Visualisation of Polynomials Used in Series Expansions

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Abstract

Boltzmann's Equation describes a myriad of phenomena from gas and fluid flow to electrons in semiconductors and hence plays an essential role in todays physics. However, calculating a solution to this seven-dimensional partial differential equation is very difficult. The high dimensionality of the equation poses a problem for its solution as traversal mechanisms for these high dimensions are not generally available. We present spherical harmonics which serve as the basis for an alternative, direct solution method to Boltzmann's equation. Here the solution is calculated by expanding the it into spherical harmonics and determining the corresponding coefficients. We visualise the spherical harmonics themselves, their changes due to the recursion relations, and compare their evolution.

1 Introduction

Series expansion has been a common and powerful method for the solution of complex equations for a long time. Polynomial series are often used for this task, as they obey clear rules and can be calculated with relative ease.

Boltzmann's equation which can be employed to describe the physics behind a large variety of problems, can also be treated in this manner. While it was originally incepted to govern the distribution of particles in gasses and fluids, it can also be used to describe the distribution of electrons in semiconductors [Vecchi et al., 1997] and in fact any phenomenon which involves particles that are not in a kind of thermodynamic equilibrium.

Spherical harmonics [Abramowitz & Stegun, 1964], which are themselves based on associated Legendre polynomials, are chosen for expansion. The visualisation of these polynomials and their specifications are the topic of this paper along with a means of solving the equation system resulting from the aforementioned expansion.

2 Boltzmann's Equation

As already mentioned, Boltzmann's equation can be used to describe electron transport in semiconductors. It is commonly given in the form presented in Equation 1.

$$\frac{\partial}{\partial t} f + \vec{v} \cdot \mathrm{grad}_r f + \vec{F} \cdot \mathrm{grad}_k f = \frac{\partial}{\partial t} f|_{\mathrm{collisions}} \tag{1}$$

Its solution depends not only on time and position (three dimensions) of the particle, but also on the particle's momentum (three dimensions), thus resulting in a seven-dimensional space in total. Due to the complexity inherent in this seven dimensional first order partial differential equation (PDE), simpler models, such as the drift-diffusion model which forms a mainstay of technology computer aided design (TCAD), are often derived from it [Selberherr, 1984] in order to increase calculation efficiency.

The ongoing development of smaller and faster semiconductor devices and circuits makes the solution of Boltzmann's equation even more pressing, as physical phenomena become influential, which simpler models cannot accommodate.

In addition other fields of research, which make use of Boltzmann's equation, such as gas dynamics or weather simulations, cannot easily make simplifications. It is therefore becoming an increasingly important matter to obtain a rigorous solution of this equation.

The established method of solving Boltzmann's equation in the field of TCAD is the Monte Carlo method [Jungemann & Meinerzhagen, 2003]. However, this method is computationally expensive and the statistical nature can cause problems in several situations. It is therefore desirable to also have different solutions methods available [Liotta & Struchtrup, 2000]. Series expansion using spherical harmonics offers one powerful alternative.

To this end the distribution function f is expanded using spherical harmonics Y_n^m in the following way

$$f = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} f_n^m \left(\vec{r}, k, t\right) Y_n^m \left(\vartheta, \varphi\right) \tag{2}$$

and inserted into Equation 1. This procedure is further discussed in Section 4.

3 Spherical Harmonics

Several fields of application from quantum mechanics, to investigations regarding gravity [S. T. Sutton, 1991] make use of spherical harmonics denoted as $Y_n^m(\vartheta, \varphi)$. In general they can be easily applied to problems with spherical symmetries, which can be expanded to multi-poles using spherical harmonics.

The expansion using spherical harmonics can also be viewed as a generalisation of a Fourier series expansion which works very well with periodic phenomena as found in semiconductor crystals. It is therefore obvious to apply spherical harmonics expansion to the momentum space of electrons, described by the vector $\vec{k}$, which is derived from this periodic structure.

The affinity to spherical symmetries becomes evident, when considering that spherical harmonics form the angular part of the solution of Laplace's equation in spherical coordinates (Equation 3).

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial f}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial f}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 f}{\partial\varphi^2} = 0 \tag{3}$$

Spherical harmonics form a complete system of orthogonal functions. In this work we make use of a normalised form which reads:

$$Y_n^m(\vartheta, \varphi) = (-1)^m \sqrt{\frac{2n+1}{4\pi}\frac{(n-m)!}{(n+m)!}}\, P_n^m\left(\cos\vartheta\right)\; e^{im\varphi} \tag{4}$$

P_n^m are associated Legendre polynomials [Abramowitz & Stegun, 1964]. Figure 1 shows an example of a spherical harmonic.

Recursion relations which link a spherical harmonic $Y_n^m(\vartheta, \varphi)$ to other spherical harmonics $Y_a^b(\vartheta, \varphi)$ of different order b and/or degree a, are among the properties inherited from the Legendre polynomials. A simple recursion

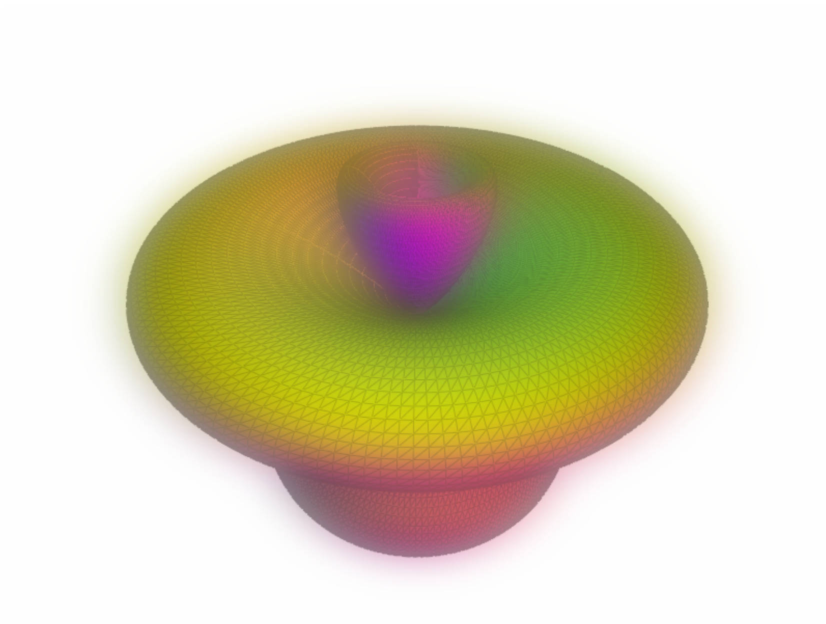

Figure 1: Spherical harmonic Y_n^m with $n = 5$ and $m = 2$.

for the index n is:

$$\cos\vartheta\ Y_n^m = \sqrt{\frac{n+m+1}{2n+1}}\sqrt{\frac{n-m+1}{2n+3}}\ Y_{n+1}^m + \sqrt{\frac{n+m}{2n-1}}\sqrt{\frac{n-m}{2n+1}}\ Y_{n-1}^m \tag{5}$$

A visualisation of this recursion relation is given in Figure 2. An example for a more complex recursion also involving the index m is

$$\begin{aligned}\frac{1}{\sin\theta}\ Y_n^m = \frac{1}{2m}\sqrt{\frac{2n+1}{2n+3}}\Big(&\sqrt{n-m+1}\sqrt{n-m+2}\ Y_{n+1}^{m-1}\\ &-\sqrt{n+m+1}\sqrt{n+m+2}\ Y_{n+1}^{m+1}\Big)\end{aligned} \tag{6}$$

It should be noted that recursions involving m are considered numerically unstable [Deuflhard, 1976], but can still greatly reduce effort, when they are used in analytical expressions. Figure 3 gives a graphical representation of this recursion.

Numerical stability has to be kept in mind not only when calculating spherical harmonics by recursion relations. The faculty in the normalising

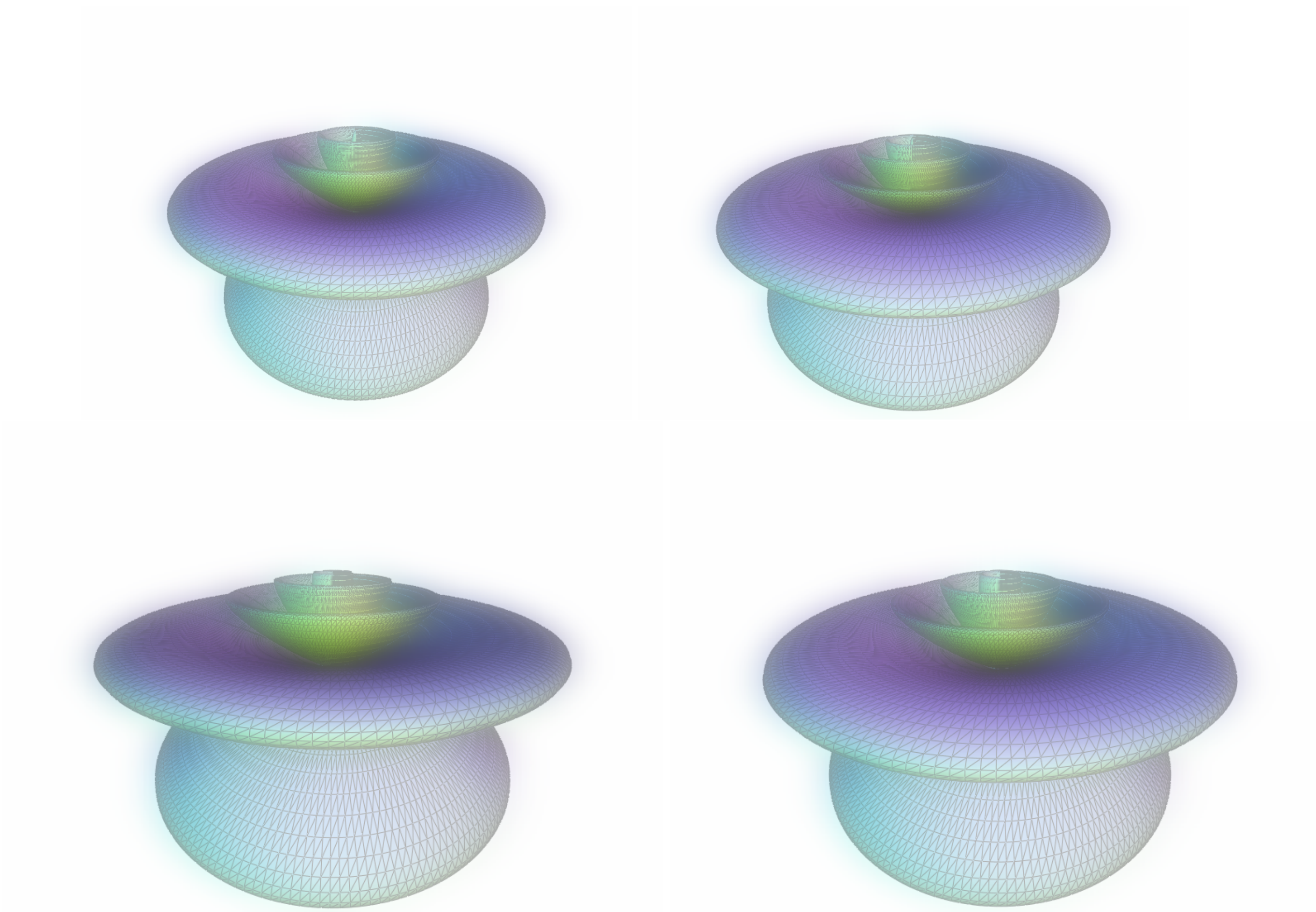

Figure 2: The recursion relation given in Equation 5. The upper left figure shows the result for $n = 8$ and $m = 2$, the upper right figure for $n = 10$ and $m = 2$. The lower left figure depicts the result of the weighted addition and corresponds to $\cos\vartheta\, Y_9^2$ and the lower right figure shows Y_9^2

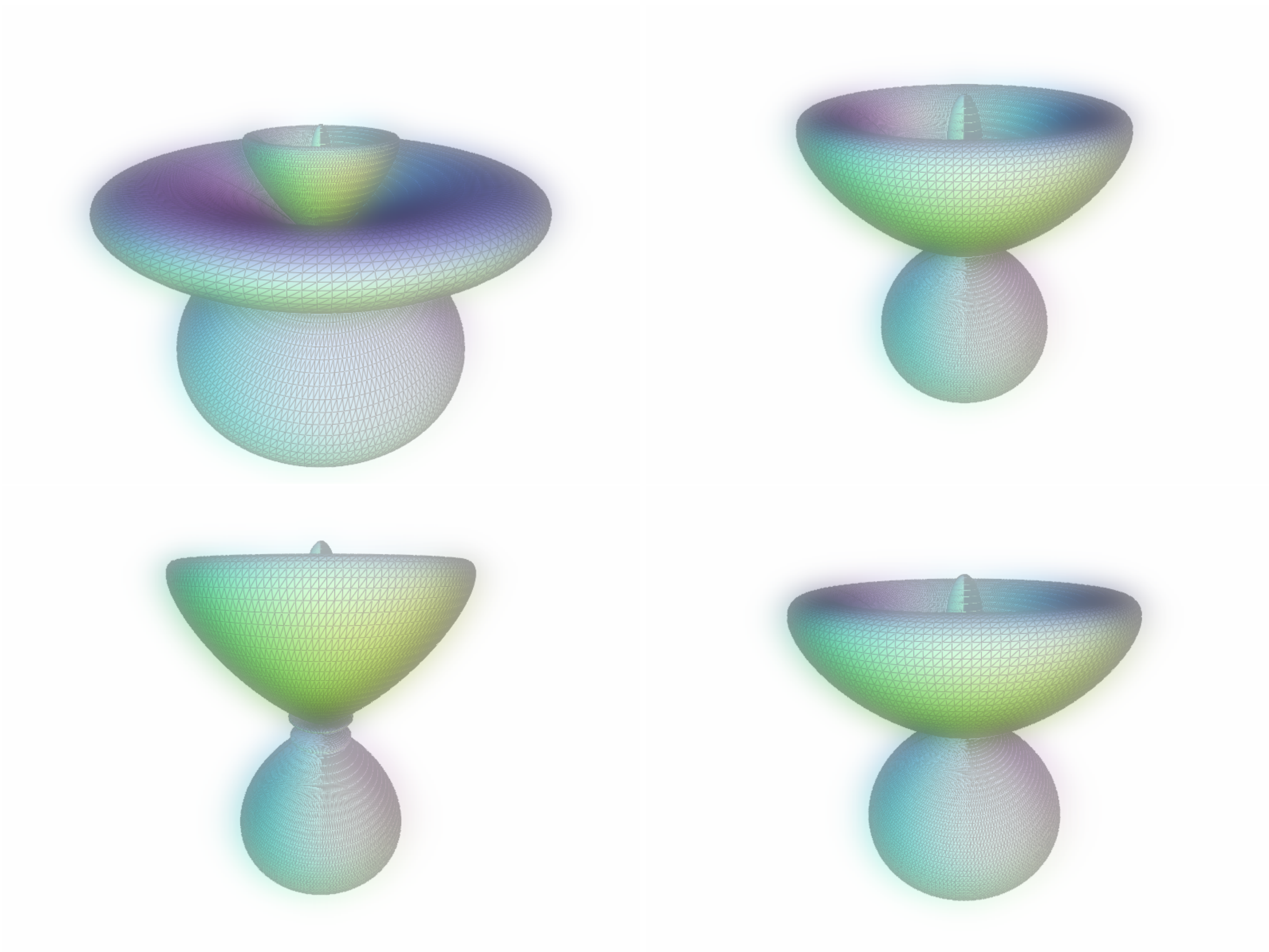

Figure 3: The recursion relation given in Equation 6. The upper left figure shows the result for $n = 6$ and $m = 2$, the upper right figure for $n = 6$ and $m = 4$. The lower left figure depicts the result of the weighted addition and corresponds to $\frac{1}{\sin\vartheta}\, Y_5^3$ and the lower right figure shows Y_5^3

factor also requires special attention for implementation, to avoid erroneous results. Simple algebra can be used to eliminate common factors in the denominator and the enumerator and data types with extended range can be used in the calculations, but these measures only push the limit of the reliably calculable spherical harmonic. While overflows of numerical values may be detected for some data types, it is not possible to discover numerical issues of recursion relations.

The left part of Figure 4 shows a spherical harmonic deformed by numerical errors. The image on the right hand side shows the correct shape of the spherical harmonic.

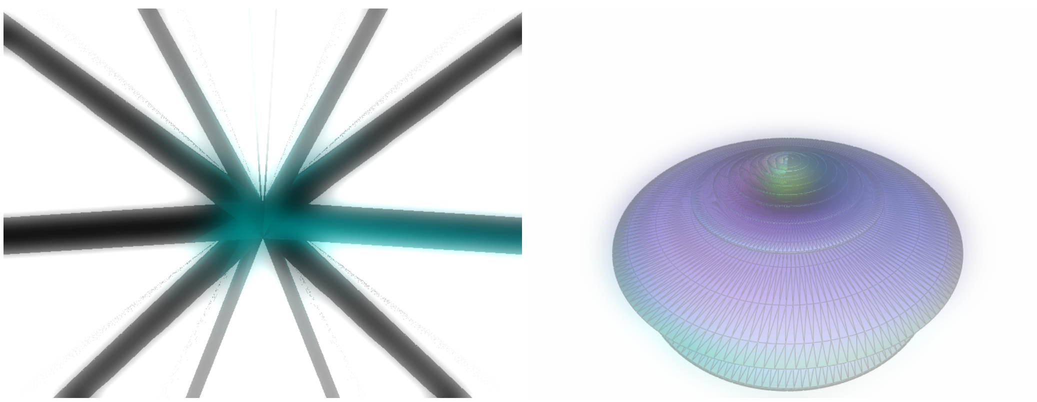

Figure 4: Two images showing Y_{21}^{2}. The spherical harmonic on the left has been calculated incorrectly by not taking proper care of numerics. The image on the right shows the result of a correct calculation.

The order of the expansion required to obtain a given accuracy depends on how well the expanding functions mimic the symmetries and the anisotropy of the solution. While it is possible to perform all calculations without any idea of the shape of the spherical harmonics, a much better understanding can be achieved when the shapes and symmetries of the expanding functions can be grasped. Visualisation of the spherical harmonic basis functions themselves is very valuable to accomplish this task.

4 Application

An equation system for the weighting factors of the spherical harmonic can be obtained by inserting the spherical harmonic expansion into Equation 1, multiplying with conjugate spherical harmonics $\overline{Y}_n^m(\vartheta, \varphi)$, and integrating over the orthogonality interval. Inserting the spherical harmonic expansion into Equation 1 and assuming that the velocity is isotropic results in:

$$\begin{aligned} &\alpha(n,m)\left[v(k)\frac{\partial}{\partial x}f_{n-1}^m + F\left(\frac{\partial}{\partial k}f_{n-1}^m - \frac{n-1}{k}\right)\right]\; Y_n^m \\ +&\beta(n,m)\left[v(k)\frac{\partial}{\partial x}f_{n+1}^m + F\left(\frac{\partial}{\partial k}f_{n+1}^m + \frac{n+2}{k}\right)\right]\; Y_n^m \end{aligned} \tag{7}$$

The integration is simple, because the $Y_n^m(\vartheta, \varphi)$ are orthogonal. In case the velocity $\vec{v}$ is anisotropic, recursion relations can be used to obtain a form that is also quite simple to integrate. The integration of Equation 7 leads directly to the matrix for the coefficients of the spherical harmonics expansion.

For the solution of Boltzmann's equation it is necessary on the one hand side to be able to integrate spherical harmonics in order to obtain the entries for the system matrix. On the other hand side it is necessary, to be able to evaluate the spherical harmonics efficiently to reassemble the solution using the appropriate coefficients.

The locality of integration and evaluation are shown in Figure 5. Evaluation yields a single point on the surface of the spherical harmonic. Integration involves the whole structure of the spherical harmonic.

5 Implementation

Our implementation of spherical harmonics makes use of several modern programming concepts such as template meta-programming to ease specification and ensure high performance. The structure of a spherical harmonic can be exploited at compile time to greatly simplify runtime calculations. This is accomplished by implementing recurrence relations as presented in Equation 5 and Equation 6 using template mechanisms [Abrahams & Gurtovoy, 2004], [Veldhuizen, 2000].

Integration of two terms containing spherical harmonics can be simplified tremendously due the orthonormality of the spherical harmonics. Because of the use of the semantic structural information available at compile time, run time evaluations of the resulting expressions are greatly simplified compared to a full integration which would otherwise have to be performed. The following C++ source code illustrates how to specify two spherical harmonics of different degree and order at compile time

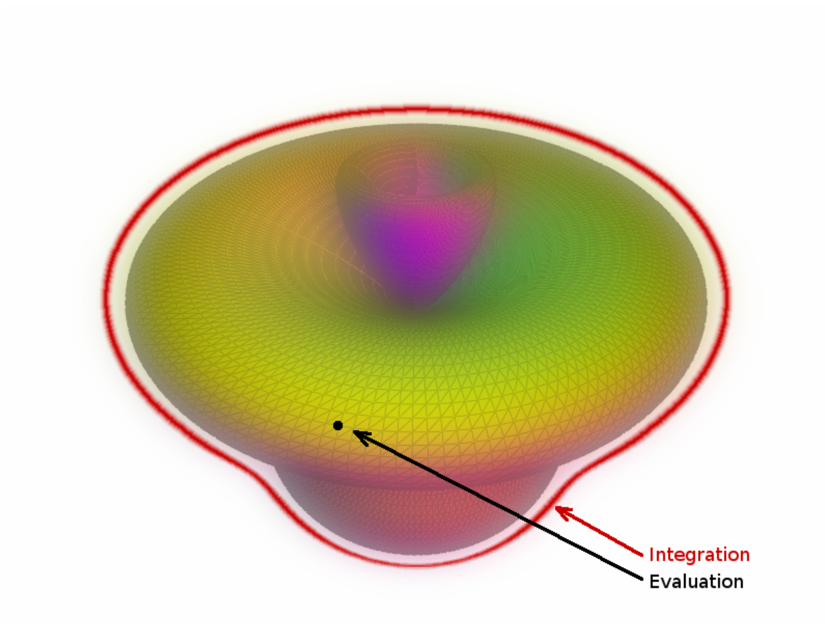

Figure 5: The locality of the operations of evaluation and integration.

```
// definition of structure
// spherical_harmonic<n,m>
spherical_harmonic<2,3> sp_2_3;
spherical_harmonic<3,0> sp_3_0;
```

Specifying degree and order defines the structure of the spherical harmonics and determines their interactions. Integration (indicated by the line surrounding the spherical harmonic in Figure 5) can make use of this structure.

```
// integration at compile time
integrate<sp_2_3, sp_3_0> integral_a;
integrate<sp_2_3, sp_2_3> integral_b;
// integral_a::value = 0
// integral_b::value = 1
```

Evaluation of single values as shown by the dot in Figure 5 can be accomplished in the following manner:

```
// evaluation at run time
std::cout << sp_2_3(0,0) << std::endl;
```

6 Conclusions

We have presented visualisations for spherical harmonics and their recurrence relations. Visualisation provides a quick and efficient way to determine, if recurrence relation based calculations are correct. It thereby provides a valuable tool for developing and debugging applications based on these methods. It also shows how naive implementations result in erroneous results, due to numerical issues.

References

[Abrahams & Gurtovoy, 2004] Abrahams, D. & Gurtovoy, A. (2004). *C++ Template Metaprogramming: Concepts, Tools, and Techniques from Boost and Beyond (C++ in Depth Series)*. Addison-Wesley Professional.

[Abramowitz & Stegun, 1964] Abramowitz, M. & Stegun, I. A. (1964). *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables*. New York: Dover.

[Deuflhard, 1976] Deuflhard, P. (1976). Algorithms for the summation of certain special functions. *Journal Computing*, 17(1), 37–48.

[Jungemann & Meinerzhagen, 2003] Jungemann, C. & Meinerzhagen, B. (2003). *Hierarchical Device Simulation. The Monte Carlo Perspective*. Springer.

[Liotta & Struchtrup, 2000] Liotta, S. & Struchtrup, H. (2000). Moment Equations for Electrons in Semiconductors: Comparison of Spherical Harmonics and Full Moments. *Solid-State Electronics*, 44, 95–103(9).

[S. T. Sutton, 1991] S. T. Sutton, H. N. Pollack, M. J. J. (1991). Spherical Harmonic Representation of the Gravitational Potential of Discrete Spherical Mass Elements. *Geophysical Journal*, 107(1), 77–82.

[Selberherr, 1984] Selberherr, S. (1984). *Analysis and Simulation of Semiconductor Devices*. Wien–New York: Springer.

[Vecchi et al., 1997] Vecchi, M., Mohring, J., & Rudan, M. (1997). An Efficient Solution Scheme for the Spherical-Harmonics Expansion of the Boltzmann Transport Equation. *Computer-Aided Design of Integrated Circuits and Systems, IEEE Transactions on*, 16, 353–361.

[Veldhuizen, 2000] Veldhuizen, T. L. (2000). Five Compilation Models for C++ Templates. In *1st Workshop on C++ Template Programming*. Available from: `http://oonumerics.org/tmpw00/`.