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Mengzhao Qin

Symplectic Geometric Algorithms for Hamiltonian Systems

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With 62 Figures

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Authors
Kang Feng (1920-1993)
Institute of Computational
Mathematics and Scientific/
Engineering Computing
Beijing 100190, China

Mengzhao Qin
Institute of Computational
Mathematics and Scientific/
Engineering Computing
Beijing 100190, China
Email: qmz@lsec.cc.ac.cn

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"... In the late 1980s Feng Kang proposed and developed so-called symplectic algorithms for solving equations in Hamiltonian form. Combining theoretical analysis and computer experimentation, he showed that such methods, over long times, are much superior to standard methods. At the time of his death, he was at work on extensions of this idea to other structures ..."

Peter Lax

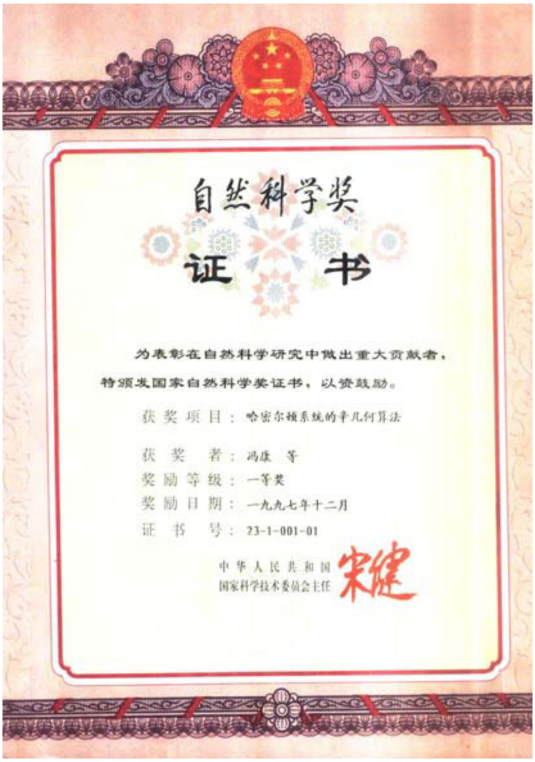
Cited from SIAM News November 1993

Kang Feng giving a talk at an international conference

" A basic idea behind the design of numerical schemes is that they can preserve the properties of the original problems as much as possible . . . Different representations for the same physical law can lead to different computational techniques in solving the same problem, which can produce different numerical results . . ."

Kang Feng (1920 – 1993)

Cited from a paper entitled "How to compute property Newton's equation of motion"



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Foreword

Kang Feng (1920–1993), Member of the Chinese Academy of Sciences, Professor and Honorary Director of the Computing Center of the Chinese Academy of Sciences, famous applied mathematician, founder and pioneer of computational mathematics and scientific computing in China.

It has been 16 years since my brother Kang Feng passed away. His scientific achievements have been recognized more and more clearly over time, and his contributions to various fields have become increasingly outstanding. In the spring of 1997, Professor Shing-Tung Yau, a winner of the Fields Medal and a foreign member of the Chinese Academy of Sciences, mentioned in a presentation at Tsinghua University, entitled "The development of mathematics in China in my view", that "there are three main reasons for Chinese modern mathematics to go beyond or hand in hand with the West. Of course, I am not saying that there are no other works, but I mainly talk about the mathematics that is well known historically: Professor Shiingshen Chern's work on characteristic class, Luogeng Hua's work on the theory of functions of several complex variables, and Kang Feng's work on finite elements." This high evaluation of Kang Feng as a mathematician (not just a computational mathematician) sounds so refreshing that many people talked about it and strongly agreed with it. At the end of 1997, the Chinese National Natural Science Foundation presented Kang Feng et al. with the first class prize for his other work on a symplectic algorithm for Hamiltonian systems, which is a further recognition of his scientific achievements (see the certificate on the previous page). As his brother, I am very pleased.

Achieving a major scientific breakthrough is a rare event. It requires vision, ability and opportunity, all of which are indispensable. Kang Feng has achieved two major scientific breakthroughs in his life, both of which are very valuable and worthy of mention. Firstly, from 1964 to 1965, he proposed independently the finite element method and laid the foundation for the mathematical theory. Secondly, in 1984, he proposed a symplectic algorithm for Hamiltonian systems. At present, scientific innovation has become the focus of discussion. Kang Feng's two scientific breakthroughs may be treated as case studies in scientific innovation. It is worth emphasizing that these breakthroughs were achieved in China by Chinese scientists. Careful study of these has yet to be carried out by experts. Here I just describe some of my personal feelings.

It should be noted that these breakthroughs resulted not only from the profound mathematical knowledge of Kang Feng, but also from his expertise in classical physics and engineering technology that were closely related to the projects. Scientific breakthroughs are often cross-disciplinary. In addition, there is often a long period of time before a breakthrough is made-not unlike a long time it takes for a baby to be born, which requires the accumulation of results in small steps.

The opportunity for inventing the finite element method came from a national research project, a computational problem in the design of the Liu Jia Xia dam. For such a concrete problem, Kang Feng found a basis for solving of the problem using his sharp insight. In his view, a discrete computing method for a mathematical and physical problem is usually carried out in four steps. Firstly, one needs to know and define the physical mechanism. Secondly, one writes the appropriate differential equations accordingly. In the third step, design a discrete model. Finally, one develops the numerical algorithm. However, due to the complexity of the geometry and physical conditions, conventional methods cannot always be effective. Nonetheless, starting from the physical law of conservation or variational principle of the matter, we can directly relate to the appropriate discrete model. Combining the variational principle with the spline approximation leads to the finite element method, which has a wide range of adaptability and is particularly suited to deal with the complex geometry of the physical conditions of computational engineering problems. In 1965, Kang Feng published his paper entitled “Difference schemes based on the variational principle”, which solved the basic theoretical issues of the finite element method, such as convergence, error estimation, and stability. It laid the mathematical foundation for the finite element method. This paper is the main evidence for recognition by the international academic community of our independent development of the finite element method.

After the Chinese Cultural Revolution, he continued his research in finite element and related areas. During this period, he made several great achievements. I remember that he talked with me about other issues, such as Thom’s catastrophe theory, Prigogine’s theory of dissipative structures, solitons in water waves, the Radon transform, and so on. These problems are related to physics and engineering technology. Clearly he was exploring for new areas and seeking a breakthrough. In the 1970s, Arnold’s “Mathematical Method of Classical Mechanics” came out. It described the symplectic structure for Hamiltonian equations, which proved to be a great inspiration to him and led to a breakthrough. Through his long-term experience in mathematical computation, he fully realized that different mathematical expressions for the same physical law, which are physically equivalent, can perform different functions in scientific computing (his students later called this the “Feng’s major theorem”). In this way, for classical mechanics, Newton’s equations, Lagrangian equations and Hamiltonian equations will show a different pattern of calculations after discretization. Because the Hamiltonian formulation has a symplectic structure, he was keenly aware that, if the algorithm can maintain the geometric symmetry of symplecticity, it will be possible to avoid the flaw of artificial dissipation of this type of algorithm and design a high-fidelity algorithm. Thus, he opened up a broad way for the computational method of the Hamiltonian system. He called this way the “Hamiltonian way”. This computational method has been used in the calculation of the orbit in celestial mechanics, in calculations for the particle path in accelerator, as well as in molecular dynamics. Later, the scope of its application was expanded. For example, it has also been widely used in studies of the atmosphere and earth sciences and elsewhere. It has been effectively applied in solving the GPS observation operator, indicating that Global Positioning System data can be dealt with in a timely manner. This algorithm is 400 times more efficient than the traditional method. In addition, a symplectic algorithm has been successfully used in the oil and gas exploration fields. Under the influence of Kang Feng, international research on symplectic algorithm has become popular and flourishing, nearly 300 papers have been published in this field to date.

Kang Feng's research work on the symplectic algorithm has been well-known and recognized internationally for its unique, innovative, systematic and widespread properties, for its theoretical integrity and fruitful results.

J. Lions, the former President of the International Mathematics Union, spoke at a workshop when celebrating his 60th birthday: "This is another major innovation made by Kang Feng, independent of the West, after the finite element method." In 1993 one of the world's leading mathematicians, P.D. Lax, a member of the American Academy of Sciences, wrote a memorial article dedicated to Kang Feng in SIAM News, stating that "In the late 1980s, Kang Feng proposed and developed so-called symplectic algorithms for solving evolution equations . . .. Such methods, over a long period, are much superior to standard methods." E. J. Marsden, an internationlly well-known applied mathematician, visited the computing institute in the late 1980s and had a long conversation with Kang Feng. Soon after the death of Kang Feng, he proposed the multi-symplectic algorithm and extended the characteristics of stability of the symplectic algorithm for long time calculation of Hamiltonian systems with infinite dimensions.

On the occasion of the commemoration of the 16th anniversary of Kang Feng's death and the 89th anniversary of his birth, I think it is especially worthwhile to praise and promote what was embodied in the lifetime's work of Kang Feng — " independence in spirit, freedom in thinking". [1] Now everyone is talking about scientific innovation, which needs a talented person to accomplish. What type of person is needed most? A person who is just a parrot or who has an "independent spirit, freely thinking"? The conclusion is self-evident. Scientific innovation requires strong academic atmosphere. Is it determined by only one person or by all of the team members? This is also self-evident. From Kang Feng's scientific career, we can easily find that the key to the problem of scientific innovation is "independence in spirit, freedom in thinking", and that needs to be allowed to develop and expand.

Kang Feng had planned to write a monograph about a symplectic algorithm for Hamiltonian systems. He had accumulated some manuscripts, but failed to complete it because he died too early due to sickness. Fortunately, his students and Professor Mengzhao Qin (see the photo on the previous page), one of the early collaborators, spent 15 years and finally completed this book based on Kang Feng's plan, realizing his wish. It is not only an authoritative exposition of this research field, but also an

[1] Yinke Chen engraved on a stele in 1929 in memory of Guowei Wang in campus of Tsinghua University.

exposure of the academic thought of a master of science, which gives an example of how an original and innovative scientific discovery is initiated and developed from beginning to end in China.

We would also like to thank Zhejiang Science and Technology Publishing House, which made a great contribution to the Chinese scientific cause through the publication of this manuscript.

Although Kang Feng died 16 years ago, his scientific legacy has been inherited and developed by the younger generation of scientists. His scientific spirit and thought still elicit care, thinking and resonance in us. He is still living in the hearts of us.

Duan, Feng
Member of Chinese
Academy of Sciences
Nanjing University
Nanjing
September 20, 2009

Preface

It has been 16 years since Kang Feng passed away. It is our honor to publish the English version of *Symplectic Algorithm for Hamiltonian Systems*, so that more readers can see the history of the development of symplectic algorithms. In particular, after the death of Kang Feng, the development of symplectic algorithms became more sophisticated and there have been a series of monographs published in this area, e.g., Sanz-Serna & M.P. Calvo's *Numerical Hamiltonian Problems* published in 1994 by Chapman and Hall Publishing House; E. Hairer, C. Lubich and G. Wanner's *Geometrical Numerical Integration* published in 2001 by Springer Verlag; B. Leimkuhler and S. Reich's *Simulating Hamiltonian Dynamics* published in 2004 by Cambridge University Press. The symplectic algorithm has been developed from ordinary differential equations to partial differential equations, from a symplectic structure to a multi-symplectic structure. This is largely due to the promotion of this work by J. Marsden of the USA and T. Bridge and others in Britain. Starting with a symplectic structure, J. Marsden first developed the Lagrange symplectic structure, and then to the multi-symplectic structure. He finally proposed a symplectic structure that meets the requirement of the Lagrangian form from the variational principle by giving up the boundary conditions. On the other hand, T. Bridge and others used the multi-symplectic structure to derive directly the multi-symplectic Hamilton equations, and then constructed the difference schemes that preserve the symplectic structure in both time and space. Both methods can be regarded as equivalent in the algorithmic sense.

Now, in this monograph, most of the content refers only to ordinary differential equations. Kang Feng and his algorithms research group working on the symplectic algorithm did some foundation work. In particular, I would like to point out three negative theorems: " non-existence of energy preserving scheme", " non-existence of multistep linear symplectic scheme", and " non-existence of volume-preserving scheme form rational fraction expression". In addition, generating function theory is not only rich in analytical mechanics and Hamilton–Jacobi equations. At the same time, the construction of symplectic schemes provides a tool for any order accuracy difference scheme. The formal power series proposed by Kang Feng had a profound impact on the later developed " backward error series" work ," modified equation" and " modified integrator".

The symplectic algorithm developed very quickly, soon to be extended to the geometric method. The structure preserving algorithm (not only preserving the geometrical structure, but also the physical structure, etc.) preserves the algebraic structure to present the Lie group algorithm, and preserves the differential complex algorithm. Many other prominent people have contributed to the symplectic method in addition to those mentioned above. There are various methods related to structure preserving algorithms and for important contributions the readers are referred to R. McLachlan & GRW Quispel " Geometric integration for ODEs" and T. Bridges & S. Reich " Numerical methods for Hamiltonian PDEs".

The book describes the symplectic geometric algorithms and theoretical basis for a number of related algorithms. Most of the contents are a collection of lectures given by Kang Feng at Beijing University. Most of other sections are a collection of papers which were written by group members.

Compared to the previous Chinese version, the present English one has been improved in the following respects. First of all, to correct a number of errors and mistakes contained in the Chinese version. Besides, parts of Chapter 1 and Chapter 2 were removed, while some new content was added to Chapter 4, Chapter 7, Chapter 8, Chapter 9 and Chapter 10. More importantly, four new chapters — Chapter 13 to Chapter 16 were added. Chapter 13 is devoted to the KAM theorem for the symplectic algorithm. We invited Professor Zaijiu Shang , a former PhD student of Kang Feng to compose this chapter. Chapter 14 is called Variational Integrator. This chapter reflects the work of the Nobel Prize winner Professor Zhengdao Li who proposed in the 1980s to preserve the energy variational integrator, but had not explained at that time that it had a Lagrange symplectic type, which satisfied the Lagrange symplectic structure. Together with J. Marsden he proposed the variational integrator trail connection, which leads from the variational integrator. Just like J. Marsden, he hoped this can link up with the finite element method. Chapter 15 is about Birkhoffian Systems, describing a class of dissipative structures for Birkohoffian systems to preserve the dissipation of the Birkhoff structure. Chapter 16 is devoted to Multisymplectic and Variational Integrators, providing a summary of the widespread applications of multisymplectic integrators in the infinitely dimensional Hamiltonian systems.

We would also like to thank every member of the Kang Feng's research group for symplectic algorithms: Huamo Wu, Daoliu Wang, Zaijiu Shang, Yifa Tang, Jialin Hong, Wangyao Li, Min Chen, Shuanghu Wang, Pingfu Zhao, Jingbo Chen, Yushun Wang, Yajuan Sun, Hongwei Li, Jianqiang Sun, Tingting Liu, Hongling Su, Yimin Tian; and those who have been to the USA: Zhong Ge, Chunwang Li, Yuhua Wu, Meiqing Zhang, Wenjie Zhu, Shengtai Li, Lixin Jiang, and Haibin Shu. They made contributions to the symplectic algorithm over different periods of time.

The authors would also like to thank the National Natural Science Foundation, the National Climbing Program projects, and the State's Key Basic Research Projects for their financial support. Finally, the authors would also like to thank the Mathematics and Systems Science Research Institute of the Chinese Academy of Sciences, the Computational Mathematics and Computational Science and Engineering Institute, and the State Key Laboratory of Computational Science and Engineering for their support.

The editors of this book have received help from E. Hairer, who provided a template from Springer publishing house. I would also like to thank F. Holzwarth at Springer publishing house and Linbo Zhang of our institute, and others who helped me successfully publish this book.

For the English translation, I thank Dr. Shengtai Li for comprehensive proofreading and polishing, and the editing of Miss Yi Jin. For the English version of the publication I would also like to thank the help of the Chinese Academy of Sciences Institute of Mathematics. Because Kang Feng has passed away, it may not be possible to provide a comprehensive representation of his academic thought, and the book will inevitably contain some errors. I accept the responsibility for any errors and welcome criticism and corrections.

We would also like to thank Springer Beijing Representation Office and Zhejiang Science and Technology Publishing House, which made a great contribution to the Chinese scientific cause through the publication of this manuscript. We are especially grateful to thank Lisa Fan, W. Y. Zhou, L. L. Liu and X. M. Lu for carefully reading and finding some misprints, wrong signs and other mistakes.

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Mengzhao Qin
Institute of Computational
Mathematics and Scientific
Engineering Computing
Beijing
September 20, 2009

Contents

Introduction

The main theme of modern scientific computing is the numerical solution of various differential equations of mathematical physics bearing the names, such as Newton, Euler, Lagrange, Laplace, Navier–Stokes, Maxwell, Boltzmann, Einstein, Schrödinger, Yang-Mills, etc. At the top of the list is the most celebrated Newton's equation of motion. The historical, theoretical and practical importance of Newton's equation hardly needs any comment, so is the importance of the numerical solution of such equations. On the other hand, starting from Euler, right down to the present computer age, a great wealth of scientific literature on numerical methods for differential equations has been accumulated, and a great variety of algorithms, software packages and even expert systems has been developed. With the development of the modern mechanics, physics, chemistry, and biology, it is undisputed that almost all physical processes, whether they are classical, quantum, or relativistic, can be represented by an Hamiltonian system. Thus, it is important to solve the Hamiltonian system correctly.

1. Numerical Method for the Newton Equation of Motion

In the spring of 1991, the first author [Fen92b] presented a plenary talk on how to compute the numerical solution of Newton classical equation accurately at the Annual Physics Conference of China in Beijing.

It is well known that numerically solving so-called mathematics-physics equations has become a main topic in modern scientific computation. The Newton equation of motion is one of the most popular equations among various mathematics-physics equations. It can be formulated as a group of second-order ordinary differential equations, $f = ma = m\ddot{x}$. The computational methods of the differential equations advanced slowly in the past due to the restriction of the historical conditions. However, a great progress was made since Euler, due to contributions from Adams, Runge, Kutta, and Stömer, etc.. This is especially true since the introduction of the modern computer for which many algorithms and software packages have been developed. It is said that the three-body problem is no longer a challenging problem and can be easily computed. Nevertheless, we propose the following two questions:

1° Are the current numerical algorithms suitable for solving the Newton equation of motion?

2° How can one calculate the Newton equation of motion more accurately?

It seems that nobody has ever thought about the first issue seriously, which may be the reason why the second issue has never been studied systematically. In this book, we will study mainly the fundamental but more difficult Newton equation of motion that is in conservative form. First, the conservative Newton equation has two equivalent mathematical representations: a Lagrange variation form and a Hamiltonian form. The latter transforms the second-order differential equations in physical space into a group of the first-order canonical equations in phase space. ***Different representations for the same physical law can lead to different computational techniques in solving the same problem, which can produce different numerical results.*** Thus making a wise and reasonable choice among various equivalent mathematical representations is extremely important in solving the problem correctly.

We choose the Hamiltonian formulation as our basic form in practice based on the fact that the Hamiltonian equations have symmetric and clean form, where the physical laws of the motion can be easily represented. Secondly, the Hamiltonian formulation is more general and universal than the Newton formulation. It can cover the classical, relativistic, quantum, finite or infinite dimensional real physical processes where dissipation effect can be neglected. Therefore, the success of the numerical methods for Hamiltonian equations has broader development and application perspectives. Thus, it is very surprising that the numerical algorithms for Hamiltonian equations are almost nonexistent after we have searched various publications. This motivates us to study the problem carefully to seek the answers to the previous two questions.

Our approach is to use the symplectic geometry, which is the geometry in phase space. It is based on the anti-symmetric area metric, which is in contrast to the symmetric length metrics of Euclid and Riemann geometry. The basic theorem of the classic mechanics can be described as "the dynamic evolution of all Hamiltonian systems preserves the symplectic metrics, which means it is a symplectic (canonical) transformation". Hence the correct discretization algorithms to all the Hamiltonian systems should be symplectic transformation. Such algorithms are called symplectic (canonical) algorithms or Hamiltonian algorithms. We have intentionally analyzed and evaluated the derivation of the Hamiltonian algorithm within the symplectic structures. The fact proved that this approach is correct and fruitful. We have derived a series of symplectic algorithms, found out their properties, laid out their theoretical foundation, and tested them with extremely difficult numerical experiments.

In order to compare the symplectic and non-symplectic algorithm, we proposed eight numerical experiments: harmonic oscillator, nonlinear Duffing oscillator, Huygens oscillator, Cassini oscillator, two dimensional multi-crystal and semi-crystal lattice steady flow, Lissajous image, geodesic flow on ellipsoidal surface, and Kepler motion. The numerical experiments demonstrate the superiority of the symplectic algorithm. All traditional non-symplectic algorithms fail without exception, especially in preserving global property and structural property, and long-term tracking capability, regardless of their accuracy. However, all the symplectic algorithms passed the tests with long-term stable tracking capability. These tests clearly demonstrate the superiority of the symplectic algorithms.

Almost all of the traditional algorithms are non-symplectic with few exceptions. They are designed for the asymptotic stable system which has dissipation mechanism to maintain stability, whereas the Hamiltonian system does not have the asymptotic stability. Hence all these algorithms inevitably contain artificial numerical dissipation, fake attractors, and other parasitics effects of non-Hamiltonian system. All these effects lead to seriously twist and serious distortion in numerical results. They can be used in short-term transient simulation, but are not suitable and can lead to wrong conclusions for long-term tracking and global structural property research. Since the Newton equation is equivalent to Hamiltonian equation, the answer to the first question is “No”, which is quite beyond expectation.

The symplectic algorithm does not have any artificial dissipation so that it can congenitally avoid all non-symplectic pollution and become a “clean” algorithm. Hamiltonian system has two types of conservation laws: one is the area invariance in phase space, i.e., Liouville–Poincaré conservation law; the other is the motion invariance which includes energy conservation, momentum and angular momentum conservation, etc. We have proved that all symplectic algorithms have their own invariance, which has the same convergence to the original theoretical invariance as the convergence order of the numerical algorithm. We have also proved that the majority of invariant tori of the near integrable system can be preserved, which is a new formulation of the famous KAM (Kolmogorov–Arnorld–Moser) theorem[Kol54b,Kol54a,Arn63,Mos62]. All of these results demonstrate that the structure of the discrete Hamiltonian algorithm is completely parallel to the conservation law, and is very close to the original form of the Hamiltonian system. Moreover, theoretically speaking, it has infinite long-term tracking capability. Hence, a correct numerical method to solve the Newton equation is to Hamiltonize the equation first and then use the Hamiltonian algorithm. This is the answer to the second question. We will describe in more detail the KAM theory of symplectic algorithms for Hamiltonian systems in Chapter 13. In the following we present some examples to compare the symplectic algorithm and other non-symplectic algorithms in solving Newton equation of motion.

(1) Calculation of the Harmonic oscillator’s elliptic orbit

Calculation of the Harmonic oscillator’s elliptic orbit (Fig. 0.1(a)) uses Runge–Kutta method (R–K) with a step size 0.4. The output is at 3,000 steps. It shows artificial dissipation, shrinking of the orbit. Fig. 0.1(b) shows the results using Adams method with a step size 0.2. It is anti-dissipative and the orbit is scattered out. Fig. 0.1(c) shows the results of two-step central difference (leap-frog scheme). This scheme is symplectic to linear equations. The results are obtained with a step size 0.1. It shows that the results of three stages for 10,000,000 steps: the initial 1,000 steps, the middle 1,000 steps, and the final 1,000 steps. They are completely in agreement.

(2) The elliptic orbit for the nonlinear oscillator

Fig. 0.2(a) shows the results of two-step central-difference. This scheme is non-symplectic for nonlinear equations. The output is for step size 0.2 and 10,000 steps. Fig. 0.2(a) shows the initial 1,000 steps and Fig. 0.2(b) shows the results between 9,000 to 10,000 steps. Both of them show the distortion of the orbit. Fig. 0.2(c) is for the second-order symplectic algorithm with 0.1 step size, 1,000 steps.

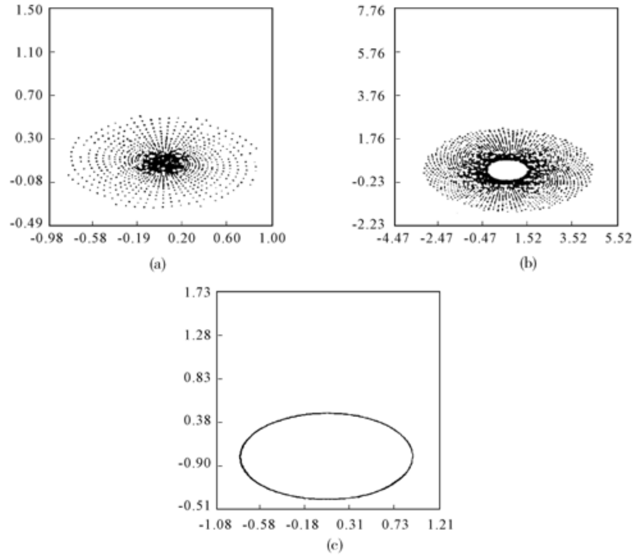

Fig. 0.1. Calculation of the Harmonic oscillator's elliptic orbit

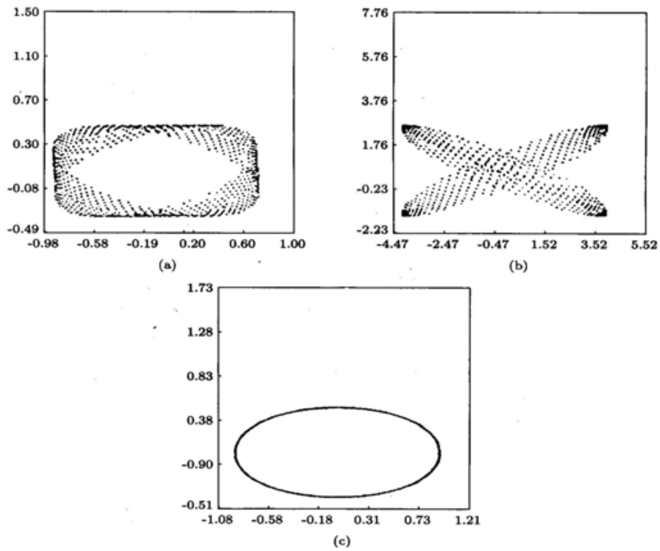

Fig. 0.2. Calculation of the nonlinear oscillator's elliptic orbit

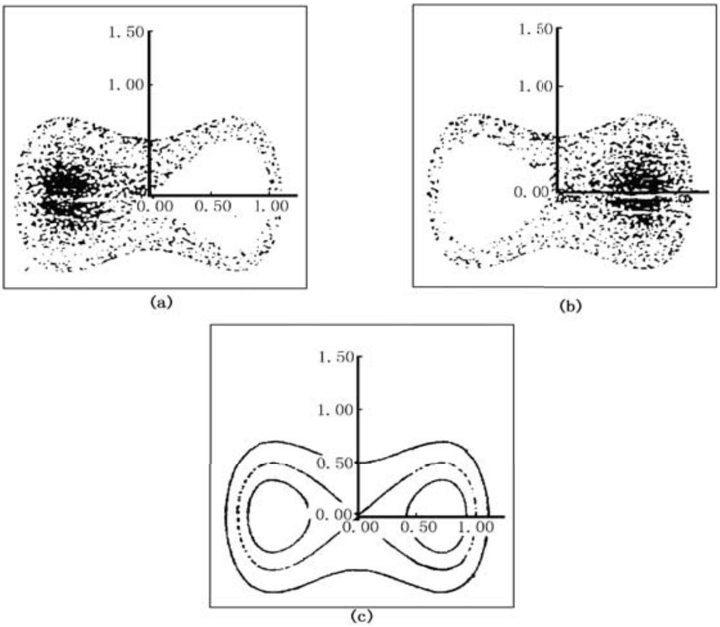

Fig. 0.3. Calculation of the nonlinear Huygens oscillator

(3) The oval orbit of the Huygens oscillator

Using the R–K method, the two fixed points on the horizontal axes become two fake attractors. The probability of the phase point close to the two attractors is the same. The same initial point outside the separatrix is attracted randomly either to the left or to the right. Fig. 0.3(a) shows the results with a step size 0.10000005 and 900,000 steps, which approach the left attractor. Fig. 0.3(b) shows the results with a step size 0.10000004 and 900,000 steps, which approach the right attractor. Fig. 0.3(c) shows the results of the second-order symplectic algorithm with a step size 0.1. Four typical orbits are plotted and each contains 100,000,000 steps: for every orbit first 500 steps, the middle 500 steps, and the final 500 steps. They are in complete agreement.

(4) The dense orbit of the geodesic for the ellipsoidal surface

The dense orbit of the geodesic for the ellipsoidal surface with irrational frequency ratio. The square of frequency ratio is 5/16, step size is 0.05658, 10,000 steps. Fig.0.4(a) is for the R–K method which does not tend to dense. Fig. 0.4(b) is for the symplectic algorithm which tends to dense.

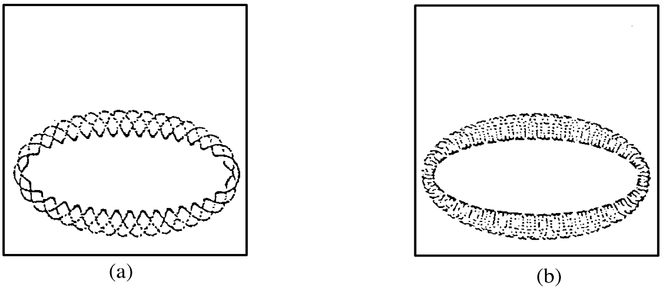

Fig. 0.4. Geodesics on ellipsoid, frequency ratio $\sqrt{5} : 4$, non dense (a), dense orbit (b)

(5) The close orbit of the geodesic for the ellipsoidal surface

The close orbit of the geodesic for the ellipsoidal surface with rational frequency ratio. The frequency ratio is 11/16, step size is 0.033427, 100,000 steps and 25 cycles. Fig.0.5(a) is for the R–K method which does not lead to the close orbit. Fig. 0.5(b) is for the symplectic algorithm which leads to the close orbit.

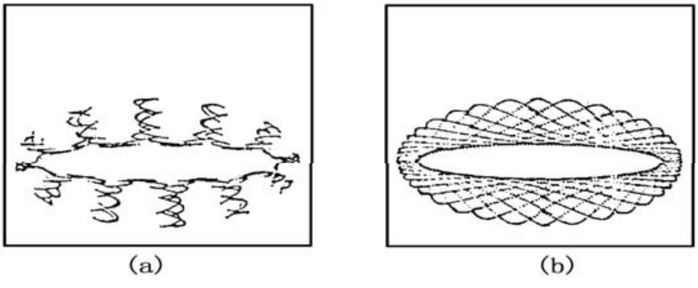

Fig. 0.5. Geodesics on ellipsoid, frequency ratio 11:16, non closed (a), closed orbit (b)

(6) The close orbit of the Keplerian motion

The close orbit of the Keplerian motion with rational frequency ratio. The frequency ratio is 11/20, step size is 0.01605, 240,000 steps and 60 cycles. Fig. 0.6(a) is for the R–K method which does not lead to the close orbit. Fig. 0.6(b)is for the symplectic method which leads to the close orbit.

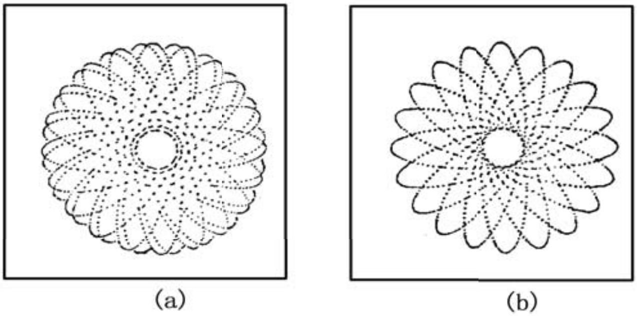

Fig. 0.6. Geodesics on ellipsoid, frequency ratio 11:20, non closed (a), closed orbit (b)

2. History of the Hamiltonian Mechanics

We first consider the three formulations of the classical mechanics. Assume a motion has n degrees of freedom. The position is denoted as $q = (q_1, \cdots, q_n)$. The potential function is $V = V(q)$. Then we have

$$m\frac{\mathrm{d}^2 q}{\mathrm{d}t^2} = -\frac{\partial}{\partial q}V,$$

which is the standard formulation of the motion. It is a group of second-order differential equations in space $\mathbf{R}^n$. It is usually called the standard formulation of the classical mechanics, or Newton formulation.

Euler and Lagrange introduced an action on the difference between the kinetic energy and potential energy

$$L(q, \dot{q}) = T(\dot{q}) - V(q) = \frac{1}{2}(\dot{q}, M\dot{q}) - V(q).$$

Using the variational principle the above equation can be written as

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{q}} - \frac{\partial L}{\partial q} = 0,$$

which is called the variational form of the classical mechanics, i.e., the Lagrange form.

In the 19th century, Hamilton proposed another formulation. He used the momentum $p = M\dot{q}$ and the total energy $H = T + V$ to formulate the equation of motion as

$$\dot{p} = -\frac{\partial H}{\partial q}, \quad \dot{q} = \frac{\partial H}{\partial p},$$

which is called Hamiltonian canonical equations. This is a group of the first-order differential equations in $2n$ phase space $(p_1, \cdots, p_n, q_1, \cdots, q_n)$. It has simple and symmetric form.

The three basic formulations of the classical mechanics have been described in almost all text-books on theoretical physics or theoretical mechanics. ***These different mathematical formulations describe the same physics law but provide different approaches in problem solving. Thus equivalent mathematical formulation can have different effectiveness in computational methods.*** We have verified this in our own simulations.

The first author did extensive research on Finite Element Method (FEM) in the 1960s [Fen65] which represents a systematic algorithm for solving equilibrium problem. Physical problems of this type have two equivalent formulations: Newtonian, i.e., solving the second-order elliptic equations, and variational formulation, i.e., minimization principle in energy functional. The key to the success of FEM in both theoretical and computational methods lies in using a reasonable variational formulation as the basic principle. After that, he had attempted to apply the FEM idea to the dynamic problem of continuum media mechanics, but not yet achieved the corresponding success, which appears to be difficult to accomplish even today. Therefore, the reasonable choice for computational method of dynamic problem might be the Hamiltonian formulation. Initially it is a conjecture and requires verification from the computational experiments. We have investigated how others evaluated the Hamiltonian system in history. First we should point out that Hamilton himself proposed his theory based on the geometric optics and then extended it to mechanics that appears to be a very different field. In 1834 Hamilton said, "This set of idea and method has been applied to optics and mechanics. It seems it can be applied to other areas and developed into an independent knowledge by the mathematicians"[Ham34]. This is just his expectation, and other peers in the same generation seemed indifferent to this set of theory, which was "beautiful but useless"[Syn44] to them. Klein, a famous mathematician, while giving a high appreciation to the mathematical elegance of the theory, suspected its applicability, and said: "... a physicist, for his problems, can extract from these theories only very little, and an engineer nothing"[Kle26]. This claim has been proved wrong at least in physics aspect in the later history. The quantum mechanics developed in the 1920s under the framework of the Hamiltonian formulation. One of the founders of the quantum mechanics, Schrödinger said, "Hamiltonian principle has been the foundation for modern physics ... If you want to solve any physics problem using the modern theory, you must represent it using the Hamiltonian formulation"[Sch44].

3. The Importance of the Hamiltonian System

The Hamiltonian system is one of the most important systems among all the dynamics systems. All real physical processes where the dissipation can be neglected can be formulated as Hamiltonian system. Hamiltonian system has broad applications, which include but are not limited to the structural biology, pharmacology, semiconductivity, superconductivity, plasma physics, celestial mechanics, material mechanics, and partial differential equations. The first five topics have been listed as "Grand Challenges" in Research Project of American government.

The development of the physics verifies the importance of the Hamiltonian systems. Up to date, it is undisputed that all real physical processes where the dissipation can be neglected can be written as Hamiltonian formulation, whether they have finite or infinite degrees of freedom.

The problem with finite degrees of freedom includes celestial and man-made satellite mechanics, rigid body, and multi-body (including the robots), geometric optics, and geometric asymptotic method (including ray-tracing approximation method in wave-equation, and WKB equation of quantum mechanics), confinement of the plasma, the design of the high speed accelerator, automatic control, etc.

The problem with infinite degrees of freedom includes ideal fluid dynamics, elastic mechanics, electrical mechanics, quantum mechanics and field theory, general relativistic theory, solitons and nonlinear waves, etc.

All the above examples show the ubiquitous and nature of the Hamiltonian systems. It has the advantage that different physics laws can be represented by the same mathematical formulation. Thus we have confidence to say that successful development of the numerical methods for Hamiltonian system will have extremely broad applications.

We now discuss the status of the numerical method for Hamiltonian systems. Hamiltonian systems, including finite and infinite dimensions, are Ordinary Differential Equations (ODE) or Partial Differential Equations (PDE) with special form. The research on the numerical method of the differential equations started in the 18th century and produced abundant publications. However, we find that few of them discuss the numerical method specifically for Hamiltonian systems. This status is in sharp contrast with the importance of the Hamiltonian system. Therefore, it is appealing and worthy to investigate and develop numerical methods for this virgin field.

4. Technical Approach — Symplectic Geometry Method

The foundation for the Hamiltonian system is symplectic geometry, which is increasingly flourishing in both theory and practice. The history of symplectic geometry can be traced back to Astronomer Hamilton in the 19th century. In order to study the Newton mechanics, he introduced generalized coordinates and generalized momentums to represent the energy of the system, which is now called Hamiltonian function now. For a system with n degrees of freedom, the n generalized coordinates and momentums are spanned into a $2n$ phase space. Thus the Newton mechanics becomes the geometry in phase space. In terms of the modern concept, this is a kind of symplectic geometry. Later, Jacobi, Darboux, Poincaré, Cartan, and Weyl did a lot of research on this topic from different points of view (algebra and geometry). However, the major development of the modern symplectic geometry started with the discovery of KAM theorem (1950s to the beginning of 1960s). In the 1970s, in order to research Fourier integral operator, quantum representation of the geometry, group representation theory, classification of the critical points, Lie Algebra, etc., people did a lot of work on symplectic geometry (e.g., Arnold[Arn89], Guillemin[GS84], Weinstein[Wei77], Marsden[AM78], etc.), which promoted the development in these areas. In the 1980s, the research on total