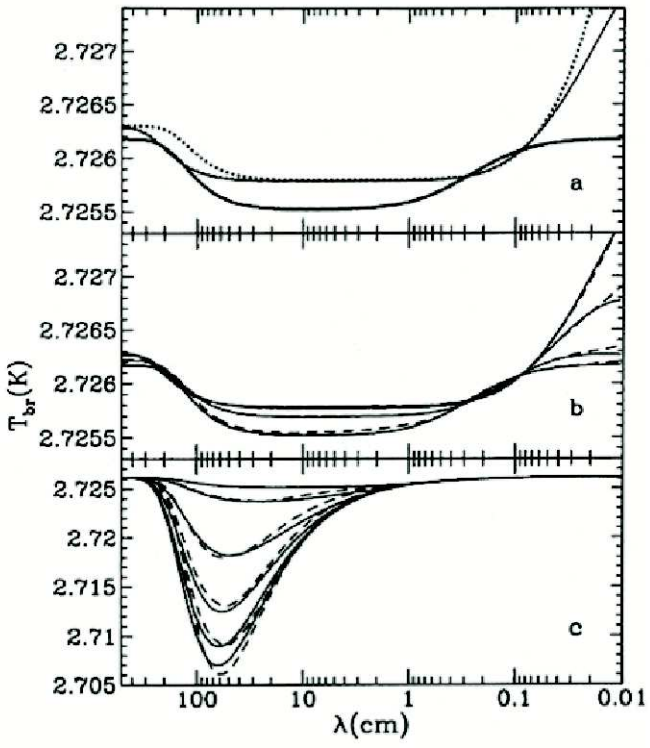

Figure 1: Some results from Burigana et al. 1995. Panel **a**): integration of the Kompaneets equation (solid lines) until today, for two cases of distortion ($\Delta\epsilon/\epsilon_i = 10^{-4}$ e $y_h = 0.25$ (thick lines) and $y_h = 0.01$ (thin lines) is compared with the analytical approximation (dotted lines). The cosmological parameters are: $H_0 = 50, \widehat{\Omega}_b = 0.03, k = 1.68, T_0 = 2.726$ K. Panel **b**): comparison between numerical solutions and corresponding semianalytical approximations for the same value of $\Delta\epsilon/\epsilon_i$ but with different epochs of the energy injection: $y_h = 0.25; 0.1; 0.025; 0.01$. Panel **c**): as in panel **b**, but for $y_h = 5; 4; 3; 2; 1; 0.5$.

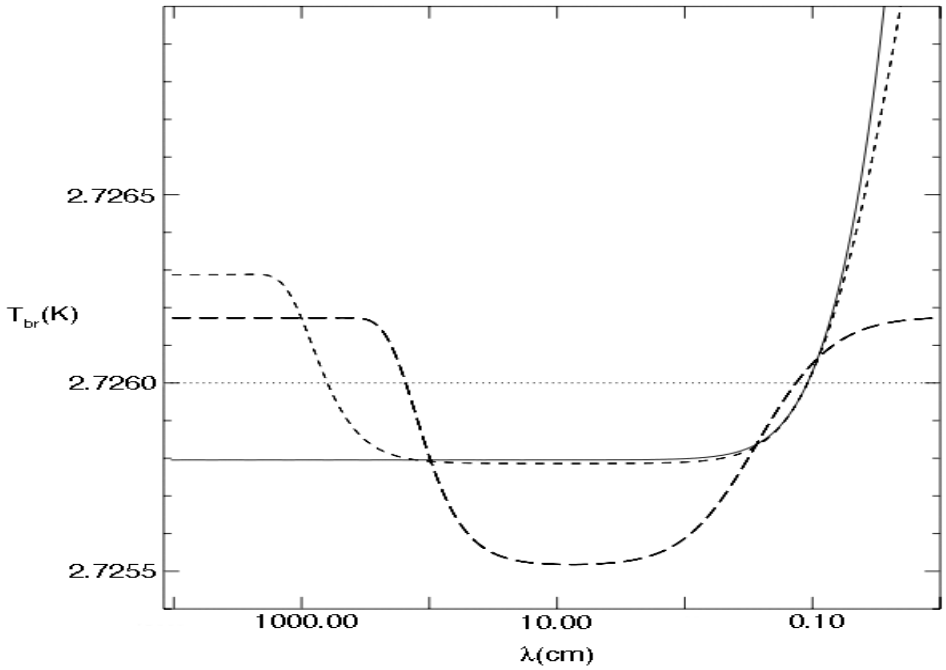

Figure 2: Results of the numeric integration obtained with the new version of the KYPRIX code. Input parameters are the same as in panel **a** of Fig. 1. Here we plot also a Planckian spectrum at 2.726 K (flat line). Note the excellent agreement with the results of panel **a** in Fig. 1: $\Delta\epsilon/\epsilon_i = 10^{-4}$, solutions for $y_h = 0.25$ (thick dashed line) and $y_h = 0.01$ (thin dashed line).

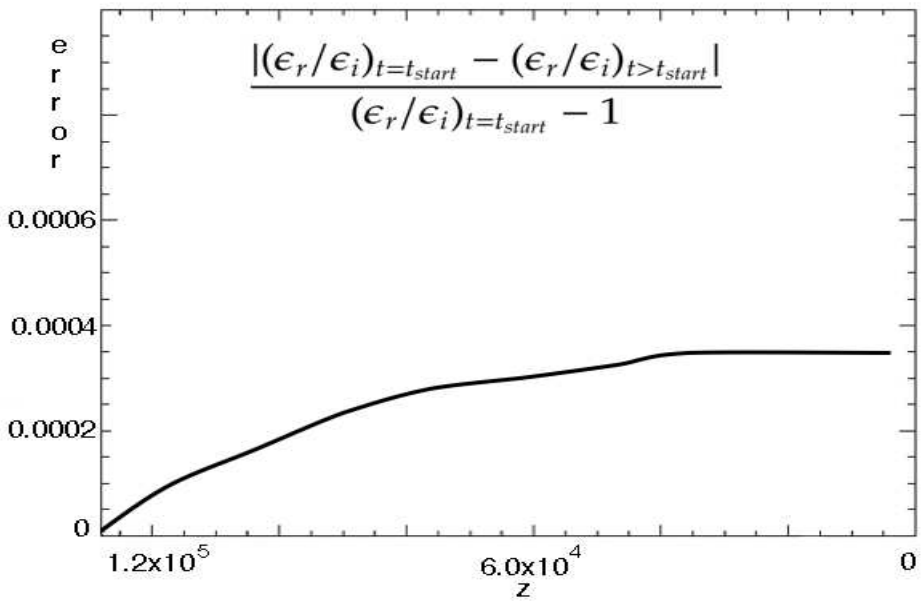

Figure 3: Time behaviour of the induced relative error on the quantity $\Delta\epsilon/\epsilon_i$.

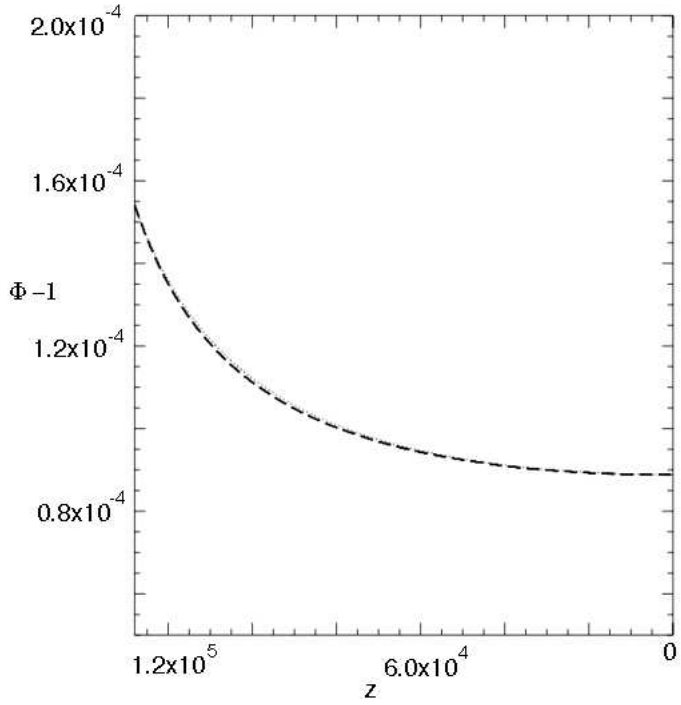

Figure 4: Time behaviour of ϕ: comparison between the analytical approximation (dotted line) and the values computed with the numerical integration (dashed line). See also the text.

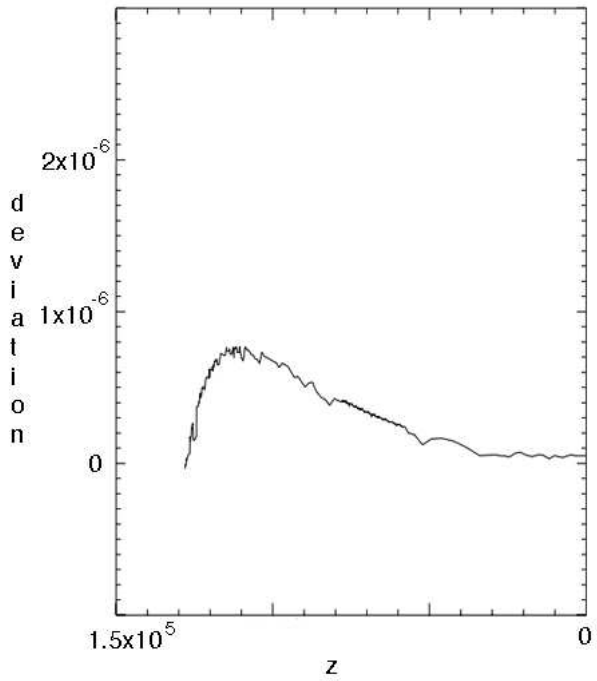

Figure 5: Deviation between the two behaviours of ϕ reported in Fig. 4. Note that the discrepancy is always less than $\simeq 1\%$.

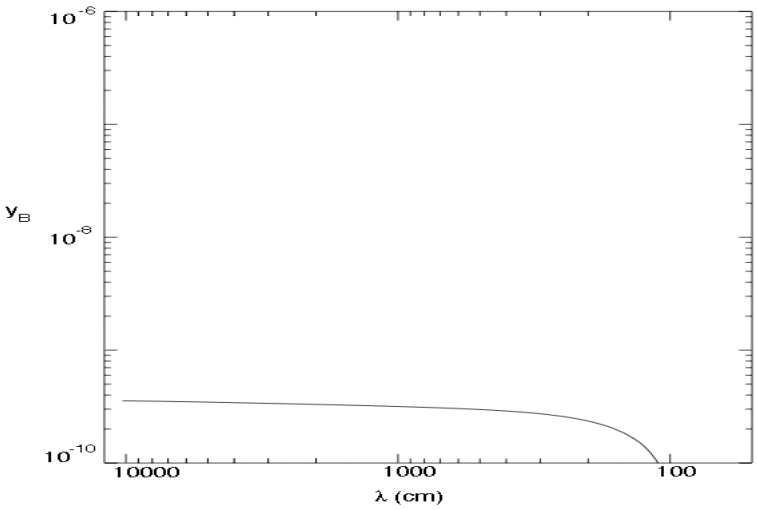

Figure 6: Behaviour of y_B with the wavelength. In the studied case we start the integration from a Planckian spectrum by keeping the electron temperature to 10^{4°K in order to simulate a reionization at ~ 20. The cosmological parameters are: $h = 0.68, \Omega_m = 1, \Omega_b = 0.047, \Omega_\Lambda = 0$. See also the text.

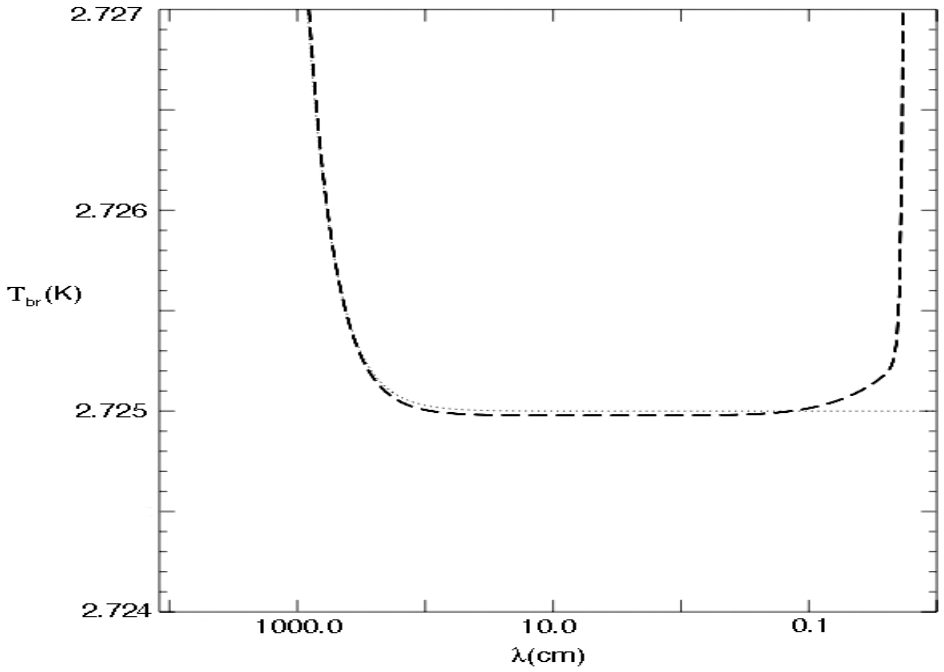

Figure 7: Comparison of the brightness temperature obtained from the analytical approximation and that obtained from the numerical integration for the same case reported in Fig. 6. See also the text.