Mathematics as an engine for computational sciences

Новая математика – движущая сила вычислительных наук

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The situation with the success of quantum computers is analyzed and a conclusion is made about the need to develop quantum computing regardless of the development of the corresponding computing base. Particularly highlighted is the role of new mathematics associated with functional integrals as a means for quantum computing. The problems of the Feynman formulation are described and it is shown how to construct an approach that allows the generation of quantum algorithms. The prospects for this approach for creating a qualitative theory of partial differential equations are indicated.

Анализируется ситуация с успехами квантовых компьютеров и делается вывод о необходимости развития квантовых вычислений безотносительно к развитию соответствующей вычислительной базы. Особо выделяется роль новой математики, связанной с функциональными интегралами, как средства для квантовых вычислений. Описаны проблемы фейнмановской формулировки и показано, как построить подход, позволяющий генерировать квантовые алгоритмы. Указаны перспективы такого подхода для создания качественной теории дифференциальных уравнений в частных производных.

INTRODUCTION

The problems of classical computing architectures are well known [1] and active attempts to find solutions to them both using graphics accelerators and switching to optical communicators are not very impressive yet. Great hopes were associated with the creation of quantum computers and the formulation of quantum supremacy, especially in the elegant formulation of R. Feynman “Nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy.” [2]. However, despite significant advances in the development and creation of quantum systems [3], the situation is far from successful and new computers are more likely to operate as analog systems. Moreover, apparently, there is a fundamental limitation associated with the Church–Turing thesis “Any computational problem that can be solved by a classical computer can also be solved by a quantum computer. Conversely, any problem that can be solved by a quantum computer can also be solved by a classical computer, at least in principle given enough time” [4]. The problems are clearly related to the need to carry out measurements after each stage of calculations, which turns a qubit into a bit and giant accelerations are possible only if the quantum computing system is a complete analogue of the one being studied.

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It seems to us that these problems are not grounds for abandoning quantum computing in principle, but, on the contrary, they need to be intensively developed to search for high-performance algorithms on emulators of quantum systems. Particularly promising is the use of new mathematics for this purpose — functional integration, which has been intensively developed specifically for quantum systems, but has been used for computational problems only from the point of view of approximate (asymptotic) methods [5]. The canonical representation for the Green's function in the form of a functional integral was proposed by Feynman [6]

$$G\ (q,t\colon q',t') = \int D\Gamma \exp\left\{\frac{i}{\hbar}\int_{t'}^{t} L(\dot{q}(\tau),q(\tau))\,d\tau\right\} \tag{1}$$

where $D\Gamma$ is "the sum over all trajectories connecting q' and q". This formulation is due to the fact that the original formula, a compact representation of which is given in [2]

$$G = \lim_{N\to\infty}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\prod_{k=1}^{N-1}\left\{dq_k\sqrt{\frac{m}{2\pi i\hbar\Delta t}}\exp\left[\frac{i}{\hbar}\left(\frac{m(q_k-q_{k-1})}{2\Delta t}-\Delta t V\left(\frac{q_k+q_{k-1}}{2}\right)\right)\right]\right\}\times\sqrt{\frac{m}{2\pi i\hbar\Delta t}}\exp\left\{\frac{i}{\hbar}\left[\frac{m(q_N-q_{N-1})}{2\Delta t}-\Delta t V\left(\frac{q_{N-1}+q_N}{2}\right)\right]\right\}, \tag{2}$$

does not allow a strict definition of the limiting transition indicated in it due to Δt in the denominator, but requires additional interpretation. R. Feynman himself understood this, so he proposed using the identity

$$\sqrt{\frac{2\pi i\hbar m}{\Delta t}} = \int d\tilde{p}_k \exp\left\{-\frac{i}{\hbar}\frac{\Delta t}{2m}\left[\tilde{p}_k-\frac{m}{\Delta t}(q_N-q_{N-1})\right]^2\right\},$$

To eliminate Δtin the denominators and go to the formulation

$$G\ (q,t\colon q',t') = \int D\Gamma \exp\left\{\frac{i}{\hbar}\int_{q'}^{q} p(\tau)dq(\tau) - \frac{i}{\hbar}\int_{t'}^{t} H(p(\tau),q(\tau))d\tau\right\}, \tag{3}$$

where now $D\Gamma$ means the sum over paths, but in phase space. But the situation is not so simple. The fact is that in formula (2) after the indicated substitution there will be a different number of integrals over q and p, so the formula can only be understood symbolically. The solution to this problem was given in the famous paper by L. Faddeev and V. Popov [7], and the result can be represented as

$$G(q,t\colon q',t') = \int_{-\infty}^{\infty}\frac{d\tilde{p}_{k_0}}{2\pi\hbar}\int_{-\infty}^{\infty}\frac{d\tilde{p}_{k_0+1}}{2\pi\hbar}2\pi\hbar\delta\left(d\tilde{p}_{k_0+1}-d\tilde{p}_{k_0}\right)\times\int\partial\widetilde{D\Gamma}\exp\left\{\frac{i}{\hbar}\left[-\int_{p'}^{\tilde{p}_{k_0}} q\,dp - E't' + E_0^{(1)}\left(t_{k_0}-\Delta t\right) - \int_{t'}^{t_{k_0}-\Delta t} H(p,q)d\tau\right]\right\}\times\int\widetilde{D\Gamma}\exp\left\{\frac{i}{\hbar}\left[-\int_{\tilde{p}_{k_0+1}}^{p} q\,dp - E_0^{(2)}\left(t_{k_0}+\Delta t\right) + Et - \int_{t_{k_0}+\Delta t}^{t} H(p,q)d\tau\right]\right\}$$

where the sign "$\sim$" means that the path in phase space connects points with a fixed coordinate and fixed momentum. Comparison with (3) shows that the passage to the limit of Δt is already meaningful. However, in a number of works the correctness of the definition of $G\ (q,t\colon q',t')$, was demonstrated directly (see, for example, [8]).

A NEW APPROACH TO EFFECTIVE QUANTUM COMPUTING

The physical meaning of this transformation is very important (see Fig. 1). The entire transition is divided into two parts, separated by a hypersurface Γ. The usual integration is carried out over the points of the hypersurface, and under the integral there are two truncated propagators in a mixed representation. The easiest way to deal with them is the approach developed by one of the authors [8]. Since canonical transformations with a unit determinant are possible in phase space [9], we perform such a transformation $(p, q) \rightarrow (Q, V)$ with a transformation generator F

$$H(P, X) \rightarrow H(Q, Y) = H(q, \partial F_1/\partial t) + \partial F_1/\partial t\,|_{Q,Y} \tag{4}$$

The following calculations are very simple. We require that the transformed H vanish, from which a first-order partial differential equation is obtained for the generator (it is obtained from (4) by vanishing the left-hand side). Then each of the truncated functional integrals turns into a functional delta function and is calculated directly.

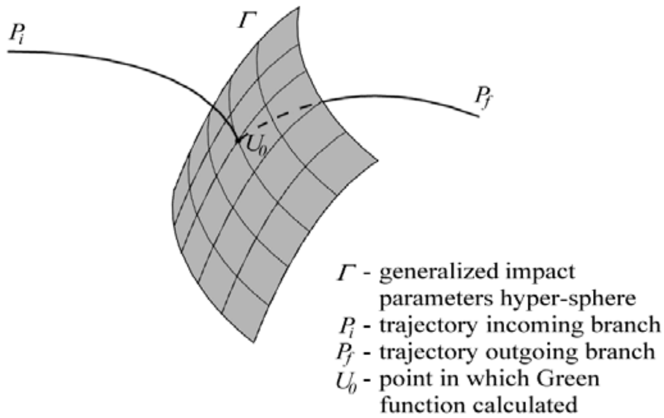

Fig. 1. Generalized impact parameters hyper-sphere and particle trajectory branches

The result looks like

$$G(P_i \rightarrow P_f) = \int dX_0 C\delta(X_0 P_0) \exp\{i/h(P_f X_f - P_i X_i) + i/hF_1|_* + i/hF_1|_* + i/hQ_i(Y_0 - Y_i) + i/hQ_f(Y_f - Y_0)\}$$

with

$$F_1\colon\ H(X, \partial F_1/\partial x) = E,$$

and " $*$ " means that it is necessary to supply the values of the phase coordinates of the corresponding branch.

From the point of view of creating high-performance algorithms, the result is almost ideal. We have a multidimensional integral with a dimension one less than the dimension of space, and under the integral, independently at each point, a set of first-order partial differential equations is solved (two for real trajectories and four for complex ones). Since solving such equations is equivalent in the method of characteristics to solving a set of ordinary differential equations, this approach is surprisingly suitable for modern computing systems with powerful CPUs with large RAM and associated GPGPUs with thousands of cores. Of course, efficient computing requires the use of virtualization and the creation of a virtual complex adapted to the algorithm [10].

1. It is worth paying attention to the special role of the hypersurface (fig. 1) from the point of view of organizing calculations in quantum systems. Obvious advantages:

1. Possibility of moving to other coordinates during rearrangement processes;
2. Possibility of localizing a quantum jump in excitation processes;
3. The ability to move this hypersurface to simplify calculations.

ADDITIONAL BENEFITS OF THE NEW APPROACH

Let us also pay additional attention to the capabilities of the proposed representation for the preliminary analysis of propagators. Since the problem comes down to calculating multidimensional integrals, and the dependence of the integral on the parameters is determined by the behavior of the integrand, it is possible to use catastrophe theory to study this dependence [11]. An effective idea of the behavior of these integrals is based on the analysis of the dynamics of the critical points of the integrand and the use of special functions to approximate the canonical integrals of catastrophe theory [11]. Considering the extensive work on obtaining functional representations for a large number of partial differential equations (including nonlinear ones) [12], the proposed approach can thus serve as a basis for constructing a qualitative theory of partial differential equations.

CONCLUSIONS

The paper proposes a new approach to the construction of efficient computational algorithms based on the ideology of quantum computing. It seems to us that the parallel algorithms derived from it are obviously suitable for adaptation to modern computing architectures. As an application, we can also point out an effective approach for the qualitative analysis of solutions to partial differential equations.

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