

SIMPLICIAL INTERPOLATIONS FOR PATH INTEGRALS [☆]

Kevin CAHILL, Sudhakar PRASAD ¹ and Randolph REEDER

Department of Physics and Astronomy, University of New Mexico, Albuquerque, NM 87131, USA

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We suggest approximating path integrals by tilting spacetime with simplexes and by interpolating the fields throughout each simplex from their values on the vertices. This simplicial interpolative method uses unaltered the action of the continuum theory. We present several tests of the method. Both in one dimension, for the harmonic oscillator, and in two dimensions, for the free massive scalar field, it was about twice as accurate as ordinary lattice theory. We also computed Wilson loops in two dimensions for free quantum electrodynamics. By using huge lattices, we achieved an accuracy of better than 0.5% and observed a remarkable restoration of translational and rotational invariance.

Because lattice gauge theory has been so successful, it is worthwhile trying to improve it. We suggest defining the fields throughout spacetime so as to be able to use the action of the continuum theory. We also suggest replacing cubes by simplexes and linearly interpolating the fields throughout each simplex from their values at the vertices. We present several tests of this simplicial interpolative method for field theories in one and two dimensions. These tests indicate that it is typically twice as accurate as ordinary lattice methods.

The simplicial interpolative method is similar in spirit to one we proposed in earlier works [1] ^{†1}, [2]. In that method one approximates path integrals by expanding the fields in terms of a complete set of functions, by truncating the expansion, and by using Monte Carlo techniques to evaluate the resulting finite-dimensional integrals. The simplicial interpolative method is also similar to the finite-element method of Bender, Guralnik and Sharp [3], and differs from it by its use of simplexes instead of cubes.

A simplex σ in d -dimensional space has $d + 1$ vertices v_i and consists of points x that are linear combinations of its vertices with nonnegative coefficients p_i which sum to one,

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¹ Institute for Modern Optics.

^{†1} In this reference "standard deviation" means that of a single measurement, not of the average.

$$x = \sum_{i=0}^d \rho_i v_i . \tag{1}$$

One may fill euclidean space of any dimension d with identical simplexes σ^α . The best way may be to use the dual root lattice A_d^* , which is probably the optimal covering lattice [4,5], and to divide its unit cell into simplexes.

Throughout each simplex, we define a field $\phi(x)$ in terms of its values at the vertices $c_i = \phi(v_i)$ as the linear interpolation

$$\phi(x) \equiv \phi(x, c) = \phi(\rho_i v_i) = \rho_i \phi(v_i) = \rho_i c_i , \tag{2}$$

where sums over i from 0 to d are understood. In this way we interpolate each field throughout spacetime in terms of the set of parameters $c \equiv \{c_i^\alpha\}$. By substituting such an interpolation for each field into the action functional $S[\phi]$ of the continuum theory and by integrating over spacetime, one may express the action as a function $S(c)$ of the parameters c . Because the interpolation is linear in the parameters, in the limit of an infinitely fine lattice of simplexes the jacobian $\det[\partial\phi(x, c)/\partial c_i^\alpha]$ cancels in ratios of path integrals. Thus one converts a path integral into an infinitely multiple integral over the parameters c . For a finite volume of spacetime and finite simplexes, the integrals over the parameters are of finite dimension. For example, the Wilson-loop functional for an abelian

gauge field $A_\mu(x)$ takes the form:

$$\langle 0|T \exp\left(ie \oint A_\mu(x) dx^\mu\right)|0\rangle \approx \left[\prod_{n=1}^N \int dc_n \exp\left(-S(c) + ie \oint A_\mu(x, c) dx^\mu\right) \right] \times \left(\prod_{n=1}^N \int dc_n \exp[-S(c)] \right)^{-1}. \quad (3)$$

One may use Metropolis' method of importance sampling [6] to compute such ratios of multi-dimensional integrals. By allotting sufficient computer time to the Monte Carlo implementation of Metropolis' method, one typically can approximate these integrals to arbitrary accuracy.

In this paper we present several applications of the simplicial interpolative method to theories in one and two dimensions. In each case, we tested the method by comparing its accuracy with that of the standard method for an equivalent lattice. We used free theories in order to be able to do the multiple integrals exactly by matrix methods rather than approximately by Monte Carlo techniques. We thus isolated the intrinsic errors of both methods.

In one dimension we computed the expected value of the square of the position operator, $\langle x^2 \rangle$, in the ground state of the harmonic oscillator. The simplicial interpolative method was more than twice as accurate as the standard one. For example, for a lattice of 11 points, it gave an accuracy of 4% as opposed to 11% for the standard method.

We applied our method to the theory of a free massive scalar field in two dimensions, for which we calculated the analogue of the Wilson loop (3). The simplicial interpolative method was typically about twice as accurate as the standard one. For example, for a 20 by 20 loop (in units of inverse mass) in a 100 by 100 lattice, our method erred by 5%; the standard one by 12%.

We also calculated Wilson loops in free two-dimensional quantum electrodynamics. Because the action of this theory has only derivatives of the fields, the two methods give identical results for the simplicial lattice obtained by slicing the usual lattice of squares along parallel diagonals. By using huge lattices, we found evidence suggesting that both methods converge

to the exact results of the continuum theory. For 200 by 200 loops (in units of inverse charge) in a 100 000 by 100 000 lattice, the errors were less than 0.5%. We observed an impressive restoration of translational and rotational symmetry. The value of a Wilson loop typically changed by only 2 parts in 10^{11} when the loop was translated in time from the center by 40 000 units and by less than 16 parts in 10^5 when it was rotated by 45° .

We derived our results for the harmonic oscillator by parameterizing the coordinate $x(t)$ in each interval $[t_i, t_{i+1}]$ of duration a as $x(t) = c_i + (t - t_i)(c_{i+1} - c_i)/a$, which is the rule (2) for $d = 1$. By substituting this parameterization into the lagrangian, $L = (\dot{x}^2 + x^2)/2$, and integrating over time, one may express the euclidean action as a quadratic form, $S = c_i M_{ij} c_j$. The expected value of $x^2(0)$ is then half the central element of the inverse of M . A similar rule applies to the standard lattice representation of $x(t)$. We used Matlab [7] to compute the required inverses for both methods with periodic boundary conditions on $x(t)$. The exact result is $\langle x^2(0) \rangle = 0.5$. For a lattice of duration 10 and for intervals of duration $a = 1.0, 0.5$, and 0.25 , the results for the simplicial interpolative method were 0.4804, 0.4949, and 0.4987; while those for the standard method were: 0.4473, 0.4851, and 0.4962. The simplicial interpolative results are from 2.7 to 3 times more accurate.

We compared the two methods in two dimensions by applying them to the theory of a free scalar field of mass m described by the Lagrange density, $L = [(\partial_\mu \phi)^2 + m^2]/2$. The quantity we evaluated is the analogue of the Wilson loop (3) that results from replacing A_μ by ϕt_μ , where t_μ is a unit vector tangent to the loop. For a square loop of side L , this quantity is

$$\langle 0|T \exp\left(ie \oint \phi(x) t_\mu dx^\mu\right)|0\rangle = \exp\left(- (2e^2 L^2 / \pi) \int_0^1 du (1-u) f(u, mL)\right), \quad (4)$$

where the function $f(u, mL)$ is defined in terms of Macdonald's function as $f(u, v) = K_0(vu) - K_0(v(u^2 + 1)^{1/2})$.

We used the simplicial lattice obtained by slicing the usual lattice of squares along parallel diagonals. We

interpolated the field ϕ in a triangle lying below a diagonal as $\phi(x, t) = c_{nm} + (c_{n+1m} - c_{nm})(t - an)/a + (c_{nm+1} - c_{nm})(x - an)/a$, with a similar rule for upper triangles. By using this parameterization and integrating over space and time, we expressed the action and the line integral of ϕ as a quadratic polynomial in the c 's. We then completed the squares by shifting the matrix c of integration variables. The shift matrix was defined by a linear system, which we solved perturbatively by identifying two small parameters of modulus less than 0.25. Thus we obtained the scalar loop (4) in terms of the shift matrix. We similarly evaluated the scalar loop for the standard square lattice. For a square loop of side 10, in units of inverse mass, the exact value of the natural logarithm of the scalar loop functional (4) divided by $-e^2 L^2$ is 0.093631. For a 50 by 50 lattice and for the lattice spacings $a = 1.0, 0.5$, and 0.25 , the results for the simplicial interpolative method were 0.087242, 0.091651, and 0.092821; while those for the standard method were 0.081301, 0.089844, and 0.092344. For a square loop of side 20 the exact value is 0.048409. For a 100 by 100 lattice and for the lattice spacings $a = 1.0, 0.5$, and 0.25 , the results for the simplicial interpolative method were 0.045833, 0.047609, and 0.047939; while those for the standard method were 0.042690, 0.046667, and 0.047689. The simplicial interpolative results are from 1.5 to 2.2 times more accurate.

We also applied the method to the calculation of Wilson loops in free two-dimensional quantum electrodynamics. To reduce the number of fields and redundant field configurations, we worked in the temporal gauge, $A_0(x, t) = 0$. The temporal-gauge action $S[A]$

$$S[A] = \frac{1}{2} \int \dot{A}^2 dx dt \quad (5)$$

in which \dot{A} is the time derivative of the remaining field variable, $A \equiv A_1$. The exact value of the Wilson-loop functional (3) for a loop of area Σ is $\exp(-e^2 \Sigma/2)$.

We used the same triangular lattice and the same parameterization for the field $A(x, t)$ as for the scalar field. In a triangle lying below a diagonal, the time derivative \dot{A} , which is the only variable in the action (5), takes the form $\dot{A}(x, t) = (c_{n+1m} - c_{nm})/a$. In terms of the matrix c and its transpose c^t , the action and the Wilson-loop integral reduce to the sum of two simple traces,

$$\begin{aligned} -S(c) + ie \oint A_\mu(x, c) dx^\mu \\ = -\text{Tr}(c^t M c) + iea \text{Tr}(c^t j) \end{aligned} \quad (6)$$

in which the matrix M is a tridiagonal with +1's along its main diagonal and -0.5 's along its upper and lower diagonals. The matrix j is nonzero only along the spatial segments of the loop. For an upright rectangular loop, j has +1's along the top and bottom of the loop and ± 0.5 's at the corners, where the sign is that of dx . We substituted the preceding expression (6) into the formula (3) for the Wilson loop, completed the squares and found the Wilson loop to be $\exp[-e^2 a^2 \times \text{Tr}(j^t M^{-1} j)/4]$. To compute the trace, we used the Linpack [8] programs `dgafa` and `dgbsl`, which are designed for large banded matrices. We used `dgafa` to factor the tridiagonal double-precision matrix M , and then used `dgbsl` to solve the system $Mb = jj^t$ for b . For square lattices of length 1000, 2000, 5000, 10000, and 100 000 (in units of inverse charge), the best square centered loops were of length 22, 32, 50, 70, and 220. For them the errors were 4.42%, 3.14%, 1.99%, 1.41%, and 0.45%, respectively. The length of the best loop is approximately 0.7 times the square root of the length of the lattice; its percent error is approximately 141 divided by the same square root. There appear to be two competing effects: the loop should be big compared to the lattice spacing a and small compared to the lattice.

We noticed a striking degree of translational and rotational invariance. For a 200 by 200 loop, the exact value of the logarithm of the Wilson loop divided by $-e^2$ is 20 000. For the 100 000 by 100 000 lattice our result for the centered loop was 19910.100398764; our results for the same loop translated in time by 10 000 and by 40 000 were 19 910.100398737 and 19 910.100398323. The larger change amounts to 2 parts in 10^{11} . Because the action (5) does not couple different points in space, our results possess a perfect but trivial invariance under spatial translations. We checked invariance under rotations by computing Wilson loops rotated by 45° , approximating such loops by loops that follow the links of the lattice. For a 10 000 by 10 000 lattice and square loops of diagonal 92, the difference between the upright and rotated loops was less than 16 parts in 10^5 , most of which was probably due to our adherence to the links.

It may be worth noting that in all these examples the computed vacuum expected value of an operator was smaller than the exact value when the operator was positive and larger when it was unitary.

We applied our method to free fermions in two dimensions, using both the right-triangular lattice and the lattice A_2^* of equilateral triangles. We also applied the finite-element method [3] to this theory. We found various forms of fermion doubling in all cases. However, the operator finite-element method [9] does appear to be free of fermion doubling.

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References

- [1] K. Cahill and R. Reeder, Phys. Lett. 136B (1984) 77.
- [2] K. Cahill, S. Prasad and R. Reeder, Phys. Lett. 143B (1984) 213.
- [3] C.M. Bender, G.S. Guralnik and D.S. Sharp, Nucl. Phys. B207 (1982) 54.
- [4] J.H. Conway and N.J.A. Sloane, IEEE Trans. Inform. Theory, IT-28 (1982) 211.
- [5] N.J.A. Sloane, Sci. Am. 250 (1984) 116.
- [6] N. Metropolis, A.W. Rosenbluth, M.N. Rosenbluth, A.H. Teller and E. Teller, J. Chem. Phys. 21 (1953) 1087.
- [7] C. Moler, Matlab user's guide, Technical Report CS81-1, Department of Computer Science, Univ. of New Mexico (1982).
- [8] J.J. Dongarra, J.R. Bunch, C.B. Moler and G.W. Stewart, Linpack user's guide (Society for Industrial and Applied Mathematics, Philadelphia, 1979).
- [9] C.M. Bender, K.A. Milton and D.H. Sharp, Phys. Rev. Lett. 51 (1983) 1815.