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UPDATING A NUMERICAL CODE FOR THE SOLUTION OF THE KOMPANEETS EQUATION IN COSMOLOGICAL CONTEXT

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SUMMARY – In this report we describe the fundamental approach and, in particular, the 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 spectral distortions under quite general assumptions. Specifically, we discuss the main subdivisions of the code and the most relevant aspects about technical specifications and code implementation. After a presentation of the equation formalism and of the boundary conditions added to the set of ordinary differential equations derived from the original parabolic partial differential equation, we provide details on the adopted space (i.e. dimensionless frequency) grid, on the output results, on the accuracy parameters, and on the used integration routines. The problem of introducing the time dependence of the ratio between electron and photon temperatures and of the radiative Compton scattering term, both of them introducing integral terms in the Kompaneets equation, is addressed in the specific context of the recent NAG versions. Finally, we describe the introduction of the cosmological constant in the terms controlling the general expansion of the universe, in agreement with the fundamental discoveries of the last years.

1 Introduction

The CMB spectrum emerges from the thermalization redshift, $z_{therm} \sim 10^6 - 10^7$, with a shape very close to a Planckian one, owing to the tight coupling between radiation and matter through Compton scattering and photon production/absorption processes, radiative Compton and bremsstrahlung. These processes were extremely efficient at early times and able to re-establish a blackbody (BB) spectrum from a perturbed one on timescales much shorter than the expansion time (see, e.g., Danese & De Zotti 1977). The value of z_{therm} (Burigana et al. 1991) depends on the baryon density parameter, Ω_b, and the Hubble constant, H_0, through the product $\widehat{\Omega}_b = \Omega_b (H_0/50)^2$ (H_0 expressed in Km/s/Mpc).

On the other hand, physical processes occurring at redshifts $z < z_{therm}$ may lead imprints on the CMB spectrum. Therefore, the CMB spectrum carries crucial informations on physical processes occurring during early cosmic epochs (see, e.g., Danese & Burigana 1993 and references therein) and the comparison between models of CMB spectral distortions and CMB absolute temperature measures can constrain the physical parameters of the considered dissipation processes.

The timescale for the achievement of kinetic equilibrium between radiation and matter (i.e. the relaxation time for the photon spectrum), t_C, is

$$t_C = t_{\gamma e} \frac{m_e c^2}{k T_e} \simeq 4.5 \times 10^{28} \, (T_0/2.7\,K)^{-1} \, \phi^{-1} \widehat{\Omega}_b^{-1} \, (1+z)^{-4} \, \mathrm{sec}\,, \tag{1}$$

where $t_{\gamma e} = 1/(n_e \sigma_T c)$ is the photon–electron collision time, $\phi = (T_e/T_r)$, T_e and $T_r = T_0(1+z)$ being respectively the electron and the CMB radiation temperature; $kT_e/m_e c^2$ (being m_e the electron mass) is the mean fractional change of photon energy in a scattering of cool photons off hot electrons, i.e. $T_e \gg T_r$; T_0 is the present radiation temperature related to the present radiation energy density by $\epsilon_{r0} = \mathrm{a} T_0^4$ (here $\mathrm{a} = 8\pi I_3 k^4/(hc)^3$, $I_3 = \pi^4/15$); a primordial helium abundance of 25% by mass is here assumed.

It is useful to introduce the dimensionless time variable $y_e(z)$ defined by

$$y_e(z) = \int_t^{t_0} \frac{dt}{t_C} = \int_1^{1+z} \frac{d(1+z)}{1+z} \frac{t_{exp}}{t_C}\,, \tag{2}$$

where t_0 is the present time and and $t_{exp} = 1/H = 1/[(da/dt)/a]$ is the expansion time, $a = 1/(1+z)$ is the cosmic scale factor normalized to the present time.

As particular cases, by neglecting the cosmological constant (or dark energy) contribution we have

$$t_{exp} \simeq 6.3{\times}10^{19} \left(\frac{T_0}{2.7\,K}\right)^{-2} (1{+}z)^{-3/2} \left[\kappa(1+z) + (1+z_{eq}) - \left(\frac{\Omega_m - 1}{\Omega_m}\right)\left(\frac{1+z_{eq}}{1+z}\right)\right]^{-1/2} \mathrm{sec}\,, \tag{3}$$

where $z_{eq} = 1.0 \times 10^4 (T_0/2.7\,K)^{-4} \widehat{\Omega}_m$ is the redshift of equal non relativistic matter and photon energy densities and $\kappa = 1 + N_\nu (7/8)(4/11)^{4/3}$, N_ν being the number of relativistic, 2–component, neutrino species (for 3 species of massless neutrinos, $\kappa \simeq 1.68$), takes into account the contribution of relativistic neutrinos to the dynamics of the universe[1], while assuming $\Omega_K = 0$, $\Omega_\Lambda = 1 - \Omega_m$, and neglecting the radiation energy density, as possible at relatively low redshifts, we have

$$t_{exp} \simeq (1/H_0) \left[\Omega_m (1+z)^3 + 1 - \Omega_m\right]^{-1/2} \mathrm{sec}\,, \tag{4}$$

[1]Strictly speaking the present ratio of neutrino to photon energy densities, and hence the value of κ, is itself a function of the amount of energy dissipated. The effect, however, is never very important and is negligible for very small distortions.

where $1/H_0 \simeq 3.1 \times 10^{17} h^{-1}$ sec ($h = H_0/100$).

The time evolution of the photon occupation number, $\eta(\nu, t)$, under the combined effect of Compton scattering and of photon production processes, namely radiative Compton (RC) (Gould 1984), bremsstrahlung (B) (Karsaz & Latter 1961, Rybicki & Lightman 1979) plus other possible contributions (EM), is well described by the complete Kompaneets equation (Kompaneets 1956, Burigana et al. 1995):

$$\frac{\partial \eta}{\partial t} = \frac{1}{\phi}\frac{1}{t_C}\frac{1}{x^2}\frac{\partial}{\partial x}\left[x^4\left[\phi\frac{\partial \eta}{\partial x} + \eta(1+\eta)\right]\right] + \left[\frac{\partial \eta}{\partial t}\right]_{RC} + \left[\frac{\partial \eta}{\partial t}\right]_{B} + \left[\frac{\partial \eta}{\partial t}\right]_{EM} . \quad (5)$$

This equation is coupled to the time differential equation governing the electron temperature evolution for an arbitrary radiation spectrum in the presence of Compton scattering, energy losses due to radiative Compton and bremsstrahlung, adiabatic cooling, plus possible external heating sources, $q = a^{-3}(dQ/dt)$,

$$\frac{dT_e}{dt} = \frac{T_{eq,C} - T_e}{(27/28)t_{e\gamma}} - \frac{2T_e}{t_{exp}} + \left[\frac{dT_e}{dt}\right]_{RC,B} + \frac{(32/27)q}{3n_e k} ; \quad (6)$$

here $T_{eq,C} = [h\int \eta(1+\eta)\nu^4 d\nu]/[4k\int \eta\nu^3 d\nu]$ is the Compton equilibrium electron temperature (Peyraud 1968, Zeldovich & Levich 1968), $t_{e\gamma} = 3m_e c/4\sigma_T \epsilon_r$, $\epsilon_r \simeq \epsilon_{r0}(1+z)^4$ being the radiation energy density, and x is the dimensionless frequency $x = h\nu/kT_0$ (ν being the present frequency).

Partial differential linear equations are divided in three classes: elliptic, parabolic and hyperbolic. The Kompaneets equation is a parabolic partial differential equation (Tricomi 1957). Solutions to this equation under general conditions have to be searched numerically, because it is impossible to find analytical solutions that accurately take into account the many kinds of cosmological scenarios and the great number of relevant physical processes. The numerical code KYPRIX (Burigana et al. 1991) was written to overcome the limited applicability of analytical solutions and to get a precise computation of the evolution of the photon distribution function for a wide range of cosmic epochs and for many cases of cosmological interest. KYPRIX makes use of the NAG libraries.

Of course, many dedicated routines have been written and available numerical algorithms have been used in this code. Among the latters, the D03PCF routine (of the current version, corresponding to D03PGF routine used the first versions of KYPRIX), has been used to reduce the Kompaneets equation into a system of ordinary differential equations. In order to use this routine, we have to put the Kompaneets equation in the form

$$\sum_{j=1}^{NPDE} P_{i,j}\frac{\partial U_j}{\partial t} + Q_i = x^{-m}\frac{\partial}{\partial x}\left(x^m R_i\right) ; \quad (7)$$

in our case $P_{i,j} = 1$ and $m = 0$ (Cartesian coordinates). Moreover, the function R_i is determined only by the inverse Compton term while the other physical processes, i.e. at least Compton scattering, Bremsstrahlung, and radiative Compton, are included in the function Q_i. In order to reduce Eq. (7) into a system of ordinary differential equations, the D03PCF routine uses the method of lines: pratically, the right member of Eq. (7) is discretized, reducing the calculation of partial derivatives in terms of finite values of the solution vector U at all the points of the x axis grid. Spatial discretization is made by the method of finite differences (Mitchell & Griffiths, 1980). The Gear's method (Gear 1971) is used to resolve the system of ordinary differential equations. The variables that enter in this equation are introduced and used in logarithmic form ($\log(x)$ and $\log(\eta)$), to have a good and essentially uniform accuracy of the solution in the whole considered frequency range. The choice of

the time parameter was driven by the need to have a very simple form of the Kompaneets equation. Finally, a "temperature independent" (time) Comptonization parameter

$$y(t) = \int \frac{dy_e}{\phi} = \int_{t_i}^{t} n_e \sigma_T c \frac{kT_r}{mc^2} dt' \,, \tag{8}$$

has found to be particularly advantageous (Burigana et al. 1991).

2 Boundary conditions

Integrating equations of the type of Eq. (7) means to calculate the time evolution of the function $U(x,t)$, for a given initial condition $U(x,0)$ (in fact, the problem is also called "problem at initial conditions"). Numerically, the derivatives of U are replaced by finite differences between values of U computed for a grid of points (in x,t) and the differential equation is replaced by a system of more simple equations. However, in presence of the only initial condition, this system is singular (Press et al. 1992). For this reason, resolving partial differential parabolic equations needs boundary conditions: the problem is at initial values for the t variable and at the boundary values for the x variable. In general, boundary conditions mean additional relations to join to the system derived from the discretization to finite differences, to the aim of having the same number of equations and unknowns.

Therefore, a good statement of the problem needs the definition of appropriate boundary conditions and, possibly, the capability of a refresh of this conditions along the time integration leads more stability to the solution evolution because of the evolution of the radiation field. Thanks to the opportunity of having the correct value of ϕ for each time step, the update of the boundary conditions can be physically motivated.

The limits of the frequency range considered are: $\log(x_{min}) = -4.3$ e $\log(x_{max}) = 1.7$. Of course, we want a solution of the Kompaneets equation over all the frequency range where it is possible to measure the CMBR and, in addition, a frequency range large enough to contain, in practice, all the energy density of the cosmic radiation field.

Also, the frequency range is so wide for two other reasons.

During the time evolution, some spurious oscillations of the solution at points close to the boundaries may appear (this effects, that could also occur independently of the need of refreshing ϕ – for example for cases at constant ϕ –, may be partially amplified if, for computational reasons discussed in the following, the necessary refresh of the electronic temperature is not made for every time step). Fixing the frequency integration range limits far from the interval where we are interested to compute the photon distribution function allows to prevent the "contamination" of the solution by this possible spurious oscillations in the frequency range of interest.

Finally, since we can generally assume that a Planckian spectrum at x_{min} is formed before recombination in a timescale shorter than the expansion time and, on the contrary, at x_{max} the shape of the spectrum is unknown, it has been implemented in the code the possibility to adopt a particular case of Neumann boundary conditions: the requirement that the current density, in the frequency space, is null at the boundaries of the integration range (Chang & Cooper, 1970):

$$\left[\phi \frac{\partial \eta}{\partial x} + \eta(1+\eta) \right]_{x=x_{min},x_{max}} = 0 \,.$$

This choice of boundary conditions formally satisfies the requirement of the problem when we integrate the Kompaneets equation in the case of Bose-Einstein like distorsions (with a

variable chemical potential μ). In fact, such distorted spectra are indistinguishable from a blackbody spectrum at sufficiently high and at low frequencies.

Of course, it is possible to make a different choice of the boundary conditions by selecting Dirichlet like conditions. In this case the photon occupation number at the boundaries of the integration interval does not change for the whole integration time. (In general cases, keeping constant conditions at the boundaries could be dangerous for the continuity of the solution. Nevertheless, for some specific problems this condition can work – typically for problems with constant ϕ).

3 A detailed view on KYPRIX

The code KYPRIX has been written to solve the Kompaneets equation in many kinds of situations. The physical processes that can be considered in KYPRIX are: Compton scattering, bremsstrahlung, radiative Compton scattering, sources of photons, energy injections without photon production, energy exchanges (heating or cooling processes) associated to $\phi \neq 1$ at low redshifts, radiative decays of massive particles, and so on. Being very versatile, this code could be easily implemented to consider other kinds of physical processes.
The data are saved into five files.
DATI. This file contains the information about the specific parameters of the considered problem with a general description of its main aspects.
DATIP. In this file we give the evolution of interesting quantities, like time, redshift, ϕ, and many another quantities inherent to physical and numerical aspects of the problem.
DATIG. It contains: the points grid for the x axis used by the main program (remember that we are using a dimensionless frequency), a Planckian spectrum at temperature T_0 and the solution vector U (that is to say $\log(\eta)$) at $y = 0$ (starting time).
DATIDE. This is the fundamental output file: it gives the solution of the Kompaneets equations at the desired cosmic epocs.
DATIT. It is similar to the file DATIDE, but it contains the solution in term of brightness temperature (i.e. equivalent thermodynamical temperature).

3.1 Main subdivisions

The code is divided in several sections and, from a general point of view, is structured as described here below.
1. Main program, in which many actions can be carried out: choice of the physical processes, choice of the cosmological parameters, characteristics of the numerical integration (accuracy, number of point of the grid, ...), time interval of interest, choice of the boundary conditions, and so on.
2. Subroutine PDEDEF. It is the subprogram where the problem is numerically defined. This subroutine is also divided in subsections to allow modifications in a simple and practical way.
3. Subroutine BNDARY. Here the boundary conditions are numerically specified.
4. Subroutines and auxiliary functions to perform specific operations.

3.2 Technical specifications and code implementation

Written in the 1990 by Carlo Burigana, the KYPRIX first version worked with the Mark 8 version of the NAG numerical library and were based on the routine D03PGF. The version of the NAG numerical library currently distributed is the Mark 20. Therefore an update of the KYPRIX code is necessary to adapt it to this new package.

Just started, KYPRIX asks all the input data, from the specifications of the output files to the integration features. In the following subsections we give a description of the various aspects of the code (and code update) more relevant for its understanding and usage.

3.2.1 Grid

The frequency integration interval is divided in a grid of points (the mesh points): larger the number of points smaller the adopted frequency step.
It is possible to used a very dense grid (for example 36001 mesh points corresponding to 36000 frequency steps). In general, it is necessary to use at least 3001 mesh points to have a solution accurate enough.

We found an important difference between the two NAG versions, not reported in the documentation of the routine D03PCF. In the first version (D03PGF), the subroutine where the partial differential equation is defined adopted the same mesh points defined in the main program. In the Mark 20 version the calculation is carried out in a different manner: the mesh points used in the subroutine PDEDEF is shifted of half spatial step with respect to the mesh defined in the main program. In this way, the mesh points in the PDEDEF subroutine will be exactly in the middle of the steps defined in the grid of the main program. For this reason, the limit of the integration interval are not considered in the mesh points in the subroutine PDEDEF and they are used only for the boundary conditions.
The effect of this feature implies the definition of new parameters that play a fundamental role in the subroutine PDEDEF. The integral quantities in the Kompaneets equation (necessary to define the radiative Compton term in the kinetic equations and the electron temperature) are computed once for any time step, inside the PDEDEF subroutine. For this computation, arrays of dimension equal to the number of mesh points of the x variable as defined in the PDEDEF subroutine are used. Therefore, a particular care must be taken in the definition of the dimension of the arrays defined in KYPRIX. Those used in the main program have dimension equal to the number of points of the mesh defined in the main program. The same dimension is given for the arrays defined for the boundary conditions. On the other hand, the major number of arrays are used in the PDEDEF subroutine to compute the integral quantities. The "inner" grid adopted in the PDEDEF subroutine is based on mesh points in the middle of the spatial steps of the main program grid, so the two grids can not work with the same point number; in fact, the arrays used in the PDEDEF subroutine have dimension $NPTS - 1$. Therefore, in the main program and in the subroutine BNDARY we have to work with arrays based on the formula:

$$X(I) = A + (I-1) \times \frac{(B-A)}{(NPTS-1)}\,, \qquad \text{with}\, 1 \leq X \leq NPTS\,,$$

to define the correspondence between the grid of $NPTS$ points and the x position, while we need another expression able to shift of half step the grid in the PDEDEF subroutine and based on $NPTS - 1$ mesh points:

$$X(I) = \left(A + (I-1) \times \frac{(B-A)}{(NPTS-1)} \right) + \left(\frac{(B-A)}{2(NPTS-1)} \right),$$

$$\text{with } 1 \leq X \leq NPTS - 1.$$

For continuity reasons, we need to define (according to the choices made in the main program) the solution vector, containing the photon initial distribution function, at the beginning of the integration also according to this grid definition. This vector is used by the PDEDEF subroutine as initial spectrum adopted for the computation of the rates of the physical processes and, of course, it is then renewed at every time step incrementation.

3.2.2 Output

Concerning the output files, the update version of KYPRIX stores a new vector containing the "inner" x grid used by the PDEDEF subroutine, XXGR (XGR refers to the main program grid).

In addition, we preferred to have the possibility to perform the conversion of the solution into equivalent thermodynamic temperature directly into the code and save it in a new output file (DATIT). The conversion relation is:

$$T_{term,equiv} = \frac{xT_0}{\ln(1 + 1/\eta)}$$

(we remember that in the code $X = \log_{10}(x)$ and $U = \log_{10}(\eta)$).
The fundamental reason to perform this conversion directly in the code is associated to the extreme accuracy required for the solution in the case of very small distorsions, of particular interest given the FIRAS results (Fixsen et al. 1996). During the first tests, the conversion of the solution in brightness temperature was performed at the same time of the solution visualization, through the IDL visualization program. The saving of the solution into files is typically performed not for all the points of the grid but for a reduced grid of, for example, 300 equidistant points along the original grid to avoid to store files of large size, unuseful for our scope, given the interest for the CMB continuous spectrum (by definition, the Kompaneets equation is not appropriate to treat recombination lines). If the considered distorsions were very small then the solution at each specific "inner" grid point could be affected by a numerical uncertainty not negligible in comparison with the very small deviations from a Planckian spectrum relevant in this cases. This numerical error is greatly reduced (becoming negligible for our purposes) by the averaging over a suitable number of grid points. Of course, the storing of the solution directly on a limited number of grid points makes this averaging no longer possible on the stored data. It were then necessary to average the solution values in intervals corresponding to the output x grid directly into the code. Anyway, in many circumstances the diagram shape derived applying the conversion to brightness temperature only on the stored averaged solution still deviates at high frequencies from the effectively computed solution displayed by considering all the "inner" grid points because of the high gradients in the photon distribution function and/or in the brightness temperature that makes difficult, or impossible, to find a general rule for the solution binning that simultaneously works properly for the two solution representations. This problem is avoided converting the solution vector in equivalent thermodynamic temperature before of the binning of its values and then applying the binning to the equivalent thermodynamic temperature. The result is then a brightness temperature diagram very clean and precise, even for very small distortions.

Other minor changes are made about the output data, where we passed from real to double precision, and for the saving frequency into the output files.

3.2.3 Equation formalism

A necessary update of the code has been performed to adapt it to the different formalism adopted by the new version of the NAG routine. This regards the expression of the Kompaneets equation in the PDEDEF subroutine. In particular, the D03PGF adopted the following expression of the partial differential equation:

$$C_i \frac{\partial U_i}{\partial t} = x^{-m} \sum_{j=1}^{NPDE} \frac{\partial}{\partial x}\left[x^m G_{ij} \frac{\partial U_j}{\partial x} \right] + F_i \,,$$

where $i = 1, 2, ..., NPDE$ (number of partial differential equations); C_i, F_i depends on $x, t, U, \partial U/\partial x$; $G_{i,j}$ depends on x, t, U and U is the set of solutions values $(U_1, U_2, ..., U_{NPDE})$. The expression now adopted by the D03PCF routine is instead:

$$\sum_{j=1}^{NPDE} P_{i,j} \frac{\partial U_j}{\partial t} + Q_i = x^{-m} \frac{\partial}{\partial x}\Big(x^m R_i \Big) \,,$$

where $P_{i,j}, Q_i, R_i$ depends on $x, t, U, \partial U/\partial x$ and the vector U is defined as above. Please note that $P_{i,j}, Q_i, R_i$ do not depend on $\partial U/\partial t$.
Translating the code from the old to the new formalism is not very difficult. In the considered case $NPDE = 1$. In this case, we have simply that R_1 contains both the function G_1 and the vector solution derivative with respect to x according to:

$$R_1 = G_{11} \times \frac{\partial U_1}{\partial x} \,.$$

At this point, it is necessary to apply only the following substitutions:

$$Q_1 = -F_1 \qquad \text{and} \qquad P_{11} = C_1 \,.$$

3.2.4 Boundary conditions

Also notable are the differences between the input expressions defining the boundary conditions. The D03PGF routine adopted an expression of the form:

$$P_i(t) U_i + Q_i(t) \frac{\partial U_i}{\partial x} = R_i(t, U) \,,$$

where $i = 1, 2, ..., NPDE$ and $P_i(t), R_i(t, U), Q_i(t)$ are functions to be defined. A quite different notation is used to provide the boundary conditions in the D03PCF routine:

$$\beta_i(x, t) R_i(x, t, U, U_x) = \gamma_i(x, t, U, U_x) \,,$$

where $i = 1, 2, ..., NPDE$ and $\beta_i(x, t) R_i(x, t, U, U_x)$ and $\gamma_i(x, t, U, U_x)$ are functions to be defined ($U_x \equiv \partial U/\partial x$).
As a consequence of this notation, Neumann like boundary conditions can be now specified according to the expression:

$$\beta(1) = 1$$

$$\gamma(1) = -XVA \times (10^{U(1)} + 1) \times \ln 10^{-2}$$

where $XVA = \eta$ computed in A and the dimension of both the equations corresponds to the differential equation number. Similar conditions are defined for the other extreme of the integration interval [A,B].

3.2.5 Accuracy parameters

Another considerable difference between the two library versions regards the definition of the integration accuracy parameter. D03PGF used three parameters for monitoring the local error estimate in the time direction, supplying a good versatility. RELERR and ABSERR were respectively the quantity for the relative and absolute component to be used in the error test. The third parameter, INORM, was used to define the error test. If $\mathrm{E}(i,j)$ is the estimated error for U_i (the vector solution) at the $j-th$ point of the x grid, then the error test was:

- $INORM = 0 \Longrightarrow \mid \mathrm{E}(i,j) \mid \leq \mathrm{ABSERR} + \mathrm{RELERR} \times \mid U(i,j) \mid$
- $INORM = 1 \Longrightarrow \mid \mathrm{E}(i,j) \mid \leq \mathrm{ABSERR} + \mathrm{RELERR} \times \max_y \mid U(i,j) \mid$
- $INORM = 0 \Longrightarrow \|\mathrm{E}(i,j)\| \leq \mathrm{ABSERR} + \mathrm{RELERR} \times \|U(i,j)\|$.

Instead, according to the new library version we have to define only one parameter ACC, a positive quantity that monitors the local error in the time integration. If $\mathrm{E}(i,j)$ is defined as above, then the error test is:

$$\mid \mathrm{E}(i,j) \mid = \mathrm{ACC} \times (1 + \mid U(i,j) \mid) .$$

3.2.6 Electron temperature

During the numerical integration, some subprograms use the distribution function calculated at that time to compute ϕ. The integrals to be computed are those that we find in the expression for $\phi_{eq,C}$:

$$\phi_{eq,C} = \frac{T_e}{T_\gamma} = \frac{\int_0^\infty \eta(\eta+1)x^4 \mathrm{d}x}{4\int_0^\infty \eta x^3 \mathrm{d}x} .$$

In this calculation, the integration range is obvioulsy the integration interval considered for the problem: $A \leq x \leq B$ (that, in terms of mesh ordering, corresponds to the range between 1 and $NPTS$ or $NPTS-1$). For computing these integrals, all the points of the grid are used. The integration is based on the NAG D01GAF routine, suitable for tabulated functions. Of course, the update value of ϕ is also used in the boundary conditions.

In the previous version of the KYPRIX code, the computation of integral quantities were performed through a specific modification of the NAG package implemented by the KYPRIX code author that allowed to recover the whole vector solution at each time step in the subroutines (and in particular in PDEDEF), while the original package maked only available in PDEDEF the solution separately at each grid point (being in fact the package originally designed for "pure" partial differential equation, without terms involving on integrals of the solution). This modification, possible thanks to the availability of the NAG sources (and, in practice, thanks to the relative simplicity of the early library versions), permitted to update the integral quantities perfectly according to the "implicit" scheme adopted by the code for the integration in time. This is no longer feasible. Therefore, the update of the integral quantities must be now performed with a "backward" scheme, saving the solution at the previous time step in a proper vector and using it in the computation at the given time step. As well known, "backward" schemes are typically less stable than implicit schemes. And, in fact, we verified the impossibility of the D03PCF routine to work implementing the update of the quantities corresponding to the integral terms in the Kompaneets equation (and in particular of ϕ) for each time step. This were likely due to numerical instabilities.

We have then introduced a new integer control parameter into the code: STEPFI. It determines the frequency for the update the dimensionless electron temperature ϕ, relevant,

of course, in the case we want to perform an integration with a variable ϕ. We have checked that updating the integral terms in the Kompaneets equation not at every time step, but after a suitable number of time steps does not affect the accuracy of the solution. This is due to the fact that the time increasing in the code is performed with very small steps while the physical variation of ϕ occurs on longer timescales [2].

3.2.7 Radiative Compton

In the computation of the radiative Compton term there is an integral term, so it is necessary to harmonize its update according to the parameter STEPFI discussed in the previous subsection. In fact, a possible asynchronous update of it and ϕ could create numerical instabilities and the crash of the code run, as physically evident from the great relevance of both radiative Compton term and electron temperature for the evolution of low frequency region of the spectrum.

3.2.8 Integration routines

Different numerical integration routines can make similar tasks, but this is made with different algorithms. Inside KYPRIX we find a practical example: in the early release of the code the NAG D01BDF routine was used to calculate integrals of a function over a finite interval. The same task can be carried out by the D01AJF routine. Anyway, this code offers a better accuracy than D01BDF (D01AJF is in fact suitable also to integrate functions with singularities, both algebric and logarithmic). After the routines substitution, the results showed a great increasing of accuracy. In particular, this improvement offers the possibility to investigate also very small distortions that requires a very precise determination of all the relevant quantities because the absolute numerical error of the integration must be much smaller than the (very small quantities) of interest in these cases. In particular, the quantity $\Delta\epsilon_r/\epsilon_i$ (where ϵ_r is the actual density energy and ϵ_i is the energy density corresponding to the imperturbed distribution function just before the energy injection) must be constant during all the integration process in the absence of energy injection terms, according to the energy conservation. The precision increase on the computation of this quantity was noteworthy, keeping now always inside a few percent of the physical value (and its possible physical variation) of the same quantity independently of the magnitude of the considered distortion, allowing to accurately check the global accuracy of the code and assuring that the integral terms appearing in the Kompaneets equation are properly computed (this is a remarkable result, because the code can now be used also for very small distortions).

4 The introduction of the cosmological constant

Up to the about 10 years ago the favourite cosmological models were CDM or CHDM models. In the recent years the relevance of the cosmological constant term (or of dark energy contributions) has been renewed by a wide set of astronomical and cosmological observables. The numerical integration code KYPRIX has been then updated to include the cosmological constant in the terms controlling the general expansion of the universe. In particular the input background cosmological parameters considered in the code are now:

[2] Of course, for physical processes with a stronger variation of the electron temperature, the accuracy parameter (see previous subsection) should be good enough to force the code to adopt sufficiently small time steps.

$T_0, \kappa, h[= H_0/(100\mathrm{Km/s/Mpc})], \Omega_m, \Omega_b, \Omega_\Lambda, \Omega_K$, i.e. the present CMB temperature, the contribution of massless neutrinos, the Hubble constant, the (non relativistic) matter and baryon energy density, the energy densities corresponding to cosmological constant and curvature terms.
In order to compute the proper cosmic evolution of the various terms we introduced a scale factor parameter ω (Silk & Stebbins 1983), defined by:

$$\omega = \frac{a}{a_1} \equiv \frac{m_e c^2}{kT_0}\frac{1}{1+z} = 1.98 \times 10^9 \Theta (1+z)^{-1},$$

with $\Theta \equiv T_0/3^\circ K$ and the index 1 is referred to a particular epoch, when the CMB energy density was equal to the electron mass: $k_T(a_1) = m_e c^2$. So the parameter ω is analogous to the scale factor a, but normalized at the epoch in which $a = a_1$, that is to say when $kT = m_e c^2$. To write a suitable expression for its time evolution we have to introduce two new key parameters

$$\beta = \frac{\rho_{m1}}{\rho_{r1}} = 3.5 \times 10^{-6}\frac{h^2}{\Theta^3}\,\Omega_{tot}$$

that is the initial ratio between matter energy density and radiation energy density, and

$$\frac{1}{\tau_{g1}} = \left(\frac{8\pi}{3}G\rho_{r1}\right)^{1/2} = \left[\frac{8\pi}{3}G\frac{a}{c^2}\left(\frac{m_e c^2}{k}\right)^4\right]^{1/2} = 0.076\mathrm{s}^{-1}$$

defined as a initial gravitational time scale. The quantities with the index 1 refer to the epoch when $a = a_1$, with the index 0 when $t = t_0$ (today); ρ_{r1} and ρ_{m1} are related to ρ_r and ρ_m by

$$\rho_r = \rho_{0r}\left(\frac{\omega_o}{\omega}\right)^4 = \rho_{r1}\frac{1}{\omega^4}; \quad \rho_m = \rho_{0m}\left(\frac{\omega_0}{\omega}\right)^3 = \rho_{m1}\frac{1}{\omega^3}\,,$$

respectively.
Now we can define an equation for the evolution of ω:

$$\frac{\dot\omega}{\omega} = \left[\frac{8\pi}{3}G\rho(\omega)\right]^{1/2} =$$

$$\frac{8\pi}{3}G\left[\frac{\rho_{r1}\kappa}{\omega^4} + \frac{\rho_{m1}}{\omega^3} + \frac{\rho_{K1}}{\omega^2} + \rho_\Lambda\right],$$

where we have included the contribution of massless relativistic neutrinos in the term κ (see also footnote 1; the term κ should be properly evaluated considering also possible energy injections after neutrino decoupling.) Then let us redefine the key parameters for the evolution:

$$\beta = \frac{\rho_{m1}}{\rho_{r1}\kappa}\ ;\ \frac{1}{\tau_{g1}} = \left(\frac{8\pi}{3}G\rho_{r1}\kappa\right)^{1/2}.$$

With this relations we can write the evolution expression for ω:

$$\frac{\dot\omega}{\omega} = \frac{1}{\tau_{g1}}\left[\frac{1}{\omega^4} + \beta\frac{1}{\omega^3} + \beta\frac{\rho_{K1}}{\rho_{m1}\omega^2} + \beta\frac{\rho_\Lambda}{\rho_{m1}}\right]^{1/2},$$

equivalent to:

$$\dot\omega = \frac{\omega}{\tau_{g1}}\left\{\frac{1}{\omega^4}\left[1 + \beta\omega\left(1 + \frac{\rho_{K1}\omega}{\rho_{m1}} + \frac{\rho_\Lambda\omega^3}{\rho_{m1}}\right)\right]\right\}^{1/2}.$$

Let's now consider the ratio $\frac{\rho_{K1}}{\rho_{m1}}\omega$ and let's write it in a more useful way:

$$\frac{\rho_{K1}}{\rho_{m1}}\omega = \frac{\left(\rho_{K1}\frac{\omega_1^2}{\omega_0^2}\right)\frac{\omega_0^2}{\omega_1^2}}{\left(\rho_{m1}\frac{\omega_1^3}{\omega_0^3}\right)\frac{\omega_0^3}{\omega_1^3}}\omega = \frac{\rho_{K0}}{\rho_{m0}}\left(\frac{\omega_1}{\omega_0}\right)\omega\,.$$

By the definition of ω we have that $\omega_1 = 1$, while ω_0 is the value that it assumes today. Through this relations we can finally write the completed and updated expression of $\frac{\mathrm{d}t}{\mathrm{d}\omega}$:

$$\frac{1}{\dot{\omega}} = \frac{\tau_{g1}\;\omega}{\left[1+\beta\;\omega\left(1+\frac{\Omega_{K/m}\;\omega}{2.164\times10^{9}}+\frac{\Omega_{\Lambda/m}\;\omega^3}{2.164\times10^{27}}\right)\right]^{1/2}}\,,$$

where $\Omega_{x/y} = \frac{\Omega_x}{\Omega_y}$.
The equation for $\dot{\omega}$ has to be inserted in the expression giving $\mathrm{d}y = a_c\mathrm{d}t$, which is inside the integral used to compute the time variable $y(\omega) = \int_{\omega_{start}}^{\omega}\mathrm{d}y$ because we set $y = 0$ when the integration starts at $\omega = \omega_{start}$ (or equivalently at $z = z_{start}$). Finally, the expression for the time evolution of ω and y are related by the variable change:

$$\mathrm{d}y = a_c\mathrm{d}t = a_c\,\frac{\mathrm{d}t}{\mathrm{d}\omega}\,\mathrm{d}\omega = a_c\,\frac{\omega}{\dot{\omega}}\,\frac{1}{\omega}\,\mathrm{d}\omega\,,$$

where $a_c = \phi/(\tau_{c1}\omega^4)$ ($\tau_{c1} = 2.638\times10^{-9}\,\Theta^3/(h^2\Omega_b)$).
Introducing the cosmological constant and curvature terms, the code KYPRIX is suitable to be applied to interesting cases at low redshifts, where Λ supplies the greatest contribution to the expansion rate of the universe evolution (remarkable examples are spectral distortions associated to the reionization of the universe).

5 Conclusion

We have described the fundamental numerical approach and, in particular, the recent update to recent NAG versions of a numerical code, KYPRIX, specifically written for the solution of the Kompaneets equation in cosmological context, aimed to the very accurate computation of the cosmic microwave background spectral distortions under quite general assumptions. Specifically, we have discussed the main subdivisions of the code and the most relevant aspects about technical specifications and code implementation. After a presentation of the equation formalism and of the boundary conditions added to the set of ordinary differential equations derived from the original parabolic partial differential equation, we have given details on the adopted space (i.e. dimensionless frequency) grid, on the output results, on the accuracy parameters, and on the used integration routines. The introduction of the time dependence of the ratio between electron and photon temperatures and of the radiative Compton scattering term, both introducing integral terms in the Kompaneets equation, has been addressed in the specific context of the recent NAG versions by discussing the solution adopted to solve the various related technical problems. We have described also the introduction of the cosmological constant in the terms controlling the general expansion of the universe, in agreement with the fundamental discoveries of the last years.

Finally, we have reported in Figs. 1–3 the input parameter files to run the code for three representative cases of cosmological interest, the evolution of an early Bose-Einstein spectrum, of a Comptonization spectrum formed at intermediate cosmic epochs, and of a simple representation of a late dissipation process roughly mimicking the effect of a heating source

associated to the reionization of the universe. In forthcoming works we will present detailed reports on the accuracy and performance of the code and on some remarkable applications aimed to illustrate the code versatility.

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```
0 1                     # REST, STAMPA: with this parameter you can decide to start the integration from
                          the beginning (REST=0, STAMPA=1) or to restart from an old stopped integration
                          (REST=1, STAMPA=read value of previous integration)
   dati.dat             # Output file containing the features of the problem.
   datig.dat            # Output file containing a planckian spectrum at T=To, the points web of x axis
                          and the initial conditions in terms of the solution vector U.
   datip.dat            # Output file. Here are saved some integration quantities of interest like:
                          redshift, time, Te/Tr, and other.
   datide.dat           # Output file. This file contains the solution of the Kompaneets equation at many
                          cosmic times.
   datit.dat            # Output file. File like the previous, but in this the solution is saved in terms
                          of brightness temperature.
   salva1.dat           # Data file. This two files serve to restart the integration (see above)
   salva2.dat           # Data file
1 1 1 0 0 0             # Choice of physical processes: Compton, freefree, double Compton,g (heating without
                          photons production), s(photons sources), vuciel (heating of electron temperature);
                          (0 = process not activated; 1 = process activated).
   2                    # Choice of the case to be esaminated (INIZ=2, this case corresponds to an integratio
                          that starts from a Bose-Einstein spectrum, that is to say a primordial cosmological
                          case).
   1.4d-6               # Chemical potential (related to INIZ=2)
   0.68  2.725  0.29  0.047  0.73
                        # Cosmological parameters: Hubble parameter, today CMBR temperature, matter density
                          parameter, barionic d.p., cosmological constant d.p.
1 0                     # VARFI=1 indicates an integration with a varying Te/Tr (if VARFI=0 Te/Tr keeps a
                          constant value during the integration; choice for a dymamical complication in
                          the universe evolution (DINAM=0 not activated).
   8                    # STEPFI: integer that determinate the refreshing frequency of both Te/Tr and the
                          rates related to the double Compton.
   1                    # CASO: 1 = stop the integration at Wric = z(recombination)
                                2 = stop at z=0 (today)
                                3 = choose a Wout
   1                    # BRUTAL: here you can choose a "brutal" stop for the ending of the integration
                          (BRUTAL=1 the integration stops with an over-flow at Wout, this way is better
                          when Yout is not known with precision; BRUTAL=0 instead corresponds to a clean
                          stop, better if Yout is well known).
   1                    # Choice of the boundary conditions type.
                          BCOND = 0 corresponds to Dirichlet boundary conditions (constant values on the edge
                          BCOND = 1 corresponds to Neumann boundary conditions (null flux on the edges).
   3.3d+3  1.d+10  5    # Wstart,Wout,nstep: time integration interval and intermediate steps in wich
                          KYPRIX gives the results.
   5.d+4                # Intermediate time step.
   9.d+5                # Intermediate time step.
   1.d+6                # Intermediate time step.
   8.d+6                # Intermediate time step.
   6.d+7                # Intermediate time step.
   1.d+9                # Intermediate time step.
   1.d-10               # ACC: the accuracy required.
-4.3 1.7  36001         # A,B,NPTS: the x range limits [A,B] and the number of mesh points on the x axis.
2500                    # Intermediate steps in wich KYPRIX gives a simpler output.
9000                    # Intermediate x step.
12000                   # Intermediate x step.
15000                   # Intermediate x step.
23000                   # Intermediate x step.
28000                   # Intermediate x step.
30000                   # Intermediate x step.
33900                   # Intermediate x step.
```

Figure 1: Example of input parameters to run the KYPRIX code. This case corresponds to an integration of the Kompaneets equation starting from a Bose-Einstein spectrum.

```
0 1                                  # REST, STAMPA: with this parameter you can decide to start the integration from
                                       the beginning (REST=0, STAMPA=1) or to restart from an old stopped integration
                                       (REST=1, STAMPA=read value of previous integration)
     dati.dat                        # Output file containing the features of the problem.
     datig.dat                       # Output file containing a planckian spectrum at T=To, the points web of x axis
                                       and the initial conditions in terms of the solution vector U.
     datip.dat                       # Output file. Here are saved some integration quantities of interest like:
                                       redshift, time, Te/Tr, and other.
     datide.dat                      # Output file. This file contains the solution of the Kompaneets equation at many
                                       cosmic times.
     datit.dat                       # Output file. File like the previous, but in this the solution is saved in terms
                                       of brightness temperature.
     salva1.dat                      # Data file. This two files serve to restart the integration (see above)
     salva2.dat                      # Data file
1 1 1 0 0 0 0                        # Choice of physical processes: Compton, freefree, double Compton,g (heating without
                                       photons production), s(photons sources), vuoiel (heating of electron temperature);
                                       (0 = process not activated; 1 = process activated).
          6                          # Choice of the case to be esaminated (INIZ=6, this case corresponds to an integratio
                                       that starts from a superposition of black bodies).
     1.d-5                           # Amount of fractional energy surplus (related to INIZ=6)
0.68  2.725  0.29  0.047  0.73       # Cosmological parameters: Hubble parameter, today CMBR temperature, matter density
                                       parameter, barionic d.p., cosmological constant d.p.
1 0                                  # VARFI=1 indicates an integration with a varying Te/Tr (if VARFI=0 Te/Tr keeps a
                                       constant value during the integration; choice for a dymamical complication in
                                       the universe evolution (DINAM=0 not activated).
          8                          # STEPFI: integer that determinate the refreshing frequency of both Te/Tr and the
                                       rates related to the double Compton.
          1                          # CASO: 1 = stop the integration at Wric = z(recombination)
                                             2 = stop at z=0 (today)
                                             3 = choose a Wout
          1                          # BRUTAL: here you can choose a "brutal" stop for the ending of the integration
                                       (BRUTAL=1 the integration stops with an over-flow at Wout, this way is better
                                       when Yout is not known with precision; BRUTAL=0 instead corresponds to a clean
                                       stop, better if Yout is well known).
               1                     # Choice of the boundary conditions type.
                                       BCOND = 0 corresponds to Dirichlet boundary conditions (constant values on the edge
                                       BCOND = 1 corresponds to Neumann boundary conditions (null flux on the edges).
2.5d+4  1.d+10  5                    # Wstart,Wout,nstep: time integration interval and intermediate steps in wich
                                       KYFRIX gives the results.
     5.d+4                           # Intermediate time step.
     9.d+5                           # Intermediate time step.
     1.d+6                           # Intermediate time step.
     8.d+6                           # Intermediate time step.
     6.d+7                           # Intermediate time step.
     1.d+9                           # Intermediate time step.
     1.d-10                          # ACC: the accuracy required.
-4.3 1.7 36001                       # A,B,NPTS: the x range limits [A,B] and the number of mesh points on the x axis.
2500                                 # Intermediate steps in wich KYFRIX gives a simpler output.
9000                                 # Intermediate x step.
12000                                # Intermediate x step.
15000                                # Intermediate x step.
23000                                # Intermediate x step.
28000                                # Intermediate x step.
30000                                # Intermediate x step.
33900                                # Intermediate x step.
```

Figure 2: This set of parameters has been used to integrate the Kompaneets equation starting from intermediate epochs; the initial condition is a Comptonization spectrum.

```
0 1                                  # REST, STAMPA: with this parameter you can decide to start the integration from
                                       the beginning (REST=0, STAMPA=1) or to restart from an old stopped integration
                                       (REST=1, STAMPA=read value of previous integration)
     dati.dat                        # Output file containing the features of the problem.
     datig.dat                       # Output file containing a planckian spectrum at T=To, the points web of x axis
                                       and the initial conditions in terms of the solution vector U.
     datip.dat                       # Output file. Here are saved some integration quantities of interest like:
                                       redshift, time, Te/Tr, and other.
     datide.dat                      # Output file. This file contains the solution of the Kompaneets equation at many
                                       cosmic times.
     datit.dat                       # Output file. File like the previous, but in this the solution is saved in terms
                                       of brightness temperature.
     salva1.dat                      # Data file. This two files serve to restart the integration (see above)
     salva2.dat                      # Data file
1 1 1 0 0 1                          # Choice of physical processes: Compton, freefree, double Compton,g (heating without
                                       photons production), s(photons sources), vuoiel (heating of electron temperature);
                                       (0 = process not activated; 1 = process activated).
   1                                 # Choice of the case to be esaminated (INIZ=1, this case corresponds to an integratio
                                       that starts from a planckian spectrum).
   0.d-0                           # Amount of fractional energy injected (related to INIZ=6)
   1.d+4                           # FIEL, the constant value of Te/Tr setted to inject energy in the radiation field.
   0.68   2.725   0.29   0.047   0.73  # Cosmological parameters: Hubble parameter, today CMBR temperature, matter density
                                       parameter, barionic d.p., cosmological constant d.p.
   0 0                             # VARFI=1 indicates an integration with a varying Te/Tr (if VARFI=0 Te/Tr keeps a
                                       constant value during the integration; choice for a dymamical complication in
                                       the universe evolution (DINAM=0 not activated).
   -                               # STEPFI: integer that determinate the refreshing frequency of both Te/Tr and the
                                       rates related to the double Compton.
   3                               # CASO: 1 = stop the integration at Wric = z(recombination)
                                          2 = stop at z=0 (today)
                                          3 = choose a Wout
   1                               # BRUTAL: here you can choose a "brutal" stop for the ending of the integration
                                       (BRUTAL=1 the integration stops with an over-flow at Wout, this way is better
                                       when Yout is not known with precision; BRUTAL=0 instead corresponds to a clean
                                       stop, better if Yout is well known).
     1                             # Choice of the boundary conditions type.
                                     BCOND = 0 corresponds to Dirichlet boundary conditions (constant values on the edge
                                     BCOND = 1 corresponds to Neumann boundary conditions (null flux on the edges).
   1.d+8  1.d+10  5                # Wstart,Wout,nstep: time integration interval and intermediate steps in wich
                                       KYPRIX gives the results.
   5.d+4                           # Intermediate time step.
   9.d+5                           # Intermediate time step.
   1.d+6                           # Intermediate time step.
   8.d+6                           # Intermediate time step.
   6.d+7                           # Intermediate time step.
   1.d+9                           # Intermediate time step.
   1.d-10                          # ACC: the accuracy required.
-4.3 1.7 36001                     # A,B,NPTS: the x range limits [A,B] and the number of mesh points on the x axis.
2500                               # Intermediate steps in wich KYPRIX gives a simpler output.
9000                               # Intermediate x step.
12000                              # Intermediate x step.
15000                              # Intermediate x step.
23000                              # Intermediate x step.
28000                              # Intermediate x step.
30000                              # Intermediate x step.
33900                              # Intermediate x step.
```

Figure 3: Input parameters for a simple simulation of a process of reionization of the universe. The initial condition is a Planckian spectrum. The integration starts at $z \sim 20$.

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