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Modified Valence Force Field Approach for Phonon Dispersion: from Zinc-Blende Bulk to Nanowires

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Adaptive quadrature for sharply spiked integrands

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Abstract A new adaptive quadrature algorithm that places a greater emphasis on cost reduction while still maintaining an acceptable accuracy is demonstrated. The different needs of science and engineering applications are highlighted as the existing algorithms are shown to be inadequate. The performance of the new algorithm is compared with the well known adaptive Simpson, Gauss-Lobatto and Gauss-Kronrod methods. Finally, scenarios where the proposed algorithm outperforms the existing ones are discussed.

Keywords Adaptive quadrature · Simpson · Gauss-Lobatto · Gauss-Kronrod

1 Introduction

With the increasing complexity of problems in science and engineering, more and more computational tasks require the use of massively parallel simulations running for hours to days. A reduction in the computational burden could translate into several hours saved and far lesser CPU time for parallel simulations. Adaptive quadrature is an essential technique to minimize the cost of integrating or simply resolving features in a function. When the cost of evaluating a function is high or if adaptive quadrature has to be used repetitively, the efficiency of the algorithm being employed becomes critical.

In the field of quantum transport it is often required to resolve sharp features in the transmission probability of a structure at different energies [3]. To convey the enormity of the problem, it is comparable to finding and integrating a Lorentzian with a full-width at half maximum (FWHM) of 10^{-10} eV over a 0.5 eV range. Numerical techniques other than adaptive quadrature have been developed [2, 6] that attempt to reduce the cost. Though these techniques are beneficial they do add a significant overhead to the computational task, since some cost is incurred by these techniques as well. In this regard any efficient adaptive quadrature method is desirable since the cost incurred by the adaptive quadrature method itself is in general minimal.

To understand why the existing adaptive quadrature methods are inadequate for such applications, the purpose and the intent behind these methods must be highlighted. Problems in computing and numerical analysis require high precision, possibly 7–8 digits. In engineering and scientific applications it is enough to have a lower precision since there are several input parameters to the simulation, that are not known to such high accuracies anyway. In device engineering a general procedure is to guide a design by many simulations that provide design trends. Absolute numbers with perfect accuracy are not required but rapid computational turn around is needed. To meet the requirements of such applications, accuracy must be traded for a reduction in cost. Further, some implementations of adaptive quadrature methods throw away function evaluations from previous iterations in the quest for accuracy, a scenario that is not desirable, given that it can be very costly to evaluate a function at every single point.

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2 Methodology: 5 point adaptive scheme

Figure 1 illustrates the procedure for the 5 point adaptive scheme for a Lorentzian placed asymmetrically in the range of integration. The Lorentzian is to be resolved and integrated as accurately as possible. After sampling the function on a widely spaced homogeneous grid, nodes are added in successive iterations. The addition of nodes in a given region, like other adaptive schemes is based on two estimates of the integral, one of which is more accurate than the other. In this case the estimates are I_5 and I_3 over a region which is typically only a small part of the entire range to be integrated over. I_5 and I_3 refer to the number of points used in evaluating the integral over a small subsection of the total range. These integrals can be performed using the mid-point rule or by fitting a quadratic function to a set of 3 points. The scheme is not very sensitive to the quadrature rule used to find I_5 and I_3 since the addition of nodes is based on the relative error of the two and not the actual values. The scheme is implemented in the following manner,

- *Step 1*: The function to be integrated is sampled on a widely spaced homogeneous grid.
- *Step 2*: I_5 using 5 points and I_3 using 3 points are computed over any set of 5 successive nodes. Typically the 2nd and the 4th points in a given set of 5 points are neglected for the purpose of computing I_3.
- *Step 3*: If the following condition,

$$|I_5 - I_3|/I_3 > \varepsilon \quad (\textit{convergence criterion}) \tag{1}$$

  is found to be true, then 4 new nodes are added in a region spanned by the original 5 successive nodes such that they bisect the 4 already existing intervals symmetrically. Otherwise no new nodes are added.
- *Step 4*: Steps 2–3 are repeated with all the nodes, till the convergence criterion is met over any set of 5 successive nodes.

The integration is done using the composite Simpson's rule by breaking the range into regions that have the same difference in successive abscissas.

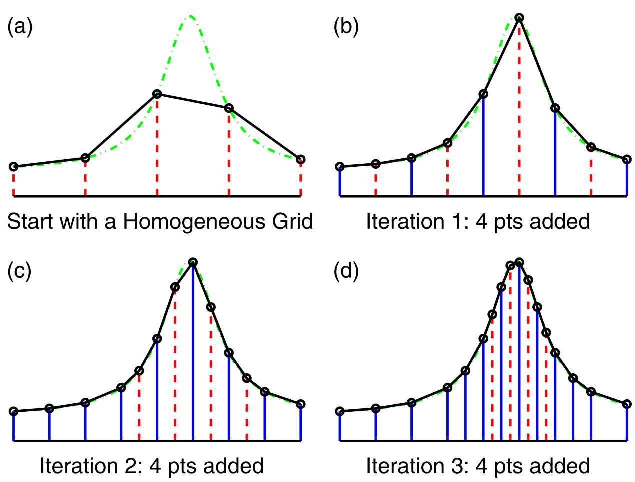


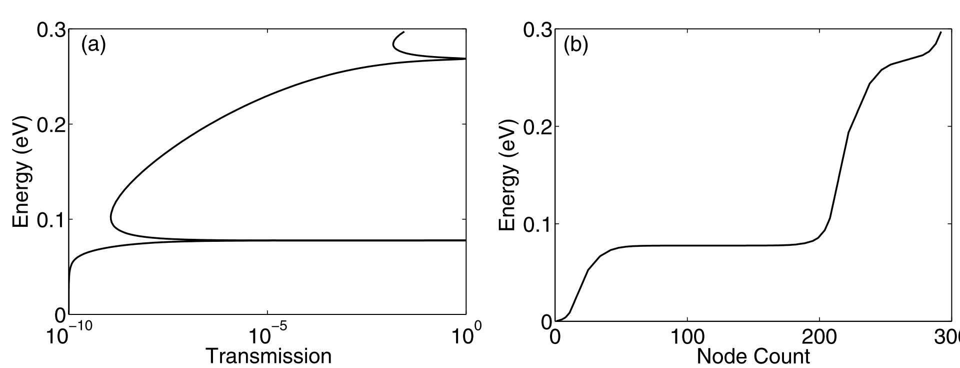
Fig. 1 Successive iterations of the adaptive refinement algorithm in the 5 point scheme are illustrated. *Vertical solid lines* denote the nodes at the beginning of each iteration. *Vertical dotted lines* denote nodes added at each iteration

3 Results and discussion: accuracy vs cost

In Fig. 2(a) the 5 point adaptive scheme is used to resolve features in the transmission through a Resonant Tunneling diode [5] at different energies. Figure 2(b) shows the distribution of nodes in energy which is indicative of the cost of resolving each features in the transmission. As is expected flatter portions of Fig. 2(b) correspond to sharper features in Fig. 2(a) since more nodes were required to resolve them. The 5 point adaptive grid scheme is running with $\varepsilon = 0.1$ in (1). A smaller ε would resolve the features even more accurately though it would increase the node count as well.

The performance of the 5 point adaptive scheme is now compared with other algorithms keeping in mind that the ideal algorithm would be one whose accuracy scales well with an increasing node count, that is, an algorithms that can give low accuracies at a low node count and high accuracies at a high node count. The 5 point adaptive scheme

Fig. 2 (**a**) Transmission as a function of energy for a Resonant tunneling device with thick barriers giving rise to very sharp features in transmission. Similar devices have been modeled in [5]. (**b**) The corresponding distribution of nodes generated using the 5 point adaptive grid scheme running with $\varepsilon = 0.1$



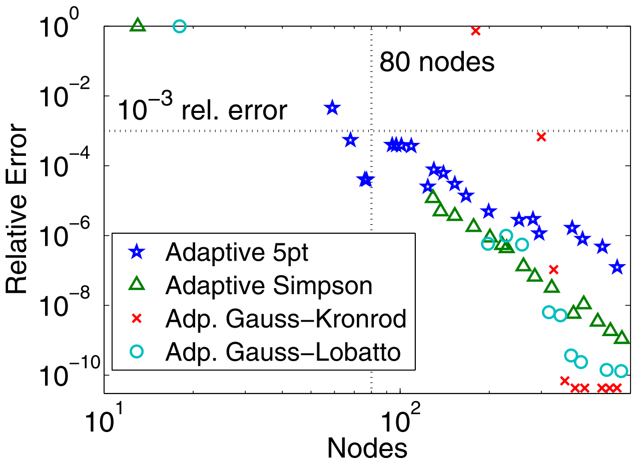


Fig. 3 The relative error as a function of node count for a normalized Lorentzian with FWHM = 10^{-3}. The different data points for a given algorithm were obtained by varying the convergence criterion (ε) for the 5 point scheme and the error tolerance for the remaining algorithms

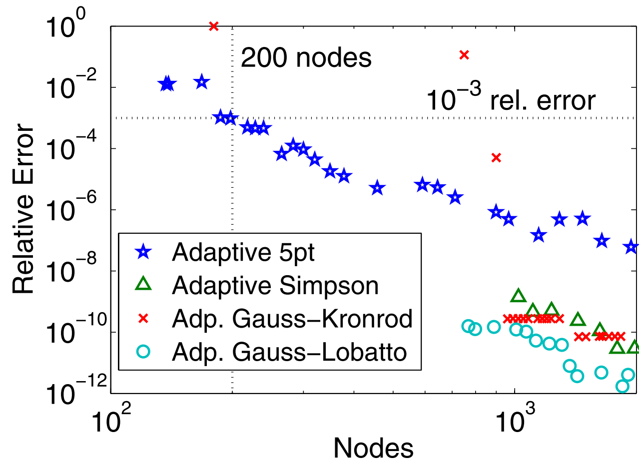


Fig. 4 The relative error as a function of node count for a normalized Lorentzian with FWHM = 10^{-7}. The different data points for a given algorithm were obtained by varying the convergence criterion (ε) for the 5 point scheme and the error tolerance for the remaining algorithms

is implemented in MATLAB and is compared with the inbuilt functions quad, quadl and quadgk which correspond to the Adaptive Simpson [8], Gauss-Lobatto [1] and Gauss-Kronrod [7] methods. The performance and implementation of these three algorithms has been discussed in [4]. A normalized Lorentzian is placed asymmetrically and integrated in the range [0, 1]. The relative error for a Lorentzian with a given FWHM is found with the corresponding node count by varying the convergence criterion for the 5 point adaptive scheme and the error tolerance in the case of the remaining adaptive quadrature methods.

Figure 3 shows how the 5 point adaptive scheme compares with the other algorithms for the case when the Lorentzian is not very sharp (FWHM = 10^{-3}). The performance of the 5 point adaptive scheme is similar to that of the adaptive Simpson's method with relative errors close to 10^{-5} being achieved with 100 nodes. A relative error close to 1 indicates that the algorithm could not resolve the feature at all, which is the case for the Simpson's and the Gauss-Lobatto methods around 15 nodes and for Gauss-Kronrod around 200 nodes. One point of distinction could be that the 5 point adaptive scheme does find the Lorentzian with even fewer nodes although with a lower accuracy. It can be argued that the three existing algorithms are missing data points in the low accuracy region (relative error between 10^{-3} and 10^{-5}) as they do not converge, but since the difference in cost between them and the 5 point adaptive scheme is not large enough the discrepancy may not be serious. However, a small node count can reduce the cost of subsequent calculations in terms of memory footprint as well as overall compute time. Accuracies of 10^{-3} may often be acceptable resulting in node reduction by a factor of 2 or more.

In Fig. 4, showing the performance for a Lorentzian of FWHM = 10^{-7}, the contrast between the 5 point adaptive scheme and the remaining methods is more evident. The 5 point adaptive scheme shows the ability to find the Lorentzian with a low accuracy (relative error between 10^{-3} and 10^{-6}) and a low node count. The remaining algorithms take larger node counts to find the Lorentzian, although to a higher accuracy. The adaptive Simpson's, Gauss-Lobatto and Gauss-Kronrod do not have any data points for high relative errors since they do not converge with low node counts.

One advantage that the 5 point adaptive scheme has that at the end of each iteration it is possible to have an estimate of the integral of the function, something that is not possible in the remaining methods. It is also possible to build safeguards that avoid getting caught in noisy integrands or that treat a certain part of the range differently than others. It has been verified that adding 4 nodes in *Step 2* of the algorithm compared to adding only one is more efficient unless there is an analysis of the integrand over the 5 points in question.

4 Conclusion

In this paper the 5 point adaptive quadrature scheme was demonstrated, that placed a greater emphasis on cost reduction, while still maintaining acceptable accuracies. Such a technique was shown to be beneficial for scientific and engineering applications. Existing techniques were shown to be inadequate despite their higher accuracies because of the prohibitive costs involved. A performance comparison was used to demonstrate the suitability of the 5 point adaptive scheme over the existing algorithms in applications where low accuracies suffice and evaluating functions at each node is expensive.

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