Hamevol1.0: a C++ code for differential equations based on Runge-Kutta algorithm. An application to matter enhanced neutrino oscillation

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Abstract: We present a C++ implementation of a fifth order semi-implicit Runge-Kutta algorithm for solving Ordinary Differential Equations. This algorithm can be used for studying many different problems and in particular it can be applied for computing the evolution of any system whose Hamiltonian is known. We consider in particular the problem of calculating the neutrino oscillation probabilities in presence of matter interactions. The time performance and the accuracy of this implementation is competitive with respect to the other analytical and numerical techniques used in literature. The algorithm design and the salient features of the code are presented and discussed and some explicit examples of code application are given.

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1. Program Summary

- Title of the program: Hamevol
- Version number: 1.0
- Available at: http://wwwteor.mi.infn.it/antonell/programs/RKutta, and mirrors
- Programming language: C++
- Platform: any platform supporting a C++ compiler (examples: Linux, Unix, Windows)
- Tested on: Pentium PC, AMD PC
- Memory requirements for execution: Standard application: 40 Kbytes
- No. of bytes in distributed program, including test data, etc: 235.000
- Keywords: Numerical algorithms, Differential equations, Hamiltonian evolution, Oscillation,
- **Nature of physical problem**: Numerical solution of Hamiltonian differential equations. Application to the numerical calculation of the oscillation probability for a quantum system (like, for instance, neutrinos of any kind propagating in a medium).

- **Method of solution**: Algorithm based on fifth order semi-implicit Runge-Kutta method.

- **Typical running time**: \( \approx 30 \) seconds for every single point on a Pentium IV PC.

### 2. Introduction. The mathematical problem.

The use of numerical algorithms and suitable computational techniques has often been very useful to find the solution of difficult problems which are of interest for mathematics and other applied science. This is particularly true in our days, when the relationships between information technology and other sciences are becoming closer and closer.

In this paper we discuss the adaptation of well known numerical techniques to a general class of problems which are described by ordinary differential equations and we present some examples taken from physics.

The numerical code and algorithm we are presenting in this work is based on the implementation of the Runge-Kutta method and it can find significant applications in the study of different physical systems. In fact the evolution of every system can be fully described once we are able to solve the differential equations that drive this evolution. The typical example is the case in which one wants to study a linear quantum system that is described by a vector \( X \equiv (X_i, i = 1..N) \), where \( X_i \) are the elements of an appropriate basis describing the system.

The system of linear differential equations we are interested in can be put in the simple form:

\[
\frac{i}{dt} X(t) = H(t)X(t),
\] (2.1)

where \( H \) is a matrix determining the evolution of the system.

In the language of physics \( H \) is the Hamiltonian of the system and Equation (2.1) is the corresponding Schrodinger equation. It is clear, however, that the system of differential equations (2.1) is very general and they can describe also problems of different nature in fields that are completely different from physics. Depending on the kind of problems one has to solve, the requirements which are fundamental for the solutions can be different. This can suggest the choice of a particular algorithm in order to fulfill these requirements in the best possible way. For instance, as we are going to discuss later, in the physical problems we are interested in, the delicate point is efficiency more than accuracy and this justifies the choice of a particular version of adaptive Runge-Kutta method that, if properly adapted to our purpose, enable us to obtain satisfactory results.

The solution of equation (2.1) can be written in terms of the fundamental system of solutions, or equivalently called evolution operator \( U(t, t_0) \), defined by the expression:

\[
U(t, t_0) = \exp \left[ -iH(t - t_0) \right],
\] (2.2)

where \( t_0 \) is the initial time at which we know the state of the system. The simple formula given above is valid for a time independent Hamiltonian. In the case in which the Hamiltonian of the
system is changing in the time (like, for instance, in presence of matter effects), formula (2.2) must be replaced by path-ordered exponential
\[ U(t, t_0) = P \exp \left[ -i \int_{t_0}^{t} d\tau H[\tau] \right]. \] (2.3)

The code we are presenting here can be used to solve in an iterative way the system of differential equations appearing in Equation (2.1). This is particularly important in the case of Hamiltonians which are explicitly time dependent or which contain terms fastly oscillating in time.

The structure of this paper is the following. We start discussing in section 3 some concrete examples, taken from physics, of situations in which the application of the algorithm presented here is particularly suited. In the next section we present the algorithmic structure and salient aspects of the code we developed. This section includes a presentation of the algorithm, all the essential informations about the distribution, the main subroutines and functions and about the way of working of a sample program. In section 5 we draw our final conclusions. An example of a sample program, with some specific Hamiltonian set up and the relative outputs are presented in the Appendices.

3. The Physical motivations.

A very interesting example is given by the study of neutrino physics, which has been one of the central topics of elementary particle physics in the last years. A detailed discussion about the main properties of neutrinos and the relevance of their study for our knowledge of the intimate structure of matter is beyond the scope of this work. Therefore we refer the interested reader to the many reviews one can find in literature [1]. Here we just recall that during the last years the answer has been given to the central question of neutrino physics, which puzzled physicists for more than seventy years, that is to discriminate whether this particle is massive or massless.

We know by now that neutrinos are massive and oscillating particles and the proof of this has been given by the important results obtained mainly in the last decade (and especially in the very last years) by the experiments looking for oscillation signals of neutrinos from different sources: solar [2, 3], reactor [4] and atmospheric [5] neutrinos.

The great relevance of these results is confirmed by the fact that this is up to now the strongest indication of oscillation we have in the leptonic sector and it is impossible to accomodate it in the usual “minimal version” of the Standard Model (the theory describing very well the electroweak interactions of elementary particles). One can say that neutrino oscillations is a hint for physical phenomena beyond to what is presently known.

All these experimental evidences in favors of the oscillation hypothesis have proved that the flavor eigenstates of neutrinos, that is the ones entering in the weak processes, are in fact quantum superspositions of different mass eigenstates (at least three different mass eigenstates are needed to explain the full set of experimental data, if one doesn’t take into account the controversial results of the LSND experiment). During the evolution the composition of this quantum system can change giving rise to the oscillation phenomenon detected in the experiments.

Any study of neutrino oscillation is necessarily based on the calculation of the so called neutrino survival (or transition) probability. This is the probability that a neutrino emitted by
a source with a certain flavor, for instance an electronic neutrino emitted in the solar fusion processes, remains with the same flavour (or is converted into a different flavor neutrino) before reaching the detector.

Hence the basic quantity to compute is the survival probability in matter for a neutrino of a certain flavor:

\[ P(\nu_i \rightarrow \nu_i; t, E_\nu) = |\langle \nu_i(t_0) | U(t, t_0) | \nu_i(t_0) \rangle|^2 \]  

(3.1)

where \( t_0 \) is the initial time at which the neutrino is assumed to be in the flavour eigenstate \( \nu_i \) (with \( i = e, \mu, \tau \)) and \( U(t, t_0) \) is the evolution operator given by Equation (2.3).

In absence of matter the basis in which the Hamiltonian is diagonal is simply the mass basis, whose eigenstates \( \nu_\alpha \) are connected to the neutrino flavor eigenstates \( \nu_i \) by means of the mixing matrix \( U \):

\[ \nu_i = \sum_\alpha U_{i\alpha} \nu_\alpha, \quad i = e, \mu, \tau \quad \text{and} \quad \alpha = 1, 2, 3. \]  

(3.2)

Using the same compact notation of Equation (2.1), we denote the set of the three neutrino mass eigenstates with the vector \( \nu \), where \( \nu \equiv (\nu_\alpha, \alpha = 1, 2, 3) \). This notation can be simply extended to the case in which one has more than three neutrinos \(^1\). The Schroedinger equation describing the evolution of the system in vacuum under the relativistic approximation and in the hypothesis of equal momentum for different mass eigenstates is:

\[ i \frac{d\nu}{dt} = H^0 \nu \]  

(3.3)

where

\[ H^0 = \text{Diag}E_\alpha = \sqrt{p^2 + m^2} \simeq E_\nu + \begin{pmatrix} m_1^2/2E_\nu & m_2^2/2E_\nu & m_3^2/2E_\nu \end{pmatrix} \]  

(3.4)

The last experimental data (both for atmospheric and solar neutrinos) have proved that to describe neutrino evolution one has to take into account also the modification of the oscillation pattern due to the very important effects of interaction with matter. This gives rise to the well known MSW effect \(^3\). The problem of calculating neutrino oscillation probability in presence of matter effects has been faced by many authors with different approaches, both numerical and analytical, in the case of two neutrino flavors \(^4\) \(^5\) \(^6\). Exact solutions to the three neutrino MSW equations were derived \(^7\) \(^8\) \(^9\) for simple matter densities. Numerical algorithms for direct computation of the solar neutrino survival probability with all three active neutrinos have been presented in \(^10\) \(^11\) \(^12\).

The purpose of our code Hamevol is to calculate the electron-neutrino survival probability for a given neutrino energy, a given density profile, given neutrino masses and mixing matrix. This set of (three) oscillation probabilities will be used subsequently by other (Fortran) programs to calculate expected signals from diverse neutrino experiments. Due to the fact that both the mixing matrix and the density function are considered input parameters of Hamevol, all kinds of neutrino oscillation problems may be tackled, including those relevant to anti-neutrinos only.

In presence of standard matter with arbitrary electron number density, the propagation is usually well described by the following system of differential equations:

\(^1\)This is the case if one introduces also sterile neutrinos in the analysis
\[
\frac{d\nu}{dt} = \left(H^0 + \rho(t)UVU^\dagger\right)\nu,
\]
where V is a matrix with \(V_{11}\) as only non-zero element, \(\rho(t)\), essentially a forward scattering amplitude, is proportional to the electron number density of the medium \(N_e(t)\)
\[
\rho(t) = \pm \sqrt{2} G_F N_e(t) \tag{3.6}
\]
and \(U\) is the mixing matrix connecting the neutrino flavor eigenstates with the mass eigenstates. In the case of three neutrino generations, adopting the Particle Data Group [15] convention for the mixing matrix, one gets:
\[
\begin{pmatrix}
\nu_e \\
\nu_\mu \\
\nu_\tau
\end{pmatrix} =
\begin{pmatrix}
c_1 c_3 & s_1 c_3 & s_3 \\
-s_1 c_2 - c_1 s_3 s_2 & c_1 c_2 - s_1 s_3 s_2 & c_3 s_2 \\
s_1 s_2 - c_1 s_3 c_2 & -c_1 s_2 - s_1 s_3 c_2 & c_3 c_2
\end{pmatrix}
\times
\begin{pmatrix}
\nu_1 \\
\nu_2 \\
\nu_3
\end{pmatrix} \tag{3.7}
\]
where \(c_i \equiv \cos \theta_i\) and \(s_i \equiv \sin \theta_i\) and the three mixing angles \(\theta_1 = \theta_{12}, \theta_2 = \theta_{23},\) and \(\theta_3 = \theta_{13}\) roughly measure mixing between mass eigenstates (1-2), (2-3), and (1-3) respectively. We have neglected the CP violating phase, which is irrelevant in this problem.

The plus/minus sign in formula of Equation (3.6) is for neutrinos/antineutrinos respectively.
The time dependence of the electron density \(N_e\) is a crucial factor involved in solving the evolution equation.

The difference of the eigenvalues of \(H^0\) (the inverse of the usually defined oscillation length) is typically considered to be, in the solar case, of the order
\[
\frac{m_i^2 - m_j^2}{2E} \approx \frac{10^{-4} - 10^{-5}}{1 \text{ MeV}} \approx 10^{-10} - 10^{-11} \text{ eV}
\]

In [10] an analytical solution of the problem has been found for the case in which the electron number density is parametrized (data taken from [16]), for sufficiently far distances from the solar core as:
\[
N_e(r) = N_0 \exp(-\lambda r) ; \lambda \simeq 10.6 \frac{r}{r_0} \tag{3.8}
\]
with \(r, r_0\) the distance from the center and solar radius respectively.

An important peculiarity of neutrino propagation in matter with respect to vacuum is that for a certain value of the parameters a resonance appears at a certain point along the neutrino trajectory. This resonance takes place if the following condition is satisfied:
\[
\rho(t_{\text{res}}) = \frac{\Delta m^2 \cos 2\theta}{E}, \tag{3.9}
\]
where \(\theta\) is the mixing angle between the 2 neutrino flavors taking part to the oscillation phenomenon. Apart from this approximate results, exact solutions have appeared for particular forms of the function \(\rho\): for linear densities, in terms of Weber-Hermite functions ([17, 18]); for functions of the form \(\rho(t) = C(1 + \tanh(\lambda t))\) in [19], and for exponentially decaying densities \(\rho(t) = ce^{-\lambda t}\) in [20, 21].

The parametrization of Equation (3.8) is the one used also in the sample program we present as an example in subsection 4.4.
In any case our numerical algorithm enables us to find a solution of the problem for every expression one chooses for the electron density number.

The capability of solving the system of Equations (3.5) and, therefore, of computing the neutrino survival (or transition) probabilities as a function of the mixing parameters is an essential ingredient in every analysis of neutrino data. The theoretical expected signal in every experiment is obtained by convoluting neutrino fluxes, oscillation probabilities, neutrino cross sections and detector energy response functions. The comparison of these expected signal as a function of the mixing parameters with the experimental results is then usually performed by means of a $\chi^2$ statistical analysis. The outcome of this kind of analyses is typically the production of exclusion plots selecting the regions of the mixing parameter plan which are in agreement with the data at a certain confidence level. The algorithm we are presenting in this work enables us to numerically solve the neutrino evolution equations for all the oscillation parameter space, without the need to introduce the approximation which are required in different approaches based on the use of semi-analytical expressions in portions of the parameter space. For a more detailed description of the full procedure we adopted for a phenomenological analysis of solar and reactor neutrino data we refer the interested reader to [20].

The numerical algorithm we are presenting here finds also other relevant applications. Some significant examples are:

a) the study of the neutrino evolution inside stochastic media and neutrino propagation in solar magnetic field [21]. In these cases one has to solve systems of differential equations where, respectively, $(2N)^2$ and $(2N)$ equations appear ($N$ is the number of neutrino species);

b) solution of the renormalization group equation for the Minimal Supersymmetric Standard Model in a Supergravity scenario. Here the number of differential equations in the systems that have to be solved simultaneously (with a complicated mixture of initial and boundary conditions) is typically between thirty and one hundred. [22]

4. Code Structure

4.1 Algorithmics

There are different ways of solving a possibly stiff set of equations and the advantages and drawbacks of each of them must be evaluated keeping in mind the kind of problem one wants to study. In our case we aim for efficiency rather than precision (a relative precision of $10^{-3} - 10^{-5}$ in conversion probabilities for example would be sufficient in a typical application in particle physics propagation problems). Therefore we opted for an adaptive Runge-Kutta (RK) algorithm.

The Runge-Kutta method [23] is particularly suitable for solving differential equations, starting from the knowledge of the function at the a fixed initial point $X$ and advancing the solution from $X$ to $X + h$, by using the evaluation of the function at intermediate points inside the interval $h$. By properly combining these evaluations one can reduce the error in the final output. The method is conventionally denoted of order $n$ if its error term is $O(h^{n+1})$.

An essential characteristic of a good Ordinary Differential Equations integrator is the capability of having an adaptive control over its progress and a mechanism for adapting its stepsize, in such a way to obtain the required accuracy with the minimal possible computational effort. This property is possessed by the algorithm we implemented. Although an implicit RK would be advised for stiff equations, there are several alternatives, such as the semi-implicit fifth-order
RK routine we have chosen. This routine requires the determination of the function at five different points in the interval between the chosen steps. They are

\[
\begin{align*}
k_1 &= hf(x_n, y_n) \\
k_2 &= hf(x_n + a_2 h, y_n + b_{21} k_1) \\
&\vdots \\
k_6 &= hf(x_n + a_6 h, y_n + b_{61} k_1 + \ldots b_{65} k_5) \\
y_{n+1} &= y_n + \sum_{i=1}^{6} c_i k_i
\end{align*}
\]

where the coefficients \(a_i, b_{ij}\) and \(c_i\) must satisfy certain constraints in order to ensure stability and convergence. This algorithm is well suited for adaptive stepping, due to the fact that among the six evaluations in Eq. \((4.1)\) there is an embedded fourth-order combination, which, although redundant, gives us an estimate of the error at each evaluation thereby allowing us to adjust the step size. Table \((1)\) gives a list of \(a_i, b_{ij}\) and \(c_i\) as determined by Cash and Karp \([23]\).

| \(i\) | \(a_i\) | \(b_{ij}\) | \(c_i\) | \(c_i^*\) |
|-----|----|-----|-----|-----|
| 1   | \(\frac{37}{378}\) | \(\frac{2825}{27648}\) |
| 2   | \(\frac{1}{3}\) | \(\frac{1}{3}\) | 0   | 0   |
| 3   | \(\frac{3}{10}\) | \(\frac{3}{10}\) | \(\frac{9}{10}\) | \(\frac{621}{48384}\) |
| 4   | \(\frac{3}{5}\) | \(\frac{3}{10}\) | \(\frac{-9}{10}\) | \(\frac{6}{5}\) | \(\frac{125}{250}\) | \(\frac{18575}{48384}\) |
| 5   | \(1\) | \(\frac{-11}{54}\) | \(\frac{5}{2}\) | \(\frac{-70}{27}\) | \(\frac{35}{27}\) | 0   | \(\frac{127}{14336}\) |
| 6   | \(\frac{7}{8}\) | \(\frac{1631}{55296}\) | \(\frac{175}{512}\) | \(\frac{575}{13824}\) | \(\frac{44275}{110592}\) | \(\frac{253}{44275}\) | \(\frac{512}{1771}\) | \(\frac{1}{4}\) |

| \(j\) | 1   | 2   | 3   | 4   | 5   |

**Table 1:** Cash-Karp coefficients for our RK routines, taken from Ref. \([23]\).

### 4.2 The distribution

The distribution of the program is contained in the tarred gzipped file `hamevol1.0.tar.gz`. In any Linux or Unix system, unpacking and untarring this distribution file will produce a local directory called `Hamevol1.0` containing the following ascii files:

- `hamevol-rungekutta.hpp` The file with the main routines.
- `hamevol-util.hpp` Some auxiliary utilities.
- `hamevol-sample.hpp` The sample program header.
- `hamevol-sample.cpp` The sample program.
- `Makefile` A simple compiling make example.

In the same Linux or Unix system the execution of the command
or directly the explicit call to the C++ compiler

```bash
make
```

```bash
./hamevol.x  
```

should produce an executable file from our sample program dedicated to solve some particular neutrino propagation problem. To run the executable the following command should be typed

```bash
./hamevol.x OPTION
```

where in our sample program `OPTION=1,0` depending on whether full Sun+Earth or only Sun propagation is demanded. As a consequence, some brief output will appear on the standard output, mainly information about parameter settings and options. In addition, as a result of the execution our sample program writes an output file `runge.out` with the neutrino conversion probabilities along the neutrino trajectory.

In our distribution, we have well separated the code corresponding to the general routines implementing the Runge-Kutta algorithm from those corresponding to a particular application (the “sample” files) of interest to us and that are presented here: the computation of oscillation neutrino probabilities. Within our sample programs, it is also well differentiated the driver code which calls the RK routines from the part where a concrete hamiltonian is built. In the most basic case, a general user should be able to use our program as a black box for his own purposes simply plugging his own definition for the hamiltonian.

In the following we will first describe the main routines included in file `hamevol-rungekutta.hpp` and then those contained in the sample programs.

4.3 The RK algorithm. Main Subroutines

The kernel code is built up with five main subroutines. They correspond to procedures and methods well known in the literature. We have improved and adapted them for our purposes. The following classes are located in file `hamevol-rungekutta.hpp`. Here it follows a brief description of any of them together with its calling sequence. For brevity, arguments which are also referenced somewhere else are omitted here.

- **void runge(CNumber y[], CNumber dydx[], CNumber (*H)(...), int n, Number x, Number h, CNumber yout[], void (*derivs)(...))**

  Given the value $y[1..n]$ of the vector state describing a physical system made up with $n$ components and evolving according to Schroedinger equation and knowing the Hamiltonian $H$ of the system, the subroutine produces the advanced solution as the function at the incremented variables $yout[1..n]$.

- **void odeint(CNumber ystart[], int nvar, Number x1, Number x2, Number eps, Number h1, Number hmin, CNumber (*H)(...), void (*derivs)(...), void (*rkqs)(...))**
This is a Runge-Kutta driver with adaptive stepsize control. It integrates the starting values \( y_{\text{start}}[1..nvar] \) from \( x_1 \) to \( x_2 \) with accuracy \( \text{eps} \), storing the intermediate results in global variables.

A value \( h_1 \) should be set as a guessed first stepsize, \( h_{\text{min}} \) as the minimum allowed stepsize (it can be zero). On output \( \text{nok} \) and \( \text{nbad} \) are the number of good and bad (but retried and fixed) steps taken, and \( y_{\text{start}} \) is replaced by values at the end of the integration interval.

- \textbf{void rkqs(CNumber} y[], CNumber dydx[], int n, Number *x, Number htry, Number eps, CNumber yscal[], Number *hdid, Number *hnext, CNumber (*H)(...), void (*derivs)(...))

This routine \textit{rkqs} is implemented in order to perform an adaptive 5th order Runge-Kutta integration. The method enables to have a monitoring of local truncation error, in order to ensure the required accuracy and adjust the stepsize. The inputs are the independent variable vector \( y[1..n] \) and its derivative \( dydx[1..n] \) at the starting value of the independent variable \( x \). Other inputs are the stepsize \( h_{\text{try}} \), the required accuracy \( \text{eps} \), and the vector \( yscal[1..n] \) against which the error is scaled. On output, \( y \) and \( x \) are replaced by their new values, \( hdid \) is the stepsize that was actually accomplished, and \( h_{\text{next}} \) is the estimated next stepsize.

- \textbf{void rkck(CNumber} y[], CNumber dydx[], int n, Number x, Number h, CNumber yout[], CNumber yerr[], CNumber (*H)(...), void (*derivs)(...))

Used in adaptive size Runge-Kutta integration. Given values for the variables \( y[1..n] \) and their derivatives \( dydx[1..n] \) known at \( x \), advance solution over an interval \( h \) and return the incremented variables as \( yout[1..n] \). Also returns an estimate of the local truncation error in \( yout \) using embedded fourth-order method.

The user supplies the routine \( H(x,i,j) \), which returns the element \( (i,j) \) of the hamiltonian of the evolution.

- \textbf{void deriv(Number} x, CNumber y[], CNumber dy[], int n, CNumber (*H)(...))

The user-supplied routine \textit{derivs} is used for calculating the right-hand side derivative. The user supplies the routine \textit{derivs}(x,y,dydx,n,H), which returns the derivatives \( dydx \) of the many variable function \( y \) with respect to the vector \( x \) at the point \( x \).

The following Auxiliary functions which will allocate the following data structures are included in the auxiliary distribution file \textit{hamevol-util.hpp}.

\begin{verbatim}
CNumber *Cvector(long nh): allocate a CNumber vector with subscript range v[1..nh]
Number *vector(long nh): a vector with subscript range v[1..nh].
int *ivector(long nh): a vector with subscript range v[1..nh].
unsigned long *lvector(long nh): a vector with subscript range v[1..nh].
unsigned char *cvector(long nh): a vector with subscript range v[1..nh].
template <class Type> Type **matrix(...) allocate a Type matrix with a subscript range.
\end{verbatim}
4.4 Sample Program and Inputs

The `void main` routine in `hamevol-sample.cpp` file takes the values of the neutrino wave functions at initial starting points for physical initial conditions which are standard for solar neutrino physics ($\nu_e(0) = 1, \nu_\mu(0) = 0, \nu_\tau(0) = 0$) and calculates the final wave function and corresponding probabilities at the target final points. The algorithm includes the following steps:

- It takes from the command line the user argument “1” (Sun) or “0” (Earth) propagation.
- It performs argument validation, set internal flags and writes to the standard output a list of current values of diverse parameters.
- It declares the output file stream `out ` runge.dat `, class ofstream included within <fstream.h>.
- It declares the `vector` objects `nu, dnu`, respectively instances of the neutrino wave function and their vector derivative. It performs diverse other initializations.
- Finally functions `odeint` and `evolve` are repeatedly called until the desired final point or the maximum number of steps is reached.

Different parameters, for example the number of equations, or in this physical case the number of neutrino species ($N = 2, 3$), have to be set in the header file `hamevol-sample.hpp`. We run the RK algorithm to obtain the transition probabilities of neutrinos produced at the sun center with a given energy and mixing angle as a function to its position along the trajectory sun-earth. The user should provide routines for computing the electron densities at Sun and the Earth along the neutrino trajectory. They appear in the matter part of the neutrino hamiltonian. We include examples of the main program and other smaller routines as appendices.

5. Conclusions

A new code based on a semi-implicit fifth order adaptive Runge-Kutta algorithm has been developed by us. It can be used as solver for many systems of differential equations, like, for instance, the ones that usually describe the evolution of a system in physics and in other fields. This algorithm is particularly suited for the solution of differential equations in which the operator driving the evolution of the system is changing in time.

Here we focus our attention to the application of this code to the study of physical problems, like solving the Schroedinger equation for a system that is a quantum superposition of different possible states. The explicit example we present is the study of the evolution and calculation of transition probability for neutrinos emitted by a source and travelling in a medium. This code has been already applied by us as a useful tool to obtain a check with respect to other possible numerical algorithms (like the ones based on the evolution operator formalism) in our phenomenological analysis of different neutrino oscillation experiments. This analysis has confirmed the validity of neutrino oscillation hypotheses and enabled us to determine the allowed region for mixing parameters, a topic of great relevance in Elementary Particle Physics.

In this paper we discuss the structure of the algorithm we developed and the main features of our code. We also present a sample program and give some typical outputs, as a concrete example of application of our algorithm.
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7. Appendices

7.1 Using Hamevol

Here we present the main sample program, corresponding to the file hamevol-sample.cpp, where we show explicitly the use of the main routines.

```c
#include "hamevol.hpp"
#include <string.h>

/* Inizialize the vacuum values (........)*/
/* #define parameters (........)*/

Number Var;
CNumber **HH0; // is the vacuum Hamiltonian in the flavour eingenstates
struct mix{  // contains the mixing matrix
    Number mass[N + 1];
    CNumber U[N + 1][N + 1];
} mixing;

/* nu are the wave functions, dnu their derivative */
CNumber *nu, *dnu;

int main(int arg, char** argv){
    Number x1=0.;
    Number x2;

    /* Argument and parameter validation (............) */
    /* Information output (.............)*/

    time_t ti, tf;
    CNumber *onu;

    nu = Cvector (N);
    dnu = Cvector (N);
    onu = Cvector (N);

    ofstream out ("runge.dat"); /* save data in runge.dat */

    srand (time (&ti));
    time (&ti);

    Var = VarI;
    Number Var0 = Var;
    Number h = (VarF - VarI) / INIT_STEPS;
    Number eps = Eps_Error;
    vacuum_values ();//
```
/* Main Routines */
odeint (nu, N, x1, x2, eps, dist, dist_min, H, deriv, rkqs);
evolute (nu, &out, Var0);

for (int nstp = 1; nstp <= MAX_STEPS; nstp++)
{ /* Take at most MAXSTP steps */
    for (int i = 1; i <= N; i++)
        onu[i] = nu[i];
    vacuum_values();
    if ((VarO + h - VarF) * (VarF - VarI) > 0.0) /* Are we done? */
        h = VarF - VarO;
    Var = VarO + h;
    odeint (nu, N, x1, x2, eps, dist, 0.0, H, deriv, rkqs);
    if (distance (nu, onu, N) > Prob_Error)
    {
        //cout << "DECREASE: h=" << h << endl;
        h *= DECREASE;
        Number htemp = ((h < 0) ? FMIN (h, -abs ((VarI - VarF) / MAX_STEPS)) : FMAX (h, abs ((VarI - VarF) / MAX_STEPS)));
        if (htemp != h)
        {
            evolute (nu, &out, Var);
            VarO = Var;
        }
        h = htemp;
    }
    else
    {
        evolute (nu, &out, Var);
        h *= INCREASE;
        Number htemp = ((h < 0) ? FMAX (h, -abs ((VarI - VarF) / MIN_STEPS)) : FMIN (h, abs ((VarI - VarF) / MIN_STEPS)));
        if (htemp != h)
            h = htemp;
        VarO = Var;
    }

    if ((Var - VarF) * (VarF - VarI) > 0.0)
    { /* Are we done? */
        cout << "t=" << time (&tf) - ti << endl;
        return 0; /* normal exit */
    }
}

cout << "Too many steps in routine evolution_matter!" << endl;
return -1;
### 7.2 Example of Hamiltonian definition

Here is the Hamiltonian we use in our sample program:

```c
#include <math.h>

/**
 * The Hamiltonian
 */

CNumber V(int i, int j) {
  return (i == j == 1) ? 1. : 0.;
}

CNumber U(int i, int j) {
  return mixing.U[i][j];
}

CNumber H(Number r, int i, int j) {
  CNumber HH = 0;
  return HH0[i][j] + V(i, j) * rho(r) * sqrt(2.) * Gf;
}

void vacuum_values() {
  mixing.mass[1] = 1.e-2;
  mixing.mass[2] = 1.e-1;
  Number th12 = M_PI / 3.;
  Number th13 = M_PI / 3.;
  Number th23 = M_PI / 3.;
  nu[1] = 1.;
  nu[2] = 0.;

  CNumber H0[N + 1][N + 1];
  HHO = matrix ((CNumber) 1, N, 1, N);
  Number sth12 = sin(th12);
  Number cth12 = cos(th12);
  Number sth13 = sin(th13);
  Number cth13 = cos(th13);
  Number sth23 = sin(th23);
  Number cth23 = cos(th23);

  /* Three neutrinos */
  (mixing.U)[1][1] = CNumber (cth12 * cth13);
  (mixing.U)[1][2] = CNumber (sth12 * cth13);
  (mixing.U)[1][3] = CNumber (sth13);
  (mixing.U)[2][1] = CNumber (-sth12 * sth23 - cth12 * sth23 * sth13);
```
(mixing.U)[2][2] = CNumber (cth12 * cth23 - sth12 * sth23 * sth13);
(mixing.U)[2][3] = CNumber (sth23 * cth13);
(mixing.U)[3][1] = CNumber (sth12 * sth23 - cth12 * cth23 * sth13);
(mixing.U)[3][2] = CNumber (-cth12 * sth23 - sth12 * cth23 * sth13);
(mixing.U)[3][3] = CNumber (cth23 * cth13);
break;
default:
  cerr << "Number of neutrina (" << N << ") not implemented!" << endl;
  exit (-1);
}
/*
cout << "Vacuum values:\n";
cout << "- Hamiltonian:\n";
Hamiltonian HH = H0();
cout << HH;
cout << "- Mixing matrix:\n";
cout << *(mixing.U);
*/

for (int i = 1; i <= N; i++)
for (int j = 1; j <= N; j++)
{
    HHO[i][j] = 0;
    /* H0 is the vacuum Hamiltonian in the mass eingenstates */
    if ((i == 1) && (j == 1))
        H0[i][i] = 1. / pow (10, Var); // This is OK for two neutrina
    else
        H0[i][j] = 0;
    /* HH0 is the vacuum Hamiltonian in the flavour eingenstates */
    for (int k = 1; k < N; k++)
        for (int l = 1; l < N; l++)
            HHO[i][j] += conj (U (k, i)) * H0[k][l] * U (l, j);
}
return;
}

The user should provide routines for computing the electron densities at Sun and the Earth along the neutrino trajectory. They appear in the matter part of the neutrino hamiltonian.

7.3 Sample outputs

The following is the verbatim output of our program
hamevol.x 0
for the values of the parameters which appears in the first information lines (included by default in the sample program).
Starting evolution in the Sun

Used parameters:
- MAX_STEPS 100000
- INIT_STEPS 10000
- DECREASE 0.1
- INCREASE 5
- VarI -2.39794
- VarF -12.3979
- Eps_Error 1e-08
- Prob_Error 0.01
- x2/VarI 0.00881916
- x2/VarF 8.81916e+07

| Var  | Eps  | Prob  | Stat  |
|------|------|-------|-------|
| -2.3979 | 1   | 0.00382 | 4.62e-44 |
| -2.4979 | 1   | 0.00382 | 4.62e-44 |
| -2.5979 | 1   | 0.00481 | -1.4e-08 |
| -2.6979 | 1   | 0.00605 | -8.5e-08 |
| -2.7979 | 1   | 0.00762 | 4.62e-44 |
| -2.8979 | 1   | 0.00959 | -1.7e-08 |
| -2.9979 | 1   | 0.0121  | 3.6e-08  |
| -3.0979 | 1   | 0.0152  | -2.8e-08 |
| -3.1979 | 1   | 0.0191  | 7.8e-08  |

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| Variable                  | default     | description                                      |
|---------------------------|-------------|--------------------------------------------------|
| hamevol-rungekutta.hpp    |             |                                                 |
| MAXSTP                    | 1000000     | RK algorithm internal parameter                 |
| TINY                      | $1.0 \times 10^{-10}$ | id.                                              |
| SAFETY                    | 0.9         | id.                                              |
| PGROW                     | -0.2        | id.                                              |
| PSHRNK                    | -0.25       | id.                                              |
| ERRCON                    | $1.89 \times 10^{-4}$ | id.                                              |
| hamevol-sample.cpp        |             |                                                 |
| MAX-STEPS                 | $1.0 \times 10^5$ | Steeper method                                  |
| MIN-STEPS                 | 10000       | id.                                              |
| INIT-STEPS                | 10000       | id.                                              |
| DECREASE                  | 0.1         | id.                                              |
| INCREASE                  | 5.0         | id.                                              |
| hamevol-sample.hpp        |             |                                                 |
| fermi-MeV                 | $1.0/197.326$ | conversion $f \rightarrow 1/MeV$               |
| m-eV                      | $\text{fermi-MeV} \times \frac{10^{15}}{10^6}$ | conversion $m \rightarrow 1/eV$               |
| Gf                        | $1.66 \times 10^{-23}$ | The Fermi constant in $1/eV^2$                  |
| Na                        | $6.022 \times 10^{23}$ | Avogadro number                                 |
| RSun                      | $6.961 \times 10^8 \times m$-eV | Radius of the Sun (1/eV)                       |
| REarth                    | $6.378 \times 10^6 \times m$-eV | Radius of the Earth (1/eV)                     |
| Eps-Error                 | $1.0 \times 10^{-8}$ |                                      |
| Prob-Error                | $1.0 \times 10^{-2}$ | number of equations                             |
| N                         | 2           | initial stepsize for Runge-Kutta                |
| dist                      | 0.000001    | minimal stepsize for Runge-Kutta                |
| dist-min                  | 0.00000001  | minimal stepsize for Runge-Kutta                |
| EARTH                     | 0           | Program option flag                             |
| SUN                       | 1           | Program option flag                             |

**Table 2:** Here is a list of the most important switches and constants

| Subroutine | Purpose                                                                                                                                 |
|------------|------------------------------------------------------------------------------------------------------------------------------------------|
| derivs     | Computes the derivatives $dy/dx$                                                                                                                                                   |
| runge      | Given the functions $y$ and their derivatives $dy/dx$, it returns the advanced solution                                                                                      |
| odeint     | RK driver with adaptive stepsize control. Integrates the starting value over an interval with a required accuracy                                                              |
| rkqs       | Used to monitor accuracy and adjust stepsize during RK integration                                                                         |
| rkck       | Returns advanced solution over an interval together with the estimate of truncation error                                                                |

**Table 3:** The main subroutines and functions used in the code are reported together with a brief explanation of their meaning.