

Implementation of WaveBlocksND's Quadrature and Inner Products in C++

Term Paper

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Seminar for Applied Mathematics
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Autumn Semester 2015

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1 Introduction

This work is part of an effort to port the WaveBlocksND project [1] from Python to C++, using the Eigen template library for linear algebra. WaveBlocksND provides a framework for quantum-physical simulations, in particular to calculate the time propagation of wavepackets in different potentials. The necessary theory for the calculations and algorithms is given in [2].

In this work, we focus on implementing quadrature and inner product calculations for the wavepackets, which is a prerequisite for the time-propagation algorithms.

This report will show formulas and rules used for numerical quadrature, the code structure for building inner products, as well as describing the additional complexity arising from multi-component wavepackets.

Because one of the main reasons of porting the code to C++ was to increase performance, run-time measurements will also show the achieved improvements.

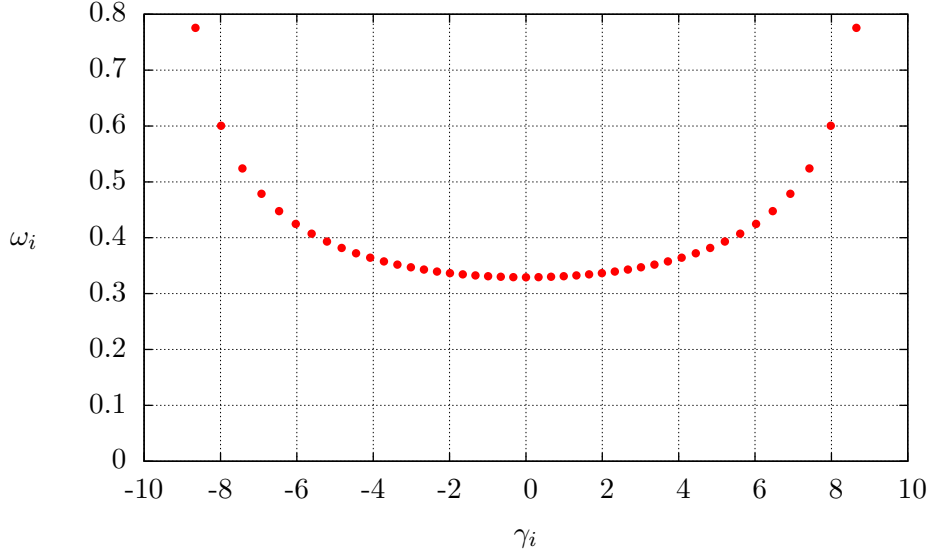


Figure 1: 45-point Gauss-Hermite nodes and weights

2 Quadrature

The central building block for evaluating inner products is the calculation of integrals between wavepackets. This is done numerically with a quadrature rule, of which there are many different kinds.

2.1 Gauss-Hermite Quadrature

The basic integration algorithm used in this project is the one-dimensional Gauss-Hermite quadrature. Like related rules, this method works by evaluating the integrand function at a defined set of nodes γ_i , the values of which are summed up with specific weights ω_i :

$$\int_{-\infty}^{\infty} g(x) dx \approx \sum_{i=1}^n f(\gamma_i) \omega_i \quad (1)$$

In its basic form, the Gauss-Hermite rule works on special integrals of the following form:

$$\int_{-\infty}^{\infty} e^{-x^2} f(x) dx \quad (2)$$

However, as we require the quadrature to work on general functions, transformations are done to the usual weights and nodes which is described in [2]. The result is a rule in the form of (1). Figure 1 shows an example of the node distribution of a Gauss-Hermite rule.

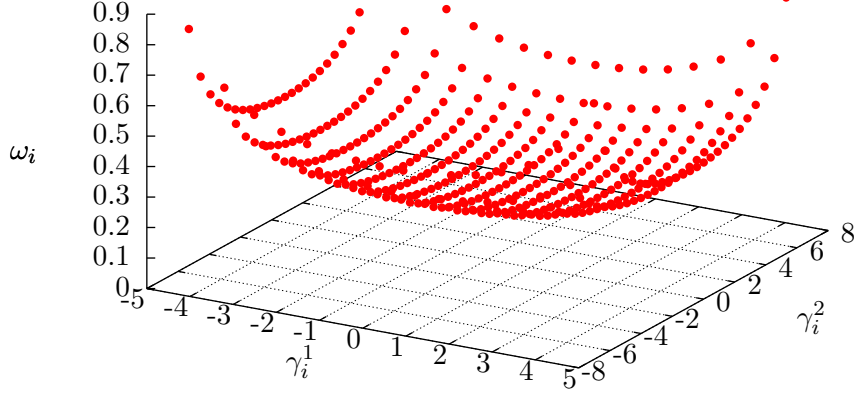


Figure 2: Tensor-product built from 16- and 25-point Gauss-Hermite rules

In the implementation of this rule, an auxiliary Python script was made to automatically generate C++-code with hardcoded tables of nodes and weights for different orders.

The source code can be found under `scripts/create_tables.py` and `waveblocks/gauss_hermite_qr.hpp`.

2.2 Tensor-Product Quadrature

The wavepackets that are processed by WaveBlocks are generally multi-dimensional. To handle this, tensor products of D one-dimensional quadrature rules can be built up.

Denoting the i -th node-weight-pair of the d -th scalar quadrature rule (γ_i^d, ω_i^d) , the resulting pair at the multi-index $j = (j_1, \dots, j_d)$ for the resulting tensor quadrature rule is:

$$(\gamma_j, \omega_j) = \left(\begin{pmatrix} \gamma_{j_1}^1 \\ \vdots \\ \gamma_{j_d}^d \end{pmatrix}, \prod_{d=1}^D \omega_{j_d}^d \right) \quad (3)$$

A two-dimensional quadrature rule is shown in figure 2.

The implementation resides in `waveblocks/tensor_product_qr.hpp`.

2.3 Result Caching

As the node positions and weight values are tabulated with an external script for Gauss-Hermite Quadrature (2.1), the code for looking up and returning those numbers is simple and fast.

However, in the case of Tensor-Product Quadrature (2.2), some calculations must be performed to yield these values. We wish to avoid recalculating node and weight vectors when the same quadrature rule is used many times, as is done in the case of wavepacket propagation over many iterations.

For this reason, the results are only calculated once for a given Tensor-Product rule, stored and re-used automatically on subsequent queries. The quadrature functions have been implemented as `static` methods, with the rule parameters given as template parameters. Therefore, the caching is done in `static` fields.

This has the advantage that the rule only has to be calculated once in the entire run of the program as long as the quadrature rule is the same, even if it is invoked in different scopes, without having to pass down an object explicitly that holds a state. On the other hand, no clean-up can be done automatically, so a method must be called manually to free the memory used by the cache.

3 Inner Products

In order to calculate wavepacket norms, various energies and other observables, it is necessary to evaluate the bracket

$$M = \langle \Psi | F | \Psi' \rangle, \quad (4)$$

where Ψ and Ψ' are wavepackets and F specifies the operator.

For the mathematical derivation of the bracket evaluation algorithms, again refer to [2].

3.1 Scalar Inner Products

In the case of scalar wavepackets Φ and Φ' the bracket is written as

$$M = \langle \Phi | f | \Phi' \rangle. \quad (5)$$

The operator f is given as a function parameter of the form

$$f(x, q) : \mathbb{C}^{D \times R} \times \mathbb{R}^D \rightarrow \mathbb{C}^R \quad (6)$$

mapping D -dimensional nodal points x and position q to the operator's values.

Here, R is the order of the quadrature. Instead of calling the operator function for the different nodes separately, all points are given to the function at once to make efficient vector calculations in its definition possible.

The inner product calculation implementation provides two different methods, `build_matrix` and `quadrature`. The first returns a $|\mathcal{R}| \times |\mathcal{R}'|$ -sized matrix, one entry for each pair of basis functions of Φ and Φ' , where \mathcal{R} is the basis shape size. `quadrature` reduces the matrix to a scalar by multiplying in the coefficient vectors c and c' of Φ and Φ' , returning $c^H M c$.

The “inhomogeneous” evaluation code for different wavepackets Φ and Φ' can be found in `waveblocks/inhomogeneous_inner_product.hpp`. If the two wavepackets are the equivalent, $\Phi = \Phi'$, a more efficient “homogeneous” algorithm can be used which is implemented in `waveblocks/homogeneous_inner_product.hpp`

3.2 Multi-component Inner Products

In the more general case the wavepackets can have multiple components:

$$\Psi = \begin{pmatrix} \Phi_1 \\ \vdots \\ \Phi_N \end{pmatrix} \quad (7)$$

$$M = \langle \Psi | F | \Psi' \rangle = \left\langle \begin{pmatrix} \Phi_1 \\ \vdots \\ \Phi_N \end{pmatrix} \middle| \begin{pmatrix} \ddots & \vdots & \ddots \\ \cdots & f_{i,j} & \cdots \\ \ddots & \vdots & \ddots \end{pmatrix} \middle| \begin{pmatrix} \Phi'_1 \\ \vdots \\ \Phi'_N \end{pmatrix} \right\rangle \quad (8)$$

The calculation of these brackets builds on top of the inhomogeneous scalar evaluation code, calling it for every pair of wavepackets (Φ_i, Φ'_j) and corresponding function $f_{i,j}$.

The source code for this algorithm is found in `waveblocks/vector_inner_product.hpp`.

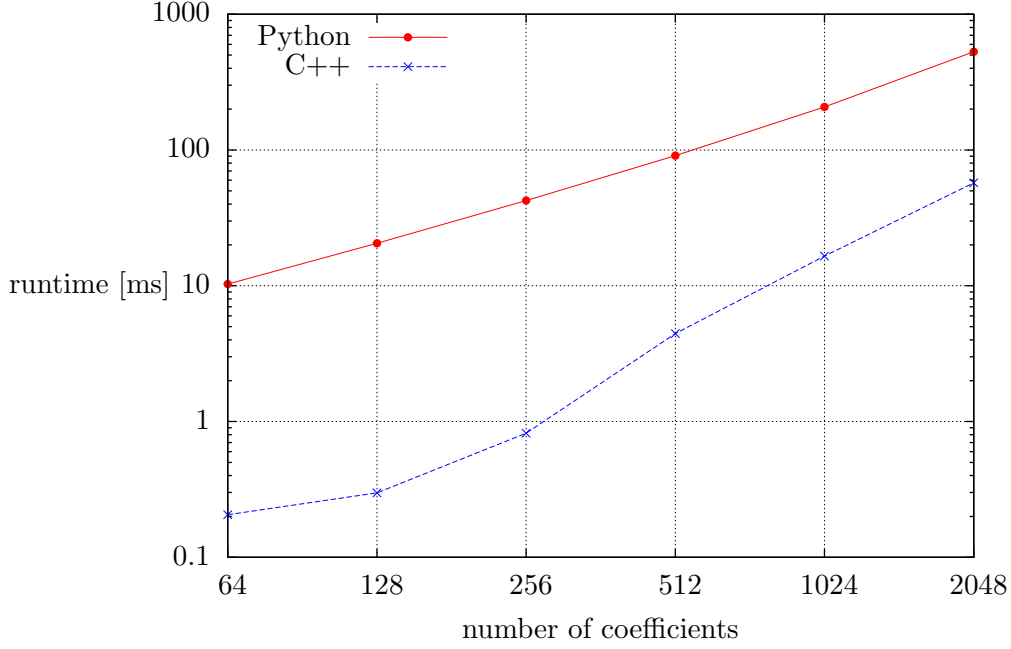


Figure 3: Run-times for 1-D homogeneous quadrature of order 8

4 Results

Since one of the main reasons of porting WaveBlocks from Python to C++ was to increase the performance, run-times for various use-cases must be measured and compared to evaluate the improvements. All tests were done using homogeneous **quadrature** with an identity operator. The computer used for benchmarking had a quad-core Intel i5-2500 processor.

Different parameters were varied to compare the scaling behaviors of the two implementations. Because the algorithms used in both cases were essentially the same, the run-times grow with the parameters roughly at the same rate, however there is a big difference in the absolute durations.

In the simplest test, the number of coefficients of a wavepacket was changed for a one-dimensional, single-component quadrature. The results in figure 3 show a huge improvement in the C++ version with a speed-up of factor 50 for smaller problems, converging to a factor of about 9 for larger ones.

The next test inspects the impact of dimensionality. As can be seen from figure 4, higher-dimensional problems can have a 20-fold speedup.

Finally, figure 5 shows the behavior for varying sizes of multi-component wavepackets. It is apparent that the speed-up is very consistently a factor of approximately 75.

In conclusion, there is no doubt that replacing the quadrature code with a

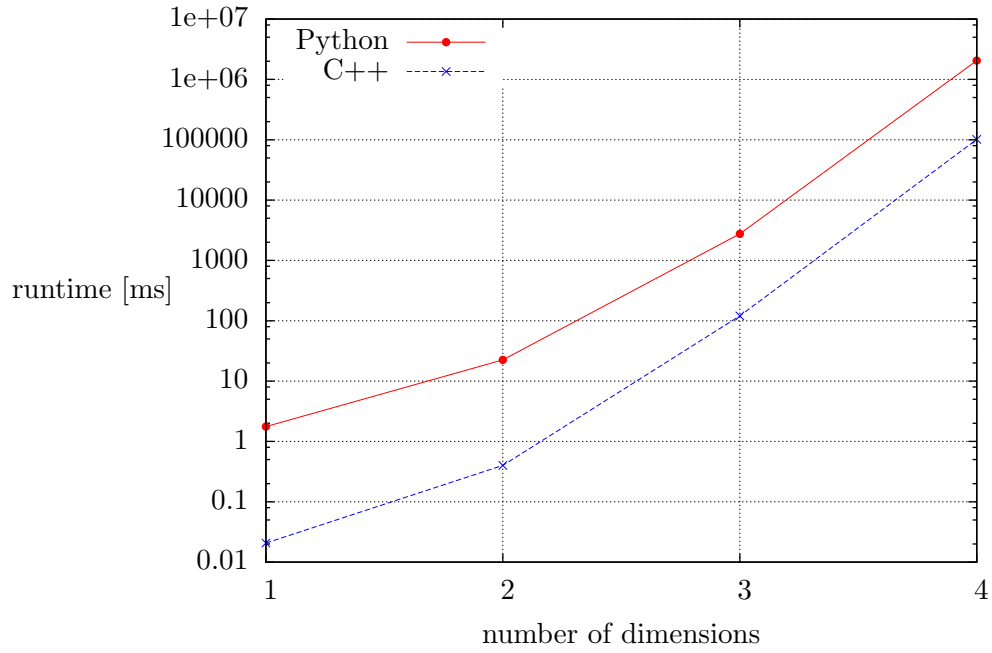


Figure 4: Run-times for multi-dimensional homogeneous quadrature of order 8 with 10 coefficients per dimension

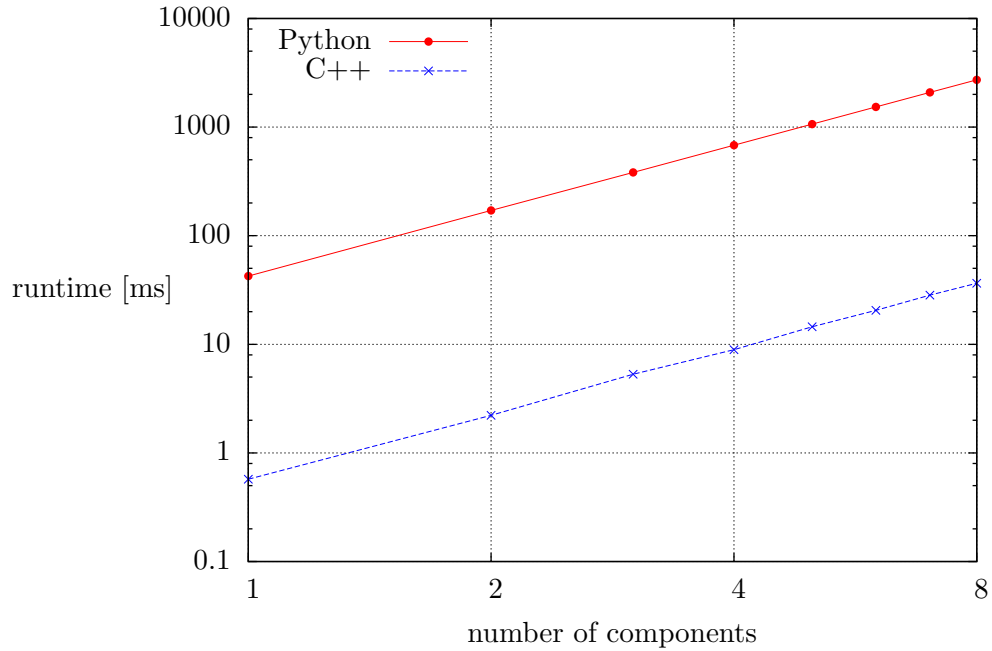


Figure 5: Run-times for multi-component 2-D homogeneous quadrature of order 8 with 10 coefficients per dimension

C++ version using the highly-optimized Eigen library brings great improvements. However, it must be noted that these are isolated measurements and the speed-up is only significant if a large part of the execution time is spent in the quadrature. This means that for smaller problems, even though the measured speed-ups are huge, there are probably bottlenecks in other parts of the code, which diminishes the total improvement.

Additionally, a noticeable trade-off is a much longer compilation time, which can hinder doing many test with small problems. If one wants to tweak some hard-coded parameter, they have to wait for the lengthy build to finish. Disabling optimization flags can help, but in this aspect the Python version has a clear advantage.

Beyond the efficiency improvements, using a statically typed language can also aid with catching more bugs at compilation time, theoretically resulting in more correct programs. Unfortunately, compiler error messages can get very complicated and confusing when using template-heavy C++ code like in this work, so some experience is needed to find and fix bugs.

References

- [1] R. Bourquin and V. Gradinaru. WaveBlocks: Reusable building blocks for simulations with semiclassical wavepackets. <https://github.com/raoulbq/WaveBlocksND>, 2010 – 2015.
- [2] Raoul Bourquin. Wavepacket propagation in d-dimensional non-adiabatic crossings. 2012. http://www.sam.math.ethz.ch/~raoulb/research/master_thesis/tex/main.pdf.