Dedicated to Professor Mihai Gavrilă's 80th Anniversary

METHODS TUNED ON THE PHYSICAL PROBLEM. A WAY TO IMPROVE NUMERICAL CODES

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We consider the problem on how the numerical methods tuned on the physical problem can contribute to the enhancement of the performance of the codes. We illustrate this on two simple cases: solution of time independent one-dimensional Schrödinger equation, and the computation of integrals with oscillatory integrands. In both cases the tuned versions bring a massive gain in accuracy at negligible extra cost.

1. INTRODUCTION

The progress in physics requites building up scientific codes with increasing complexity, and quite often the resulting codes are of a form that asks for big computational resources. The usual way to face this problem consists in using computation platforms with improved facilities, such as clusters for parallel computation. Still, there is also another way. It consists in selecting numerical methods tuned on the problem and, if so is done, the computational effort is substantially diminished and then the area of problems to be approached on the existing platforms is significantly enlarged. The simple case of the eigenvalue problem for the one-dimensional Schrödinger equation represents an illustration for such an attitude. If this problem is solved by the Runge-Kutta method then not only the values of the eigenfunctions at the mesh points are obtained but also those of their first derivative. Now, if these eigenfunctions are further used for computing matrix elements then, with standard "off the shelf" quadrature formulas (e.g. Simpson formula), only the values of the eigenfunctions are involved. Formulae which use also the first derivative exist, and it is clear that these non standard formulae will improve the accuracy with no significant extra effort. The adaptation of codes then implies an examination of the flow-chart of the code along two lines.

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First, the specific properties of the problem have to be considered on each step separately with the aim of identifying the properties which are potentially helpful from numerical point of view. Second, at each new step in the flow-chart it is important to be aware of what are the data available from the previous steps and then try improving the approach on that step in a way which ensures that as many existing data as possible are exploited. Tuned methods exist for a limited number of specific problems, and the development of new methods of this type is one of the main areas of concern in the literature of computational physics. In this paper we present some of the tuned methods for solving the Schrödinger equation and for performing integrals. For simplicity reasons we consider only the one-dimensional cases.

2. NUMERICAL SOLUTION OF THE SCHRÖDINGER EQUATION

We consider the one-dimensional Schrödinger equation which is written with the standard notation in the literature of numerical methods, that is by taking a system of units such that $\hbar^2/2m = 1$ by default, and using x for the independent variable and y for the wavefunction. The equation is

$$y'' = \left[V(x) - E\right] y, \quad x \in [a, b], \tag{1}$$

where E is the energy and $V(x)$ is the potential function which is assumed smooth. As a matter of fact, the latter condition may be considered as quite restrictive. For example, in the case of the radial equation, where x stands for the radial distance r, the domain is $(0, \infty)$. The potential function contains the centrifugal term and therefore it is singular at the origin. Still, after dividing the domain in three regions $I_1 = (0,a)$, $I_2 = [a,b]$ and $I_3 = (b,\infty)$, where a is close to the origin and b is placed in the asymptotic region, then simple forms of the solution are available on I_1 (so called solution close to the origin) and I_3 (asymptotic solution) such that only the solution on I_2, where $V(x)$ is smooth, is of concern from numerical point of view.
Two problems are actually addressed with respect to eq. (1):
Initial value problem (IVP), that is solving for $y(x)$ when either $y(a), y'(a)$ or $y(b), y'(b)$ are given. These are usually called as representing forwards and backwards propagation, respectively.
Eigenvalue problem (EVP), that is determining the eigenenergies E_n and eigenfunctions $y_n(x)$ for given data at a and b, in particular when the logarithmic derivatives $y'(a)/y(a)$ and $y'(b)/y(b)$ are known.

Since the two problems are so different it may be expected that the corresponding numerical methods must be also different but this holds true only partially. Direct methods for the EVP exist indeed, and these are based on writing the algorithm in

matrix form, whose eigenvalues are computed by usual algebraic techniques. However, much more efficient is a procedure based on the solution of the IVP, known as the shooting procedure. A point x_c in [*a, b*], called matching point, is fixed, and for each given value of E in some interval the solutions propagated from the two endpoints towards the matching point are compared. A mismatch function is defined on this basis and successive values of E are tried until the mismatch function is vanishing. The value of E at which the mismatch function vanishes is the eigenenergy E_n searched for in that interval, and to obtain the whole energy spectrum the same procedure is repeated on new energy intervals.
The accuracy in the eigenenergies obtained in this way reflects directly the accuracy of the numerical solution when propagated from the two ends of the interval [*a, b*]. The quality of any code for the solution of the one-dimensional Schrödinger equation then depends on the method used for the IV problem.

Quite often standard methods for ordinary differential equations are applied. Two of them, the method of Numerov and the Runge-Kutta method, are perhaps the most widely used, see e.g., [1], [2]. The method of Numerov has been introduced for differential equations of the form $y'' = f(x, y)$; notice that y' does not appear in f. Its algorithm is

$$y(X-h) + a_1 y(X) + y(X+h) = h^2 \left[b_0 \left(y''(X-h) + y''(X+h) \right) + b_1 y''(X) \right] \quad (2)$$

where h is the stepwidth. For eq. (1) this becomes

$$y_{k-1} + a_1 y_k + y_{k+1} = h^2 \left\{ b_0 \left[(V_{k-1} - E) y_{k-1} + (V_{k+1} - E) y_{k+1} \right] + b_1 (V_{k-1} - E) y_{k-1} \right\} \quad (3)$$

and then it allows computing y_{k+1} when y_{k-1} and y_k are known (forwards propagation), or y_{k-1} when y_k and y_{k+1} are known (backwards propagation). The standard coefficients are

$$a_1 = -2,\ b_0 = 1/12,\ b_1 = 5/6. \quad (4)$$

The algorithm with these coefficients works well when the solution of the equation is smooth enough. In particular it is exact when the true solution is a polynomial of the fifth degree.

The problem is that the solution of the Schrödinger equation is not a polynomial. Its behaviour depends on E. For a mathematical description of this behaviour let us assume that on the interval $[X-h, X+h]$ the approximation of the potential $V(x)$ by a constant $\bar{V}$ is satisfactory, $\bar{V} = V(X)$, for example. The general solution is a linear combination with x dependent coefficients f_1 and f_2 of two linear independent solutions of the approximating equation $\bar{y}'' = (\bar{V} - E)\bar{y}$, that is

$$y(x) = f_1(x)\sin(\omega x) + f_2(x)\cos(\omega x),\ \omega = \sqrt{E - \bar{V}}, \quad (5)$$

in a classically allowed region, that is $E > \bar{V}$, and

$$y(x) = f_1(x)\sinh(\lambda x) + f_2(x)\cosh(\lambda x),\ \lambda = \sqrt{\bar{V} - E}, \tag{6}$$

in a classically forbidden region, $E < \bar{V}$. The dependence on x of the coefficients reflects the deviation of $V(x)$ with respect to $\bar{V}$; if the original $V(x)$ happens to be just that constant then the coefficients are also constants.

The written forms suggest that in both regions the solution is smooth enough only if E and $\bar{V}$ are close to each other but this behaviour is more and more altered when the distance between E and $\bar{V}$ increases. The typical practical consequence is that the Numerov method with the standard coefficients (4) is satisfactory for low lying energies (for computing the ground and a few excited states, for example) but it will meet more and more difficulties for higher excited states or when problems in the continuous spectrum are of concern. In the later case acceptable accuracies can be obtained only if the step h is drastically diminished but this makes the computation more costly. Such a difficulty is not serious for this simple example but it becomes certainly a problem when many-channel problems with a big number of channels are addressed.

A standard way to overcome such problems consists in using computation equipment with increased performance, which allows parallel computation, for instance. Still, there exists also another way. It consists in making the code more effective by introducing better numerical methods, tuned on the problem. In our case this means replacing the standard Numerov method by a version whose coefficients take into account that the solution is of the form (5)-(6). This can be done by the exponential fitting (EF) procedure. The EF procedure allows building up numerical methods tuned on functions of the form

$$y(x) = g_+(x)\exp(\mu x) + g_-(x)\exp(-\mu x) + g_0(x) \tag{7}$$

where $g_{\pm}(x)$ and $g_0(x)$ are smooth enough. The solution of the Schrödinger equation is of this type, with real $\mu = \lambda$ in a classically forbidden region and imaginary $\mu = i\omega$ in a classically allowed region, and $g_0 = 0$. Four levels of tuning exist for the Numerov scheme, and they correspond to four distinct versions denoted S_i, i = 0, 1, 2, 3. To obtain the coefficients for each version it is required that eq.(2) is satisfied exactly for $y(x)$ of the form (7) with specific restrictions, as follows:

S_0. This is standard version. The restrictions are that $g_{\pm}(x) = 0$ and $g_0(x)$ is a polynomial of the fifth degree. The coefficients (4) result in this way.

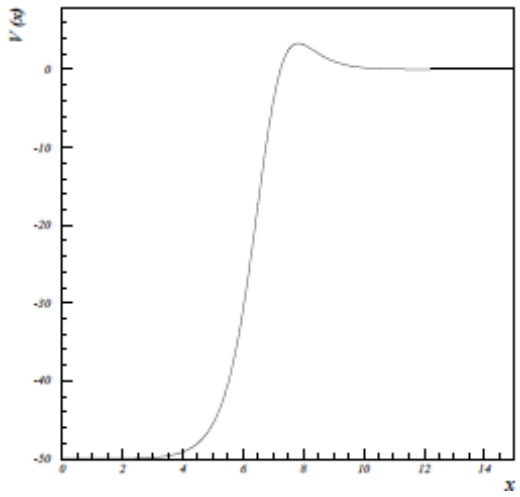

Fig. 1 – Woods-Saxon potential (8).

S_1. $g_{\pm}(x)$ are constants and $g_0(x)$ is a polynomial of the third degree, [3]. The resulting coefficients in ready-to-program form are (hereinafter we use notations $Z=\left(\bar{V}-E\right)h^2$ and $\theta=\sqrt{|Z|}$): $a_1=-2$,

$$b_0(Z)=\begin{cases}\dfrac{1}{Z}\left[1-\dfrac{Z}{4\sinh^2(\theta/2)}\right] & \text{if} \quad Z>T\\ \dfrac{1}{12}-\dfrac{1}{240}Z+\dfrac{1}{6048}Z^2-\dfrac{1}{172800}Z^3+\dfrac{1}{5322240}Z^4 & \text{if} \quad -T\le Z\le T\\ \dfrac{1}{Z}\left[1+\dfrac{Z}{4\sin^2(\theta/2)}\right] & \text{if} \quad Z<-T\end{cases}$$

and $b_2(Z) = 1-2b_1(Z)$.

S_2. $g_{\pm}(x)$ and $g_0(x)$ are linear polynomials, [4]. The coefficients are: $a_1 = -2$,

$$b_0(Z)=\begin{cases}\dfrac{1}{Z}\left[1-\dfrac{2}{\theta}\tanh(\theta/2)\right] & \text{if} \quad Z>T\\ \dfrac{1}{12}-\dfrac{1}{120}Z+\dfrac{17}{20160}Z^2-\dfrac{31}{362800}Z^3+\dfrac{691}{79833600}Z^4 & \text{if} \quad -T\le Z\le T\\ \dfrac{1}{Z}\left[1-\dfrac{2}{\theta}\tan(\theta/2)\right] & \text{if} \quad Z<-T\end{cases}$$

$$b_1(Z)=\begin{cases}\dfrac{2}{Z}\left[-1+\dfrac{2}{\theta}\tanh(\theta/2)\cosh(\theta)\right] & \text{if} \quad Z>T\\ \dfrac{5}{6}+\dfrac{1}{60}Z+\dfrac{5}{2016}Z^2-\dfrac{29}{181440}Z^3+\dfrac{139}{7983360}Z^4 & \text{if} \quad -T\le Z\le T\\ \dfrac{2}{Z}\left[-1+\dfrac{2}{\theta}\tan(\theta/2)\cos(\theta)\right] & \text{if} \quad Z<-T\end{cases}$$

S_3. $g_{\pm}(x)$ are second degree polynomials and $g_0(x) = 0$, [5]. In this case the resulting coefficients are:

$$a_1(Z)=\begin{cases}-\dfrac{2\left[2\theta+\cos(\theta)\left(3\sin(\theta)-\theta\cos(\theta)\right)\right]}{3\sin(\theta)+\theta\cos(\theta)} & \text{if} \quad Z>T\\ -2+\dfrac{1}{240}Z^3-\dfrac{1}{2016}Z^4 & \text{if} \quad -T\le Z\le T\\ -\dfrac{2\left[2\theta+\cosh(\theta)\left(3\sinh(\theta)-\theta\cosh(\theta)\right)\right]}{3\sinh(\theta)+\theta\cosh(\theta)} & \text{if} \quad Z<-T\end{cases}$$

$$b_0(Z)=\begin{cases}\dfrac{\sin(\theta)-\theta\cos(\theta)}{Z\left(3\sin(\theta)+\theta\cos(\theta)\right)} & \text{if} \quad Z>T\\ \dfrac{1}{12}-\dfrac{1}{80}Z+\dfrac{41}{20160}Z^2-\dfrac{1219}{3628800}Z^3+\dfrac{8887}{159667200}Z^4 & \text{if} \quad -T\le Z\le T\\ \dfrac{\sinh(\theta)-\theta\cos(\theta)}{Z\left(3\sinh(\theta)+\theta\cosh(\theta)\right)} & \text{if} \quad Z<-T\end{cases}$$

$$b_1(Z)=\begin{cases}\dfrac{2\left[2\theta-\cos(\theta)\left(\sin(\theta)+\theta\cos(\theta)\right)\right]}{Z\left(3\sin(\theta)+\theta\cos(\theta)\right)} & \text{if} \quad Z>T\\ \dfrac{5}{6}+\dfrac{1}{40}Z+\dfrac{17}{2016}Z^2-\dfrac{1811}{1814400}Z^3+\dfrac{13817}{79833600}Z^4 & \text{if} \quad -T\le Z\le T\\ \dfrac{2\left[2\theta-\cos(\theta)\left(\sinh(\theta)+\theta\cosh(\theta)\right)\right]}{Z\left(3\sinh(\theta)+\theta\cosh(\theta)\right)} & \text{if} \quad Z<-T\end{cases}$$

The introduction of the cutting parameter T is necesary because the analytic expressions exhibit a 0/0 undeterminacy at $Z = 0$. The value of T depends on the accuracy needed in the results. If this is of 14 exact figures we can take $T = 10^{-2}$.

The classical version is not tuned at all on the form (5)-(6) of the solution but the others are increasingly tuned on this and S_3 represents the best tuned version. This is described mathematically by the behaviour of the error. All versions are of order 4 but the dependence of the error with respect to E varies with the version. When E is increased then the error increases as E^3 for S_0, E^2 for S_1, $E^{3/2}$ for S_2 but only as E for the best tuned S_3. The price to be paid is that the coefficients must be updated but this is not compulsory to be done on each new step. One and the same set of coefficients can be well used on a sequence of successive steps where $V(x)$ does not vary significantly and therefore the coefficients are updated only a few times along $[a, b]$. The following test case illustrates this.

We take the Woods-Saxon potential

$$V(x)= v_0/(1+t)+v_1 t/(1+t)^2,\ \ t = \exp[(x - x_0)/a],\ x \geq 0, \tag{8}$$

where $v_0 = -50$, $x_0 = 7$, $a = 0.6$ and $v_1 = v_0/a$, see Fig. 1. Its shape is such that only two values for $\bar{V}$ are sufficient: $\bar{V} = -50$ for $0 \leq x \leq 6.5$ and $\bar{V} = 0$ for $x \geq 6.5$, and therefore the coefficients must be updated only twice for each E.

We solve the resonance problem which consists in the determination of the positive eigenvalues corresponding to the boundary conditions

$$y(0) = 0,\ y(x)= \cos(E^{1/2} x) \text{ for big } x.$$

The physical interval is truncated at $b = 20$ and the eigenvalues are obtained by shooting at $x_c = 6.5$. For any given E the solution is propagated forwards with the starting values $y(0) = 0$, $y(h) = h$ up to $x_c + h$, and backwards with the starting conditions $y(b)= \cos(E^{1/2}b)$, $y(b-h)= \cos(E^{1/2}(b-h))$ up to x_c. If E is an eigenvalue the forwards (f) and backwards (b) solutions are proportional and then the numerical values of the products $y^f(x_c + h)y^b(x_c)$ and $y^b(x_c + h)y^f(x_c)$ must coincide. The resonance eigenenergies searched for are then the roots of the mismatch function

$$\Delta(E)= y^f(x_c + h)y^b(x_c) - y^b(x_c + h)y^f(x_c),$$

which can be evaluated directly on the basis of the available data. The error in the eigenvalues will then reflect directly the quality of the solvers for the two mentioned initial value problems.

In Table 1 we list the absolute errors in three such eigenvalues for all four schemes of the Numerov method. It is seen that, as expected, all these versions are of order four but the way in which the error increases with the energy differs from one version to another. For one and the same h the accuracy clearly increases with each new level of tuning.

EF-based tunings are available also for other methods; see [6]-[10] for the Runge-Kutta methods.

The way of deriving tuned methods via exponential fitting uses for input the knowledge on the qualitative behaviour of the solution but tunings based on different types of information are also possible. In particular, information behind the *piecewise perturbation methods* refers to the form of the equation: eq.(1) is of such a form that expressions of the potential function exist such that the one step initial value problem has analytic solution, [11]. Examples are the constant (CP) and the linear potentials (LP). The two linear independent solutions are expressed by elementary functions (sin and cos, or a pair of exponential functions) in the first case, and by Airy functions in the second case. If on the considered step the value of the constant in CP or of the two numerical parameters in LP are fixed by a fit of the given $V(x)$ then the solution on that interval is the sum of the analytic solution for the reference potential $\bar{V}(x)$ derived in this way and perturbation corrections from

$$\Delta V(x) = V(x) - \bar{V}(x).$$

Table 1

Absolute errors $E_{exact} - E_{comput}$ in 10^{-6} units from the four versions of the Numerov method for the resonance eigenenergy problem in the Woods– Saxon potential (8). The empty areas indicate that the corresponding errors are bigger than the format adopted in the table

h	S_0	S_1	S_2	S_3
E_{exact} = 53.588852				
1/16	−259175	6178	−1472	587
1/32	−15872	367	−84	35
1/64	−989	22	−5	1
1/128	−62	1	0	0
E_{exact} =163.215298				
1/16		9579	−9093	721
1/32	−595230	4734	−525	46
1/64	−36661	292	−32	2
1/128	−2287	18	−1	0
E_{exact} = 341.495796				
1/16		661454	−40122	1600
1/32		36703	−2116	126
1/64	−560909	2215	−126	7
1/128	−34813	136	−8	0

The real problem is of whether the perturbation corrections can be computed efficiently and in this respect CP is superior: if $\Delta V(x)$ is a polynomial then all perturbation corrections have analytic expressions, and this is why the CP methods (CPM) received a particular attention. For the single channel equation we find versions of orders between 2 (when no correction is taken) and 6 (with two

corrections) in [11], up to 12 in [12] and up to 18 in [13], while for the many channel equation between 2 and 6 in [11,14], and up to 10 in [15]. Except that so big orders are available, other salient advantages are that the CP methods can be coded in an architecture which makes them extremely fast, and that the error of the computation is practically *independent* of E; notice that for the EF-based methods this increases for large E. Computer codes are also available: SLCPM12,[12], of order 12 for the single channel equation, and LILIX [14] of order 6 for the coupled channel case. As a matter of fact, the resonance energies taken for reference in Table 1 have been computed by a slightly adapted version of SLCPM12 with h =1/4.

3. OTHER OPERATIONS

Computation of the solution of the Schrödinger equation is only one step in a code. It is followed by other steps where the obtained wavefunctions are exploited as, for example, when the solutions have to be presented as graphs or when they are used to compute matrix elements. Take for example the case of the third resonance in Table 1. If this has been computed by the method SLCPM12 with h = 1/4 the meshpoints at which the values of the wavefunctions are available are too distanced from each other to produce a nice graph directly, and interpolated data have to be added. However, standard interpolation techniques are useless because the wave function has one or two zeros within each step, and then tuned methods must be used. The specific features to be used for tuning are that (i) not only $y(x_k)$ are available but also $y'(x_k)$ (if methods like Runge-Kutta or CPM were used for the Schrödinger equation) and $y''(x_k) = \left(V(x_k) - E\right) y(x_k)$, and (ii) the values of ω or λ in (5-6) are also available. Interpolation techniques tuned for such features can be found in [16] and [17].

As for the quadrature procedure, here is an illustration on how the quality of the input information on the integrand influences the accuracy of the integral. We compute

$$I(\omega) = (\omega+1)\int_0^1 dx\, y(x), \tag{9}$$

where

$$y(x) = \frac{1}{(1+x)^2}\cos\left[(\omega+1)x\right]. \tag{10}$$

Its exact value is

$$I(\omega) = (\omega+1)F(x;\omega+1)\Big|_{x=0}^{1}, \tag{11}$$

where

$$F(x;\omega) = -\frac{\cos(\omega x)}{1+x} + \omega\left\{\sin(\omega)\mathrm{Ci}\left[\omega(1+x)\right] - \cos(\omega)\mathrm{Si}\left[\omega(1+x)\right]\right\}. \quad (12)$$

We divide the interval [0, 1] in 20 equal subranges and apply a three-point quadrature rule on each subrange.
Let us denote the current subrange as $[X-h, X+h]$. In our case h =1/40, of course. We use three different versions (rules).

Rule 1. Assume that only the values of the integrand at points $x_1 = X - h$, $x_2 = X$ and $x_3 = X + h$ are known. This is covered by the standard Simpson rule

$$\int_{x_1}^{x_3} dx\, y(x) \approx h\left[y(x_1) + 4y(x_2) + y(x_3)\right]/3. \quad (13)$$

The rule is exact if $y(x)$ is a polynomial of the third degree.

Rule 2. Assume that not only the values of the integrand are known but also those of its first derivative. This allows using the extended form of the Simpson formula,

$$\int_{x_1}^{x_3} dx\, y(x) \approx h\left[7y(x_1) + 16y(x_2) + 7y(x_3) + h\left(y'(x_3) - y'(x_1)\right)\right]/15. \quad (14)$$

see[18]. This formula is exact when the integrand is a polynomial of the fifth degree.

Rule 3. Here it is assumed that the values of the integrand and of its first derivative are known, as before, but we also use information that the integrand is an oscillatory function of the form

$$y(x) = f_1(x)\sin(\omega x) + f_2(x)\cos(\omega x), \quad (15)$$

with smoothly varying $f_1(x)$ and $f_2(x)$, a case covered by the exponential fitting procedure, see [16, 19]. The weights of the rule will now depend on $\theta = \omega h$ but we do not enter into details on how their expressions are derived. The quadrature rule is now

$$\int_{x_1}^{x_3} dx\, y(x) \approx h\left[a_1(\theta)\left(y(x_1)\right) + y(x_3) + a_2(\theta)y(x_2) + a_1(\theta)h\left(y'(x_3) - y'(x_1)\right)\right] \quad (16)$$

where $a_1(\theta)$ and $a_2(\theta)$ are computed numerically by means of the subroutine EFEXTQS in the CD attached to [16]. This rule is exact when $f_1(x)$ and $f_2(x)$ are polynomials of the second degree. It is interesting to remark that the numerical values of the components $f_1(x)$ and $f_2(x)$ are irrelevant; they do not appear in the quadrature rule. Also instructive is that frequency ω is assumed to govern the oscillation in eq. (16) although in our test case the frequency is actually ω+1. The reason for such an alteration was that of placing the discussion in a realistic situation when the frequency is known with some approximation only.

The quantity $-\log\left[\left|I(\omega)-I^{comput}(\omega)\right|\right]$ represents roughly the number of exact figures in $I(\omega)$ after the decimal point. This is displayed on Fig. 2 for the three versions and for $0 < \omega < 100$. We see that, as expected, each new level of tuning enhances the accuracy. However, the degree of enhancement depends on ω. When ω is small the gain brought by the first derivative is more important than that from the form of the integrand and this is just normal. In fact, the effective value of θ is also small in this case, that is close to the default value $\theta = 0$ which corresponds to rule 2. The things change when ω is increased. The gain due to the tuning corresponding to the first derivative becomes less and less important, in contrast to the one due to the tuning with respect to the shape of the integrand.

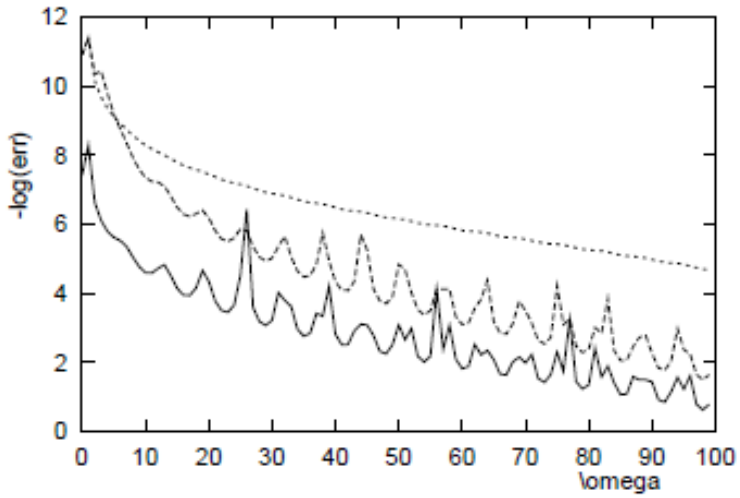

Fig. 2 – A comparison of the accuracies produced by the three quadrature rules for integral (11): Simpson (solid), extended Simpson (long-dashed), and extended Simpson with frequency dependent coefficients (short-dashed).

This was only an example but the possibility of formulating tuned quadrature rules is seen as one of the major factors for enhancing the efficiency in a number of current large scale applications. In [20] a code aimed at creating virtual experiments on high performance and grid architectures is presented, which enables the study of electron scattering from H-like atoms and ions at intermediary energies. As noted by these authors, the bottleneck of the code is the large number of two-dimensional radial integrals, the so-called Slater integrals, and they want to remove this by replacing the current subroutine for these integrals by one where the quadrature rule is the 14-point EF-based extended Newton-Cotes rule developed in [21], which is by three decimal figures more accurate and by two orders of magnitude faster.

4. CONCLUSIONS

We presented two simple problems where successive levels of tuning enhance significantly the accuracy at negligible extra cost. These problems should be seen as representing only some illustrations on how the codes can be improved but we must also mention that in many cases tuned versions still have to be developed. Just for a suggestion, quadrature formulae which involve the integrand and a number of successive derivatives of this exist, but no formula is available when some of these derivatives are missing, for example when we dispose of y and y'' but not of y'. A direct application will be on the case when the integrand involves the solution of the Schrödinger equation by the method of Numerov.

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