On Convergence Acceleration of Multipolar and Orthogonal Expansions*

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Abstract

Multipolar expansions arise in many branches of the computational sciences. They are an example of orthogonal expansions. We present methods for the convergence acceleration of such expansions. As an example, the computation of the electrostatic potential and its multipolar expansion is treated for the case of a two-center charge density of exponential-type orbitals. This potential may also be considered as a special molecular integral, namely as a three-center nuclear attraction integral. It is shown that in this example, the extrapolation to the limit of the corresponding expansions via suitable nonlinear sequence transformations leads to a pronounced convergence acceleration.
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1 Introduction

Multipole expansions and expansions in spherical harmonics are prominent examples of orthogonal expansions and play an important rôle in the sciences. Consequently, there is an immense literature regarding this topic. In chemistry, such expansions are important

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- for the transitions between molecular states induced by an interaction with electromagnetic radiation in the context of time-dependent perturbation theory [1], Chap. 16,
- for the description of NMR (*Nuclear Magnetic Resonance*) experiments [2],
- for the description of intermolecular interactions that are fundamental for the classical description of many-body systems, for instance in terms of induced multipole moments like polarizability [3], Chap. 15
- in particular for the computation of the electrostatic potential of molecular charge distributions, e.g., by solving the Poisson equation [4], with applications also in density functional programs (deMon),
- for the characterization of molecules by electrostatic multipole moments (dipole, quadrupole, octupole and hexadecapole moments) where the first non-vanishing multipole moment is independent of the choice of the origin [5] that is in most cases chosen to be the center of mass of the molecule
- for the determination of effective atomic charges (partial charges) [6], [7] for force-field, molecular mechanics and molecular modeling calculations by fits to the electrostatic potentials of molecules [8], [9], [10], [11], [12], [13], [14] as an alternative to charges derived from population analysis [15], [16], [17], [18] or also to empirical charges that are derived on the basis of interaction energies and distances (CHARMm, [19], [20]) or properties of fluids [21], [22], [23], [24], [25], [26], [27], [28],
- for determining effective atomic multipole moments, also for molecular force-field calculation, where the effective forces between two molecules are represented as a sum of electrostatic interactions of such distributed atomic multipole moments of pairs of atoms [29], [30]
- in the *Fast Multipole Method* (FMM) of Greengard and Rokhlin [31], [32], [33], [34], [35], [36], [37], [38], [39], where the computational effort — like in some other methods, compare the next item — scales *linearly* with the number of atoms and which is currently used for molecular dynamics calculation of macro molecules with a complete description of long-range Coulomb interactions [40], [41], [42], [43] and will be part of the new quantum chemistry program Q-Chem of Johnson, Gill and Head-Gordon [1],

[1] According to an E-mail message of W. Koch [kochw@argon.chem.TU-Berlin.DE,

- in the *Distributed Parallel Multipole Tree Algorithm* (DPMTA) where the computational effort also scales linearly with system size and that also has been used in molecular dynamics simulations of macro molecules [2],

- in tight-binding Hartree-Fock calculations of polymers [44],

- for the calculation of molecular integrals (mostly with exponential-type basis functions) [45], [46], [47], [48], [49], [50], [51], [52], [53], [54], [55], [56], [57], [58], [59], [60], [61], [62], [63], [64], [65], [66], [67], [68], [69], [70], [71], [72], [73], [74], in particular in combination with addition theorems and/or one-center expansions. [75], [76], [77], [78], [79], [80], [81], [82], [83], [84], [85], [86], [87], [88], [89], [90], [91], [92], [93], [94], [95], [96], [97], [98], [99], [100], [101], [102],[103], [104], [105], [106], [107], [108], [109], [110], [111], [112], [113], [114], [115], [116], [117]

These expansions can be regarded as generalized Fourier series. Since such expansions often converge rather slowly, there is a need for methods to accelerate the convergence. The basic approach is to transform the sequence of partial sums of the series into a new sequence that converges faster, while using only very simple arithmetics. As we will see, such methods can also improve drastically the convergence even in cases where the original series is already converging relatively fast. Such methods may even be used to calculate a meaningful value of divergent series. The additional calculational effort for the calculation of the sequence transformation is very low, and may often be neglected in comparison to the calculation of the terms of the series.

Not many successful methods for the convergence acceleration of Fourier series and orthogonal expansions are known. Some new methods have been introduced recently by the author [118], [119], [120], [121], [122], [123], [124], [125]. Methods for the convergence acceleration of expansions in orthogonal polynomials will be discussed in Sec. 4.

We study here the convergence acceleration of a one-center multipole expansion in comparison to an expansion of the exact electrostatic potential in spherical harmonics.

An extension of the results to the convergence acceleration of distributed multipole expansions where the electrostatic potential is represented by a sum of truncated multipole expansions at various centers (mostly the atoms), can simply be obtained by separate convergence acceleration of each of these expansions and subsequent summation.

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[2] Programm namd, University of Illinois, http://www.ks.uiuc.edu:1250/Research/namd/.

As a first step, we limit attention to expansions in Legendre polynomials that arise for rotationally symmetric problems. It is believed that more general types of expansions can be treated similarly. This, however, is still under investigation.

First, we will recall some basic facts on multipole expansions of electrostatic potentials. Then, we go on to point out the connection to three-center nuclear attraction integrals. Before going on to a specific example, we discuss methods for convergence acceleration of such orthogonal expansions based on nonlinear sequence transformations. As a simple example, we treat a two-center density that could arise in molecular LCAO[3] calculations. Numerical tests are presented that show that the extrapolated values obtained by using the nonlinear sequence transformation converge much faster than the original expansions, both for the multipole expansion of the potential, and for its exact expansion in spherical harmonics.

2 Multipole Expansion of the Electrostatic Potential

For the calculation of the electrostatic potential U of a charge density ρ one can use the equation (in atomic units)

$$U(\vec{r}) = \int \frac{\rho(\vec{r}')}{|\vec{r} - \vec{r}'|} \, \mathrm{d}^3 r' \tag{1}$$

Inserting the Laplace expansion

$$\frac{1}{|\vec{r} - \vec{r}'|} = 4\pi \sum_{\ell m} \frac{Y_\ell^m(\vec{r}/r) \, Y_\ell^{m*}(\vec{r}'/r')}{2\ell + 1} \frac{r_<^\ell}{r_>^{\ell+1}} \tag{2}$$

with the abbreviations $r = |\vec{r}|$, $r' = |\vec{r}'|$, $r_< = \min(r, r')$ and $r_> = \max(r, r')$ and the complex spherical harmonics Y_ℓ^m in the phase convention of Condon and Shortley [126] as defined in [127], p. 3, Eq. (1.2-1), and interchanging the order of integration and summation yields

$$U(\vec{r}) = 4\pi \sum_{\ell m} \frac{Y_\ell^m(\vec{r}/r)}{2\ell + 1} \int \rho(\vec{r}') \frac{r_<^\ell}{r_>^{\ell+1}} Y_\ell^{m*}(\vec{r}'/r') \, \mathrm{d}^3 r' \, . \tag{3}$$

This can be interpreted as orthogonal expansion in the complete orthonormal system of spherical harmonics.

[3] Linear Combination of Atomic Orbitals

If the charge density vanishes outside of a sphere of radius a with center at the origin and if $r > a$ holds then $r > r'$ is satisfied for all $\vec{r}'$ for which $\rho(\vec{r}') \neq 0$ holds, and the relation

$$U(\vec{r}) = 4\pi \sum_{\ell m} r^{-\ell-1} \frac{Y_\ell^m(\vec{r}/r)}{2\ell+1} \int \rho(\vec{r}') r'^{\ell} Y_\ell^{m*}(\vec{r}'/r') \, \mathrm{d}^3 r' \tag{4}$$

follows.

Introduction of the multipole moments

$$Q_\ell^m = \int r'^{\ell} Y_\ell^m(\vec{r}'/r') \rho(\vec{r}') \, \mathrm{d}^3 r' \tag{5}$$

allows to represent the potential by an infinite series of the form

$$U(\vec{r}) = U_Q(\vec{r}) = 4\pi \sum_{\ell m} \frac{1}{r^{\ell+1}} \frac{Y_\ell^m(\vec{r}/r)}{2\ell+1} Q_\ell^{m*} \tag{6}$$

that is usually called the multipole expansion. In particular, for a charge distribution $\rho(\vec{r})$ that is invariant under rotations with axis $\vec{R}$, the multipole moments have the form

$$Q_\ell^{m*} = Y_\ell^{m*}(\vec{R}/R) \, q_\ell \, , \tag{7}$$

and the addition theorem

$$\frac{4\pi}{2\ell+1} \sum_m Y_\ell^m(\vec{r}/r) Y_\ell^{m*}(\vec{R}/R) = P_\ell \left(\frac{\vec{r} \cdot \vec{R}}{r \, R} \right) \tag{8}$$

of the spherical harmonics yields an expansion in Legendre polynomials P_ℓ

$$U_Q(\vec{r}) = \sum_{\ell=0}^{\infty} P_\ell \left(\frac{\vec{r} \cdot \vec{R}}{r \, R} \right) \frac{q_\ell}{r^{\ell+1}} \, . \tag{9}$$

This form of the electrostatic potential is also implied by the fact that the Laplace equation $\nabla^2 U = 0$ holds outside of a charge distribution. The only solutions of this equation for $r \to \infty$ in spherical coordinates are linear combinations of irregular solid harmonics $\mathcal{Z}_\ell^m(\vec{r}) = r^{-\ell-1} Y_\ell^m(\vec{r}/r)$ and thus, taking rotational symmetry around the direction $\vec{R}/R$ into account, only linear combinations of $r^{-\ell-1} P_\ell(\cos\alpha)$ occur in the multipole expansion of U where α is the angle between the position vector and the direction $\vec{R}/R$.

If the charge distribution does not have compact support in $\mathbb{R}^3$, the above multipole expansions only hold approximately for large $r = |\vec{r}|$. In this case, the inequality $r > r'$ does *not* hold for all $\vec{r}'$ for which $\rho(\vec{r}') \neq 0$.

The difference between the exact potential U and the multipole expansion U_Q in Eq. (6) is given by

$$U(\vec{r}) - U_Q(\vec{r}) = 4\pi \sum_{\ell m} \frac{Y_\ell^m(\vec{r}/r)}{2\ell+1} \int \rho(\vec{r}') \left\{ \frac{r_<^\ell}{r_>^{\ell+1}} - \frac{r'^\ell}{r^{\ell+1}} \right\} Y_\ell^{m*}(\vec{r}'/r')\, \mathrm{d}^3 r' \,. \tag{10}$$

Because of

$$\frac{r_<^\ell}{r_>^{\ell+1}} - \frac{r'^\ell}{r^{\ell+1}} = 0 \quad \text{for } r' \le r \tag{11}$$

the difference $U - U_Q$ can also be represented as

$$U(\vec{r}) - U_Q(\vec{r}) = 4\pi \sum_{\ell m} \frac{Y_\ell^m(\vec{r}/r)}{2\ell+1} \int_{r'>r} \rho(\vec{r}') \left\{ \frac{r^\ell}{r'^{\ell+1}} - \frac{r'^\ell}{r^{\ell+1}} \right\} Y_\ell^{m*}(\vec{r}'/r')\, \mathrm{d}^3 r' \,. \tag{12}$$

If $\rho(\vec{r})$ decays sufficiently rapidly for large arguments, the contributions with angular momentum quantum number ℓ to the difference $U - U_Q$ will go to zero for large r (unless they vanish anyway by symmetry). In the case of the example $\rho(\vec{r}) = \exp(-\gamma r)$ with $\gamma > 0$, only the term with $\ell = 0$ survives the angular integration and one obtains

$$U(\vec{r}) - U_Q(\vec{r}) = 4\pi \int_r^\infty \exp(-\gamma r') \left\{ \frac{1}{r'} - \frac{1}{r} \right\} r'^2\, \mathrm{d}r' = -4\pi \frac{\exp(-\gamma\, r)\,(2+\gamma\, r)}{r\,\gamma^3}. \tag{13}$$

Hence, the difference $U - U_Q$ vanishes for large r exponentially in this simple model example.

Note that the multipole expansion U_Q for $\vec{r} \neq 0$ is a solution of the Laplace equation $\nabla^2 U_Q = 0$. But the exact electrostatic potential U satisfies the Poisson equation (atomic units)

$$\nabla^2 U(\vec{r}) = -4\pi \rho(\vec{r}) \,. \tag{14}$$

This implies that also the difference $U - U_Q$ is a solution of this Poisson equation. A further consequence is that the multipole expansion can only be a good approximation to U where the charge density is small, i.e., for large distances from the origin.

An advantage of the multipole expansion is that the moments Q_ℓ^m or q_ℓ, respectively, to a given charge distribution ρ can be computed once and for all, and then, the multipole approximation $U_Q(\vec{r})$ of $U(\vec{r})$ can be computed very easily for very many arguments $\vec{r}$. The exact expansion (3) of $U(\vec{r})$ on the other hand is more demanding computationally. It requires the calculation of the integrals

$$\tilde{Z}_\ell^m(r) = \int \rho(\vec{r}') \frac{r_<^\ell}{r_>^{\ell+1}} Y_\ell^m(\vec{r}'/r')\, \mathrm{d}^3 r' \,, \tag{15}$$

that depend also on the distance r to the expansions centre. If the charge density ρ is rotationally symmetric around the direction $\vec{R}$, then in analogy to Eq. (7) we have

$$\tilde{Z}_\ell^m(r) = Y_\ell^m(\vec{R}/R)\,\tilde{z}_\ell(r)\,, \tag{16}$$

and hence, the expansion (3) simplifies to

$$U(\vec{r}) = 4\pi \sum_{\ell m} \frac{Y_\ell^m(\vec{r}/r)}{2\ell+1} Y_\ell^{m*}(\vec{R}/R)\,\tilde{z}_\ell(r) = \sum_{\ell=0}^{\infty} P_\ell\left(\frac{\vec{r}\cdot\vec{R}}{r\,R}\right)\,\tilde{z}_\ell(r)\,. \tag{17}$$

This corresponds to the cylindrical symmetry of the problem since only the coordinates r and θ with $rR\cos\theta = \vec{r}\cdot\vec{R}$ enter. Thus, one obtains an expansion in Legendre polynomials that may or may not converge rapidly.

3 Three-center Nuclear Attraction Integrals

In the context of a LCAO (*Linear Combination of Atomic Orbitals*) calculation of the matrix elements of the molecular Hamilton operator, integrals of the form

$$I[\phi_j,\phi_k](\vec{r}) = \int \frac{\phi_j^*(\vec{r}')\,\phi_k(\vec{r}')}{|\vec{r}-\vec{r}'|}\,\mathrm{d}^3r' \tag{18}$$

occur. Here, $\phi_j(\vec{r})$ and $\phi_k(\vec{r})$ are two spatial orbitals that are centered each at an atom, i.e., functions $\mathbb{R}^3 \to \mathbb{C}$, the so-called *atomic orbitals* that are also called basis functions in the following, and the (spatial) molecular orbitals $\psi_\alpha(\vec{r})$ are linear combinations of the form

$$\psi_\alpha(\vec{r}) = \sum_j c_{j,\alpha}\phi_j(\vec{r})\,. \tag{19}$$

A basis function $\phi_j(\vec{r})$ with center $\vec{R}_j$ can be written as

$$\phi_j(\vec{r}) = \chi_j(\vec{r}-\vec{R}_j) \tag{20}$$

where in quantum chemistry the χ_j factorize in a radial and an angular part according to $\chi_j(\vec{r}) = \rho_j(r)\sigma_j(\theta,\phi)$ For cartesian basis functions, the angular part is proportional to products of the form $x^a y^b z^c$, for spherical basis functions, it is given by spherical harmonics $Y_\ell^m(\theta,\phi)$. The radial part has the form $P(r)\exp(-\alpha r^\tau)$, where P is a polynomial. Gaussian-type orbitals (GTO) correspond to $\tau = 2$, and exponential-type orbitals (ETO) correspond to $\tau = 1$. The simplest representatives of these two classes of basis functions are the 1s GTO

$$G(\alpha,\vec{r}) = \exp(-\alpha r^2) \tag{21}$$

and the 1s ETO

$$e(\alpha, \vec{r}) = \exp(-\alpha r)\,. \tag{22}$$

The latter is, up to a constant factor, on the one hand nothing but the special case $n = 1$, $\ell = m = 0$ of the most popular ETOs, the Slater-type Orbitals (STO) (cp. [128] and [46], Eq. (2.1))

$$\chi^m_{n,\ell}(\alpha, \vec{r}) = (\alpha\, r)^{n-1}\, \exp(-\alpha r)\, Y^m_\ell(\theta, \phi)\,, \tag{23}$$

and on the other hand it is identical to the most simple B function that are defined by [46], Eq. (2.14)

$$B^m_{n,\ell}(\alpha, \vec{r}) = \frac{1}{2^{n+\ell}(n+\ell)!)}\, \hat{k}_{n-1/2}(\alpha r)\, (\alpha r)^\ell\, Y^m_\ell(\theta, \phi) \tag{24}$$

and are the ETOs with the most simple Fourier transform. The latter are tensorial generalizations of the reduced Bessel functions $\hat{k}_\nu$ defined by [108], p. 275, Eq. (3.1):

$$\hat{k}_\nu(z) = \left(\frac{2}{\pi}\right)^{1/2} z^\nu K_\nu(z) \tag{25}$$

in terms of the modified Bessel functions $K_\nu(z)$ of the second kind [129], p. 66.

The integrals I are called *nuclear attraction integrals*. They are examples of the previously mentioned molecular integrals.

There are three center in the case of nuclear attraction integrals (the origin, $\vec{R}_j$, $\vec{R}_k$ in the case of $I[\phi_j, \phi_k](\vec{r})$) that can, however, coincide. The corresponding one- and two-center nuclear attraction integrals are usually computationally much simpler than the three-center nuclear attraction integrals. The latter are the topic of the present section.

Depending on the choice of basis functions, the calculation of nuclear attraction integrals may be complicated or simple.

In the case of GTOs the computation of the nuclear attraction integrals is relatively simple since products of GTOs at two centers can be easily represented by GTOs at a single center. This implies that for GTOs three-center nuclear attraction integrals are easily expressed in terms of two-center integrals.

In the case of ETOs the computation of three-center nuclear attraction integrals is substantially more difficult. Using the Fourier transformation method for such integrals with B functions, one can use a two-dimensional integral representation in combination with numerical quadrature. [51], [52], [55]. This contains, however, oscillating terms that limit the achievable accuracy for large distances of the centers. Thus, there is a need for methods

that work for large distances. One alternative is the use of expansions in spherical harmonics or of multipole expansions.

The idea is relatively simple:

For real basis functions, the product $\rho_{jk}(\vec{r}) = \phi_j(\vec{r})\phi_k(\vec{r})$ can be regarded as a charge density. The associated electrostatic potential then corresponds exactly to the nuclear attraction integral I, as may be seen easily from a comparison of Eqs. (1) and (18).

Especially, the exact expansion (3) with respect to spherical harmonics and the approximate multipole expansion (6) can be applied in this context as well.

Recently, procedures of this kind have been studied, mainly by Fernández Rico and coworkers [80], [81], [82], [83], [84], [85], [86], [87], [88] and by Jones and coworkers [90], [91], [92], [93], [94], [95], [96], [97], [98], [99].

This work has been taken up by the group around Bouferguene and in some papers [78], [79], these authors tried to apply convergence accelerators to expansions that are analogous to Eq. (3) using mainly the ϵ algorithm.

Since orthogonal expansions are involved it is to be expected that special methods for this type of series are advantageous.

4 Extrapolation Methods for Orthogonal Expansions

For extrapolation of expansions in orthogonal polynomials of the form

$$s(x) = \sum_{j=0}^{\infty} c_j \, P_j(x) \tag{26}$$

with partial sums

$$s_n(x) = \sum_{j=0}^{n} c_j \, P_j(x) \, , \tag{27}$$

not many methods are known to work well. Besides the well-known ϵ algorithm of Wynn and the $d^{(m)}$ transformations [130], there are methods based on the acceleration of related complex power series [121], [124], [125]. If one does not like to work with complex arithmetics, one may use also the so-called $\mathcal{K}$ transformation [120]. The $\mathcal{K}$ transformation may be regarded as a generalization of the $\mathcal{I}$ transformation that has proved to be useful for trigonometric Fourier series [119], [123]. Both transformations are obtained by iteration of a simple transformation.

We sketch the main ideas that lead to the $\mathcal{K}$ transformation.

Consider the sequence of the partial sums s_n to be extrapolated as given in Eq. (27), and write it in terms of the limit s and a tail t_n as

$$s_n = s + t_n \ , \qquad t_n = -\sum_{j=n+1}^{\infty} c_j \, P_j(x) \ . \tag{28}$$

By using the usual three-term recurrence relation of the orthogonal polynomials $P_n(x)$ repeatedly, one may express the tail as

$$t_n = \alpha_{n+1}(x) P_{n+1}(x) + \beta_{n+1}(x) P_{n+2}(x) \tag{29}$$

One may express $P_{n+2}(x)$ as linear combination of $P_{n+1}(x)$ and $Q_{n+1}(x)$ with x-dependent coefficients.

Remark This is always possible in the cases of interest, at least asymptotically for large n. For example, specializing to Legendre functions $P_n(x)$ and $Q_n(x)$ that satisfy the recurrence relation $w_{n+1}(x) = (2n+1)xw_n(x)/(n+1) - nw_{n-1}/(n+1)$ with the initial conditions $P_0(x) = 1$, $P_1(x) = x$, $Q_0(x) = log((1+x)/(1-x))/2$, $Q_1(x) = xQ_0(x) - 1$, one has the asymptotic relation[130] $P_n(\cos\theta) - \mathrm{i}\frac{2}{\pi} Q_n(\cos\theta) = \exp(\mathrm{i}n\theta) k n^{-1/2} \, (1 + O(1/n))$ for large n where k is a constant. An easy calculation then shows $P_{n+1}(\cos\theta) = (1 + 1/n)^{-1/2} (\cos\theta \, P_n(\cos\theta) + 2 \sin\theta \, Q_n(\cos\theta)/\pi)(1 + O(1/n))$ for large n.

Using this method, it is possible to rewrite the tails as

$$t_n = A_{n+1}(x) P_{n+1}(x) + B_{n+1}(x) Q_{n+1}(x) \tag{30}$$

Assuming that the leading behavior of $A_n(x)$ and $B_n(x)$ for large n is up to constants c and d given by remainder estimates ω_n, model sequences of the form

$$s_n = s + \omega_n \, (c \, \tilde{P}_n(x) + d \, \tilde{Q}_n(x)) \tag{31}$$

are obtained where the $\tilde{P}_n(x) = P_{n+1}(x)$ and $\tilde{Q}_n(x) = Q_{n+1}(x)$ obey the three-term recursion

$$\zeta_n^{(0)} v_n + \zeta_n^{(1)} v_{n+1} + \zeta_n^{(2)} v_{n+2} = 0 \tag{32}$$

where the coefficients $\zeta_n^{(j)}$ for $j = 0, 1, 2$ are x dependent. Rewriting this as

$$\frac{s_n - s}{\omega_n} = c \, \tilde{P}_n(x) + d \, \tilde{Q}_n(x) \tag{33}$$

and applying the recursion relation (32) to both sides of the equation, one obtains

$$\zeta_n^{(0)} \frac{s_n - s}{\omega_n} + \zeta_n^{(1)} \frac{s_{n+1} - s}{\omega_{n+1}} + \zeta_n^{(2)} \frac{s_{n+2} - s}{\omega_{n+2}} = 0 \; . \tag{34}$$

This may be solved for s. Then, we obtain

$$s = \frac{\zeta_n^{(0)} \dfrac{s_n}{\omega_n} + \zeta_n^{(1)} \dfrac{s_{n+1}}{\omega_{n+1}} + \zeta_n^{(2)} \dfrac{s_{n+2}}{\omega_{n+2}}}{\zeta_n^{(0)} \dfrac{1}{\omega_n} + \zeta_n^{(1)} \dfrac{1}{\omega_{n+1}} + \zeta_n^{(2)} \dfrac{1}{\omega_{n+2}}} \; , \tag{35}$$

i.e., we can calculate the exact limit s for model sequences of the form (31). If a given sequence s_n differs from this model, one cannot expect to calculate the limit exactly by this simple formula, but applying it is expected to yield a sequence of approximations that is closer to the limit if the problem sequence is "close" to the model. Thus, one obtains a sequence transformation given by the expression

$$s_n^{(1)} = \frac{\zeta_n^{(0)} \dfrac{s_n}{\omega_n} + \zeta_n^{(1)} \dfrac{s_{n+1}}{\omega_{n+1}} + \zeta_n^{(2)} \dfrac{s_{n+2}}{\omega_{n+2}}}{\zeta_n^{(0)} \dfrac{1}{\omega_n} + \zeta_n^{(1)} \dfrac{1}{\omega_{n+1}} + \zeta_n^{(2)} \dfrac{1}{\omega_{n+2}}} \; . \tag{36}$$

We say that this transformation is exact for model sequences of the form (31) since it allows to calculate the exact limit s for such model sequences. This is the simple sequence transformation mentioned above that is to be iterated.

Iteration leads to the recursive scheme

$$\begin{aligned}
&\mathrm{N}_n^{(0)} = s_n/\omega_n \; , \qquad \mathrm{D}_n^{(0)} = 1/\omega_n \; , \\
&\mathrm{N}_n^{(k+1)} = \left(\zeta_{n+k}^{(0)} \mathrm{N}_n^{(k)} + \zeta_{n+k}^{(1)} \mathrm{N}_{n+1}^{(k)} + \zeta_{n+k}^{(2)} \mathrm{N}_{n+2}^{(k)} \right) \Big/ \delta_n^{(k)} \; , \\
&\mathrm{D}_n^{(k+1)} = \left(\zeta_{n+k}^{(0)} \mathrm{D}_n^{(k)} + \zeta_{n+k}^{(1)} \mathrm{D}_{n+1}^{(k)} + \zeta_{n+k}^{(2)} \mathrm{D}_{n+2}^{(k)} \right) \Big/ \delta_n^{(k)} \; , \\
&\mathcal{K}_n^{(k)}(\{\delta_n^{(k)}\}, \{\zeta_n^{(j)}\}, \{s_n\}, \{\omega_n\}) = \mathrm{N}_n^{(k)}/\mathrm{D}_n^{(k)}
\end{aligned} \tag{37}$$

that defines the $\mathcal{K}$ transformation. Here, the $\delta_n^{(k)}$ are auxiliary quantities. This transformation is a nonlinear sequence transformation, if the ω_n depend on the s_n.

We make the important observation that in each step of the iteration numbered by k, a new sequence of remainder estimates is used according to $\omega_n^{(k)} = 1/D_n^{(k)}$, and that the lower index of the recursion coefficients $\zeta_n^{(j)}$ is shifted by k. Note that the remainder estimates $\omega_n^{(k)}$ depend only on the original remainder estimates $\omega_n = \omega_n^{(0)}$ and the auxiliary quantities $\delta_n^{(k)}$. Note

that the recursion relations for the numerators and denominators are nothing but the application of the three-term recurrence relation for $P_{n+k}(x)$ (up to a scaling inducing by the $\delta_n^{(k)}$). Thus, the sequence transformation eliminates approximately contributions of orthogonal functions $P_n(x)$ (and $Q_n(x)$) for successive higher values of n.

We specialize to the case of expansions in Legendre polynomials. Here, the input sequence s_n of partial sums (27) is transformed into a new sequence

$$\{s_n\} \longrightarrow \{s'_n\} = \{\mathcal{K}_{n-2[\![n/2]\!]}^{([\![n/2]\!])}(\{\delta_n^{(k)}\}, \{\gamma_n^{(j)}\}, \{s_n\}, \{\omega_n\})\} \tag{38}$$

with $\gamma_n^{(0)} = n+2$, $\gamma_n^{(1)} = -(2n+5)x$ and $\gamma_n^{(2)} = n+3$. The latter correspond to the three-recurrence relation for P_{n+1}. By $[\![x]\!]$ we denote the integer part of x.

The transformed sequence converges normally much faster than the original one if the coefficients c_j in (26) do not oscillate itself, and also considerably faster than the estimates obtained using the ϵ algorithm. [120] For further information on the extrapolation of orthogonal expansions see also [131], [121].

If the maximal value of n is $2N$, i.e., if only partial sum up to s_{2N} are available, then s_{2N} is a polynomial of degree $2N$ in x. In this case, the transformed quantities $s'_{2N} = \mathcal{K}_0^{(N)}(\{\delta_n^{(k)}\}, \{\gamma_n^{(j)}\}, \{s_n\}, \{\omega_n\})\}$ are a rational function in x of the form

$$s'_{2N} = \frac{p_{2N}(x)}{q_N(x)} \tag{39}$$

where $p_{2N}(x)$ is a polynomial of degree $2N$ and $q_N(x)$ is a polynomial of degree N. For instance, for $\delta_n^{(k)} = 1/(n+1)$, $\omega_n = c_n$, and $N = 2$ we have

$$\begin{aligned} s'_4 = -\frac{1}{2}(&x^4\, c_4\, c_1\, c_3\, c_2 + (-196\, {c_1}^2\, c_3\, c_4 + 492\, c_4\, c_1\, {c_2}^2 - 300\, c_1\, c_2\, {c_3}^2)\, x^3 \\ &+ (-c_1\, c_2\, c_3\, c_4 - 196\, c_1\, c_3\, c_4\, c_0 + 328\, c_4\, {c_1}^2\, c_2 - 180\, c_1\, {c_2}^2\, c_3)\, x^2 + (\\ &114\, c_2\, c_3\, c_4\, c_0 - 164\, c_4\, c_1\, {c_2}^2 + 328\, c_4\, c_1\, c_2\, c_0 + 180\, c_1\, c_2\, {c_3}^2 \\ &- 120\, {c_1}^2\, c_2\, c_3 - 114\, {c_1}^2\, c_3\, c_4)x + 60\, c_1\, {c_2}^2\, c_3 - 120\, c_1\, c_2\, c_3\, c_0 \\ &- 114\, c_1\, c_3\, c_4\, c_0)c_0 \Big/ (98\, x^2\, c_4\, c_1\, c_3\, c_0 \\ &+ (-164\, c_4\, c_1\, c_2\, c_0 - 57\, c_2\, c_3\, c_4\, c_0)\, x + 6\, c_1\, c_2\, c_3\, c_4 + 60\, c_1\, c_2\, c_3\, c_0 \\ &+ 57\, c_1\, c_3\, c_4\, c_0) \end{aligned}$$

and

$$s_4 = \frac{35}{8}\, c_4\, x^4 + \frac{5}{2}\, c_3\, x^3 + (\frac{3}{2}\, c_2 - \frac{15}{4}\, c_4)\, x^2 + (c_1 - \frac{3}{2}\, c_3)\, x + c_0 - \frac{1}{2}\, c_2 + \frac{3}{8}\, c_4\ .$$

If the evaluation of the expansion at many values of x is required, then it pays to compute the coefficients of numerator and denominator polynomial once and for all from the known coefficients c_j, and then, the additional numerical effort in comparison to the term-wise summation of the expansion is the additional evaluation of a polynomial of degree N. As we will see, the resulting expression s'_{2N} is much more accurate than s_{2N}. For instance, s'_4 is often 1000fold more accurate than s_4.

Although this approach of fixing the maximum value of n throughout is very cost-effective, it has some disadvantages: The accuracy is not uniform, ie., not the same for all angles. Further, as seen from the explicit expression for s'_4, there are some values of $x = \cos\theta$ for which the denominator polynomial vanishes. These angles may easily be identified in advance. In the vicinity of these angles either the explicit summation or linear convergence [132], [133] acceleration may be used. Then, however, convergence is much slower usually. Thus, a hybrid algorithm would have to be designed. Alternatively, by using the whole sequence of the s'_n as computed via the recursive scheme defining the $\mathcal{K}$ transformation, one can stop the calculation when the difference between consecutive approximations lies below a threshold. This method will result in more uniform approximations. Also, for nonlinear convergence accelerators, one may use progressive forms and particular rules to avoid the rare cases that the denominators vanish (cp. [131], and [134] and references therein). Alternatively, the simple device to replace an accidentally vanishing denominator by a small number near the smallest floating point number and simply to go on with the recursive algorithm, has proven to work surprisingly well. [135] The latter approach can also be implemented in the programs for the $\mathcal{K}$ transformation that were used in the present work.

We further remark that in the vicinity of the singularities of the Legendre series the convergence of the original series may become exceedingly slow (like $O(1/n^\alpha)$ for small α). In this case, convergence acceleration is especially desirable. Straightforward application of nonlinear convergence accelerators is not the best way to evaluate the sum of the orthogonal series. Instead, it is much better to use the $\tau-$fold frequency approach. (τ: "tau") This is essentially the application of a convergence acceleration method to the sequence $\{s_{\tau n}\}_{n=0}^{\infty} = \{s_0, s_\tau, s_{2\tau}, \ldots\}$ for some suitable integer $\tau > 1$. In the case of the $\mathcal{K}$ transformation, this produces approximations

$$ {}^{\tau}s_n = \mathcal{K}_{n-2\lfloor n/2 \rfloor}^{(\lfloor n/2 \rfloor)}(\{\delta_n^{(k)}\}, \{\gamma_n^{(j)}\}, \{s_{\tau\, n}\}, \{{}^{\tau}\omega_n\}) \tag{40} $$

using $\gamma_n^{(0)} = n + 2$, $\gamma_n^{(1)} = -(2n + 5)\, x_\tau$, and $\gamma_n^{(2)} = n + 3$ corresponding to the three-term recurrence relation of Legendre polynomials at the argument

$$ x_\tau = \cos(\tau \arccos(x)) \, . \tag{41} $$

One may choose the remainder estimated in this approach for instance as ${}^{\tau}\omega_n = c_{\tau n}$, i.e., as suitable coefficients of the Legendre series. For further details of the $\tau-$fold frequency approach, the interested reader is referred to the literature [121], [122], [123], [124], [125]. We are not going to use this approach in the following for simplicity.

5 A Simple Example

We study as a simple example a charge density

$$\rho(\vec{r}) = \exp(-\alpha r)\exp(-\beta|\vec{r}-\vec{R}|) \tag{42}$$

corresponding to a two-center product of 1s-ETOs. For the electrostatic potential of this density, we have

$$\begin{aligned} U(\vec{r}) &= \int \frac{\exp(-\alpha r')\exp(-\beta|\vec{r}'-\vec{R}|)}{|\vec{r}-\vec{r}'|}\,\mathrm{d}^3r' \\ &= 4\pi\sum_{\ell m}\frac{Y_\ell^m(\vec{r}/r)}{2\ell+1}\int\frac{r_<^\ell}{r_>^{l+1}}Y_\ell^{m*}(\vec{r}'/r') \\ &\times\exp(-\alpha r')\exp(-\beta|\vec{r}'-\vec{R}|)\,\mathrm{d}^3r' \\ &= 4\pi\sum_{\ell m}\frac{Y_\ell^m(\vec{r}/r)}{2\ell+1}\int\frac{r_<^\ell}{r_>^{\ell+1}}Y_\ell^{m*}(\vec{r}'/r')\exp(-\alpha r') \\ &\times\frac{-4\pi}{\sqrt{r'R}}\sum_{\ell'm'}Y_{\ell'}^{m'}(\vec{r}'/r')Y_{\ell'}^{m'*}(\vec{R}/R) \\ &\times\left(\frac{\partial}{\partial\beta}\right)I_{\ell'+1/2}(\beta r'_<)K_{\ell'+1/2}(\beta r'_>)\,\mathrm{d}^3r' \end{aligned} \tag{43}$$

with $r'_< = \min(r', R)$ and $r'_> = \max(r', R)$. Here, the addition theorem [117], [78]

$$\exp(-\lambda\sqrt{r^2+\rho^2-2r\rho\cos\theta}) = -\sum_{\ell=0}^{\infty}(2\ell+1)\,P_\ell(\cos\theta)\frac{1}{\sqrt{r\rho}}\frac{\partial}{\partial\lambda}[I_{\ell+1/2}(\lambda r)K_{\ell+1/2}(\lambda\rho)] \tag{44}$$

of the exponential function was used that holds for $r < \rho$. Further, the addition theorem (8) of the spherical harmonics was used. Now, the orthonormality of the spherical harmonics yields

$$\begin{aligned} U(\vec{r}) &= \frac{-4\pi}{\sqrt{R}}\sum_{\ell=0}^{\infty}P_\ell\left(\vec{r}\cdot\vec{R}/(rR)\right)\int_0^\infty r'^{3/2}\frac{r_<^\ell}{r_>^{\ell+1}}\exp(-\alpha r') \\ &\times\left(\frac{\partial}{\partial\beta}\right)I_{\ell+1/2}(\beta r'_<)K_{\ell+1/2}(\beta r'_>)\,\mathrm{d}r'\ . \end{aligned} \tag{45}$$

The remaining radial integral can be computed with the help of Maple. This approach avoids rounding errors that can easily spoil the calculation of the integral [78]. We note that the result is of the form (17), with

$$\tilde{z}_\ell(r) = \frac{-4\pi}{\sqrt{R}} \int_0^\infty r'^{3/2} \frac{r_<^\ell}{r_>^{\ell+1}} \exp(-\alpha r') \left(\frac{\partial}{\partial\beta}\right) I_{\ell+1/2}(\beta r'_<) K_{\ell+1/2}(\beta r'_>)\, \mathrm{d}r' \,. \tag{46}$$

Analogously, one obtains for the multipole expansion of this charge density an equation of the form (9),

$$\begin{aligned} U_Q(\vec{r}) = \frac{-4\pi}{\sqrt{R}} \sum_{\ell=0}^\infty P_\ell\left(\vec{r}\cdot\vec{R}/(rR)\right) \int_0^\infty r'^{3/2} \frac{r'^\ell}{r^{\ell+1}} \exp(-\alpha r') \\ \times \left(\frac{\partial}{\partial\beta}\right) \left[I_{\ell+1/2}(\beta r'_<) K_{\ell+1/2}(\beta r'_>)\right] \mathrm{d}r' \,, \end{aligned} \tag{47}$$

and for the multipole moments follows

$$q_\ell = \frac{-4\pi}{\sqrt{R}} \int_0^\infty r'^{3/2+\ell} \exp(-\alpha r') \left(\frac{\partial}{\partial\beta}\right) \left[I_{\ell+1/2}(\beta r'_<) K_{\ell+1/2}(\beta r'_>)\right] \mathrm{d}r' \tag{48}$$

which can also be computed advantageously with Maple.

6 Numerical Tests

We study the charge density $\rho(\vec{r}) = \rho(x,y,z)$ of Eq. (42) in the last section for $\alpha = 3/10$, $\beta = 1$ and $\vec{R} = 2\vec{e}_z$, where $\vec{e}_z$ is the unit vector in z direction. It is rotationally symmetric around the z axis. This density is also plotted in http://www.chemie.uni-regensburg.de/ECCC/4/rho.ps as a function of x and z for $y = 0$.

The corresponding electrostatic potential is also rotationally symmetric around the z axis, a function of z and $\sqrt{x^2+y^2}$ only or, equivalently, only of $r = \sqrt{x^2+y^2+z^2}$ and θ with $\cos\theta = z/r$. This is also valid for the multipole expansion (47) and the exact expansion (45) in spherical harmonics.

6.1 Multipole Expansion

The multipole moments q_ℓ are displayed in Tab. 1. They grow relatively fast with ℓ.

In Tabs. 2-5 we display for various combinations of r and θ the partial sums

$$s_\ell = \sum_{j=0}^{\ell} P_j\left(\cos\theta\right) \frac{q_j}{r^{j+1}} \tag{49}$$

and the transformed values

$$s'_\ell = \mathcal{K}^{([\![\ell/2]\!])}_{\ell-2[\![\ell/2]\!]}(\{(\ell+1)^{-1}\}, \{\gamma^{(j)}_\ell\}, \{s_\ell\}, \{q_\ell/r^{\ell+1}\})\} \tag{50}$$

with $\gamma^{(0)}_\ell = \ell+2$, $\gamma^{(1)}_\ell = -(2\ell+5)\cos\theta$ and $\gamma^{(2)}_\ell = \ell+3$ corresponding to the recursion of the Legendre polynomials $P_{\ell+1}(\cos\theta)$. These values are rounded and can not display more than 16 exact decimal digits. The definition Eq. (37) of the $\mathcal{K}$ transformation is used. Also displayed is for both sequences s_ℓ and s'_ℓ the number of exact digits. This is defined as the negative decadic logarithm of the relative error as indicated also in the table headers.

Also, we display in Figures 1, 2, and 3 graphically the performance of the acceleration method for the multipole expansion using partial sums s_ℓ up to $\ell = 20$. Plotted are the achievable number of exact digits without (Fig. 1) and with acceleration (Fig. 1), and the gain, i.e., the additional digits achieved using the acceleration method, as a function of r and $x = \cos(\theta)$. For simplicity, the τ-fold frequency approach was not used, and hence the performance is better for larger distances from the singularity at $r =$ and $x = 1$.

From these tables and figures, one observes a clear increase of the accuracy by using the extrapolation method. Already for smaller values of ℓ, there is a drastic reduction of the error. A gain of three and more digits is typical and corresponds to a reduction of the error by a factor of 1000 or more.

Let us remark that the additional numerical effort for the extrapolation is very low in comparison to the evaluation of the multipole moments.

6.2 Exact Expansion in spherical harmonics

In Tabs. 6-8 we plot for various combinations of r and θ the partial sums

$$s_\ell = \sum_{j=0}^{\ell} P_j(\cos\theta)\,\tilde{z}_j(r) \tag{51}$$

of the exact expansion (45) and the transformed values

$$s'_\ell = \mathcal{K}^{([\![\ell/2]\!])}_{\ell-2[\![\ell/2]\!]}(\{(\ell+1)^{-1}\}, \{\gamma^{(j)}_\ell\}, \{s_\ell\}, \{\tilde{z}_\ell(r)\})\} \tag{52}$$

with $\gamma^{(0)}_\ell = \ell+2$, $\gamma^{(1)}_\ell = -(2\ell+5)\cos\theta$ and $\gamma^{(2)}_\ell = \ell+3$ corresponding to the recursion of the Legendre polynomials $P_{\ell+1}(\cos\theta)$. As in the case of the multipole expansion the values are rounded to 16 decimal digits. The definition Eq. (37) of the $\mathcal{K}$ transformation is used. Also, we plot for both sequences s_ℓ and s'_ℓ the corresponding number of exact digits. As before, this

number is defined as the negative decadic logarithm of the relative error as indicated also in the table headers.

Comparison of Tabs. 2 with 6, 3 with 7 and 4 with 8, that have been computed for the same point, respectively, reveals that the converged extrapolated values differ considerably. This means that in this way the difference $U - U_Q$ can be evaluated.

Let us remark that also in this case the additional numerical effort for the extrapolation is very low in comparison to the evaluation of the coefficients of the orthogonal expansion.

In summary, it can be stated that the acceleration of the expansion in Legendre polynomials via the $\mathcal{K}$ transformation leads to pronounced error reduction, as well in the case of the multipole expansion as well as in the case of the exact computation of the electrostatic potential. Put another way, for achieving a certain accuracy, considerably less multipole moments or expansion coefficients, respectively, are necessary if a problem adapted extrapolation method as the $\mathcal{K}$ transformation is used.

7 Tables

For detailed explanations of the meaning of the displayed data see Sec. 6.

8 Figures

For detailed explanations of the meaning of the displayed data see Sec. 6.

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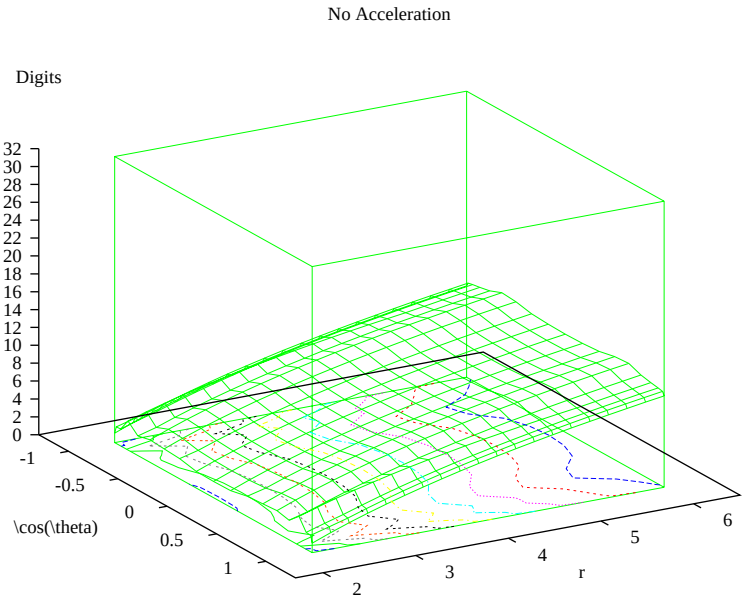

Figure 1: Without Acceleration (eps-file[4])

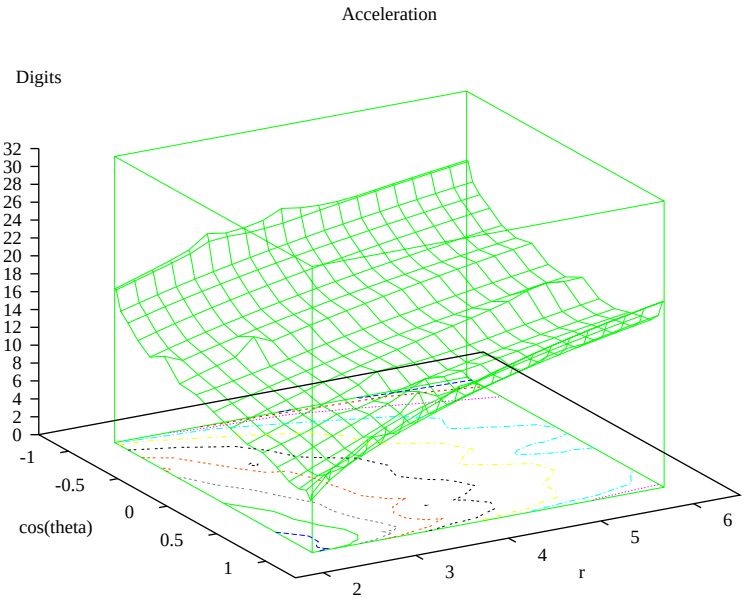

Figure 2: With Acceleration (eps-file[5])

Table 1: Multipole Moments q_ℓ

ℓ	q_ℓ	ℓ	q_ℓ
0	$9.6145542836957232 \cdot 10^{0}$	15	$5.6126132139082320 \cdot 10^{4}$
1	$1.5111468162060430 \cdot 10^{1}$	16	$1.0526398832720890 \cdot 10^{5}$
2	$2.4972140819932912 \cdot 10^{1}$	17	$1.9791327162842600 \cdot 10^{5}$
3	$4.2508094215318600 \cdot 10^{1}$	18	$3.7295814285560472 \cdot 10^{5}$
4	$7.3829280479536656 \cdot 10^{1}$	19	$7.0429819898685744 \cdot 10^{5}$
5	$1.3014160081924070 \cdot 10^{2}$	20	$1.3325858332275628 \cdot 10^{6}$
6	$2.3205220342856620 \cdot 10^{2}$	21	$2.5258921378457704 \cdot 10^{6}$
7	$4.1759801415517728 \cdot 10^{2}$	22	$4.7958001073652480 \cdot 10^{6}$
8	$7.5724460859402144 \cdot 10^{2}$	23	$9.1198033217610032 \cdot 10^{6}$
9	$1.3819758024471442 \cdot 10^{3}$	24	$1.7367785134246278 \cdot 10^{7}$
10	$2.5360253549353620 \cdot 10^{3}$	25	$3.3120638623127288 \cdot 10^{7}$
11	$4.6760909010975208 \cdot 10^{3}$	26	$6.3243038872318152 \cdot 10^{7}$
12	$8.6583940808828048 \cdot 10^{3}$	27	$1.2090777865352850 \cdot 10^{8}$
13	$1.6092055362945430 \cdot 10^{4}$	28	$2.3141623269443344 \cdot 10^{8}$
14	$3.0007868261207612 \cdot 10^{4}$	29	$4.4340905859803936 \cdot 10^{8}$

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Table 2: $\mathcal{K}$ transformation of the multipole expansion for $r = 4$ and $\theta = 60$ degree

ℓ	s_ℓ	s'_ℓ	$-\lg\lvert 1 - s_\ell/s\rvert$	$-\lg\lvert 1 - s'_\ell/s\rvert$
11	2.7418043436441288	2.7418396451187988	4.9	8.5
13	2.7418444420453968	2.7418396360933220	5.8	9.8
15	2.7418400997161048	2.7418396365510044	6.8	11.3
17	2.7418393319135280	2.7418396365368780	7.0	13.2
19	2.7418396810712432	2.7418396365366408	7.8	13.6
21	2.7418396408021740	2.7418396365367192	8.8	14.6
23	2.7418396335310588	2.7418396365367116	9.0	∞
25	2.7418396369949232	2.7418396365367116	9.8	∞

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Table 3: $\mathcal{K}$ transformation of the multipole expansion for $r = 4$ and $\theta = 2$ degree

ℓ	s_ℓ	s'_ℓ	$-\lg\lvert 1 - s_\ell/s\rvert$	$-\lg\lvert 1 - s'_\ell/s\rvert$
5	4.0055910661641912	4.0310298596769504	2.2	6.0
7	4.0258375726969488	4.0310259627927432	2.9	8.1
9	4.0299452870267560	4.0310259342473168	3.6	10.3
11	4.0307974518518776	4.0310259340256136	4.2	12.5
13	4.0309770827258808	4.0310259340268592	4.9	14.2
15	4.0310154000570728	4.0310259340268832	5.6	∞
17	4.0310236476902344	4.0310259340268832	6.2	∞
19	4.0310254353074664	4.0310259340268832	6.9	∞

Table 4: $\mathcal{K}$ transformation of the multipole expansion for $r = 12$ and $\theta = 2$ degree

ℓ	s_ℓ	s'_ℓ	$-\lg\lvert 1 - s_\ell/s\rvert$	$-\lg\lvert 1 - s'_\ell/s\rvert$
2	0.9205147491201462	0.9229094827555278	2.6	5.1
4	0.9228521264440244	0.9229028304339108	4.3	9.7
6	0.9229017067530020	0.9229028306219438	5.9	11.5
8	0.9229028050126544	0.9229028306190520	7.6	∞
10	0.9229028300243444	0.9229028306190520	9.2	∞

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Table 5: $\mathcal{K}$ transformation of the multipole expansion for $r = 3$ and $\theta = 45$ degree

ℓ	s_ℓ	s'_ℓ	$-\lg\lvert 1 - s_\ell/s\rvert$	$-\lg\lvert 1 - s'_\ell/s\rvert$
14	4.3489633745055632	4.3493388832962536	4.1	8.4
16	4.3492565069391536	4.3493388972986296	4.7	9.5
18	4.3493913460628168	4.3493388992014864	4.9	10.0
20	4.3493504034221608	4.3493388987593184	5.6	11.1
22	4.3493312030632704	4.3493388987929736	5.8	12.6
24	4.3493372120197552	4.3493388987948584	6.4	12.8
26	4.3493400696609064	4.3493388987940592	6.6	13.7
28	4.3493391551806856	4.3493388987941480	7.2	∞

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Table 6: $\mathcal{K}$ transformation of the expansion in spherical harmonics for $r = 4$ and $\theta = 60$ degree

ℓ	s_ℓ	s'_ℓ	$-\lg\lvert 1 - s_\ell/s\rvert$	$-\lg\lvert 1 - s'_\ell/s\rvert$
5	2.6360864318669988	2.6377072675101864	3.2	5.2
6	2.6374837369057832	2.6377515327293168	4.0	5.0
7	2.6378518176502576	2.6377253830860056	4.3	6.0
8	2.6378042659979908	2.6377219784704452	4.5	6.4
9	2.6377350134378020	2.6377230006666316	5.3	8.6
10	2.6377151544952184	2.6377230256403856	5.5	8.2
11	2.6377179511190400	2.6377230015625168	5.7	8.7
12	2.6377222605455336	2.6377230070377540	6.5	10.9
13	2.6377235638641044	2.6377230071786740	6.7	10.2
14	2.6377233701261704	2.6377230069889060	6.9	11.1
15	2.6377230603586148	2.6377230070087064	7.7	12.7
16	2.6377229633254132	2.6377230070085216	7.8	12.8
17	2.6377229782819236	2.6377230070080356	8.0	13.5
18	2.6377230028127904	2.6377230070081392	8.8	14.2
19	2.6377230106880184	2.6377230070081228	8.9	∞
20	2.6377230094424720	2.6377230070081228	9.0	∞

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Table 7: $\mathcal{K}$ transformation of the expansion in spherical harmonics for $r = 4$ and $\theta = 2$ degree

ℓ	s_ℓ	s'_ℓ	$-\lg\lvert 1 - s_\ell/s\rvert$	$-\lg\lvert 1 - s'_\ell/s\rvert$
10	4.5865590596837048	4.5866525846910224	4.7	6.4
12	4.5866776132666136	4.5866544475900856	5.3	7.7
14	4.5866762505499168	4.5866543754774488	5.3	8.5
16	4.5866652462194176	4.5866543587750376	5.6	9.4
18	4.5866588085511440	4.5866543606914784	6.0	10.8
20	4.5866559736808440	4.5866543607829960	6.5	11.4
22	4.5866548859890528	4.5866543607630656	6.9	13.1
24	4.5866545102511760	4.5866543607625712	7.5	13.5
26	4.5866543942048184	4.5866543607627224	8.1	15.3
28	4.5866543637663352	4.5866543607627240	9.2	15.5

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Table 8: $\mathcal{K}$ transformation of the expansion in spherical harmonics for $r = 12$ and $\theta = 2$ degree

ℓ	s_ℓ	s'_ℓ	$-\lg\lvert 1 - s_\ell/s\rvert$	$-\lg\lvert 1 - s'_\ell/s\rvert$
2	0.9205059009697086	0.9228996042830154	2.6	5.1
3	0.9225472237960400	0.9228930830704692	3.4	6.0
4	0.9228417168669332	0.9228922656178376	4.3	8.2
5	0.9228847832640386	0.9228922593965848	5.1	9.8
6	0.9228911451439840	0.9228922591923836	5.9	10.3
7	0.9228920922347056	0.9228922592384774	6.7	11.4
8	0.9228922340878756	0.9228922592424316	7.6	12.6
9	0.9228922554386146	0.9228922592422232	8.4	13.6
10	0.9228922586651554	0.9228922592421988	9.2	15.0
11	0.9228922591544072	0.9228922592421998	10.0	15.7
12	0.9228922592288100	0.9228922592421998	10.8	16.0

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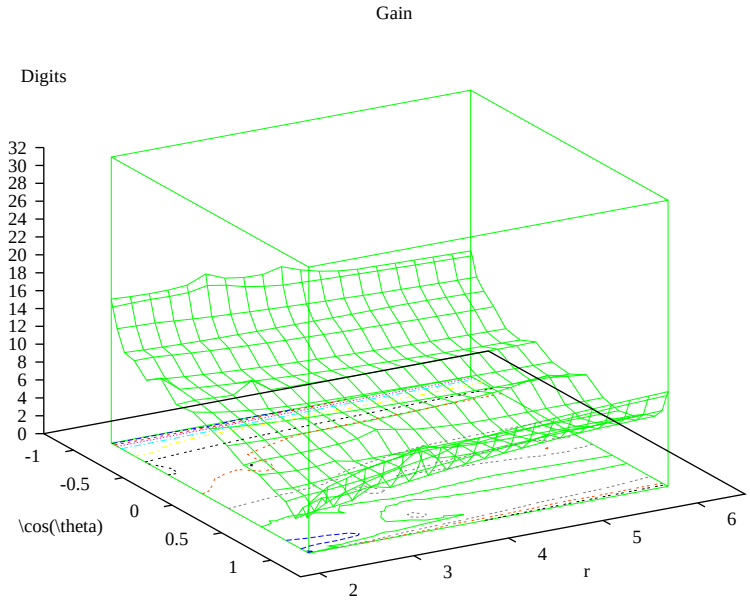

Figure 3: Gain (eps-file[6])

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