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Oscillations over long times in numerical Hamiltonian systems

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1 Introduction

The numerical treatment of ordinary differential equations has continued to be a lively area of numerical analysis for more than a century, with interesting applications in various fields and rich theory. There are three main developments in the design of numerical techniques and in the analysis of the algorithms:

- *Non-stiff differential equations.* In the 19th century (Adams, Bashforth, and later Runge, Heun and Kutta), numerical integrators have been designed that are efficient (high order) and easy to apply (explicit) in practical situations.
- *Stiff differential equations.* In the middle of the 20th century one became aware that earlier developed methods are impractical for a certain class of differential equations (stiff problems) due to stability restrictions. New integrators (typically implicit) were needed as well as new theories for a better understanding of the algorithms.
- *Geometric numerical integration.* In long-time simulations of Hamiltonian systems (molecular dynamics, astronomy) neither classical explicit methods nor implicit integrators for stiff problems give satisfactory results. In the last few decades, special numerical methods have been designed that preserve the geometric structure of the exact flow and thus have an improved long-time behaviour.

The basic developments (algorithmic and theoretical) of these epochs are documented in the monographs [HNW93], [HW96], and [HLW06]. Within geometric numerical integration we can also distinguish between non-stiff and stiff situations. Since here the main emphasis is on conservative Hamiltonian systems, the term "stiff" has to be interpreted as "highly oscillatory".

The present survey is concerned with geometric numerical integration with emphasis on theoretical insight for the long-time behaviour of numerical solutions. There are several degrees of difficulty:

- *Non-stiff Hamiltonian systems — backward error analysis.* The main theoretical tool for a better understanding of the long-time behaviour of numerical methods for structured problems is backward error analysis (Sect. 2). Rigorous statements over exponentially long times have been obtained in [BG94, HL97, Rei99] for symplectic integrators. Unfortunately, the analysis is restricted to the non-stiff situation, and does not provide any information for problems with high oscillations.
- *Highly oscillatory problems — modulated Fourier expansion.* The main part of this survey treats Hamiltonian systems of the form

$$\ddot{q} + \Omega^2 q = -\nabla U(q), \tag{1.1}$$

  where Ω is a diagonal matrix with real entries between 0 and a large ω, and $U(q)$ is a smooth potential function. The additional difficulty is the presence of two time scales, and the crucial role of harmonic actions in the long-time analysis. Basic work for the analytic solution is in [BGG87]. Section 3 presents the technique of modulated Fourier expansions which permits to prove simultaneously the conservation of energy and actions for the analytic and the numerical solution (where the product of the time step size and ω is of size one or larger). This is developed in [HL01, CHL03] for one high frequency and in [CHL05] for several high frequencies.
- *Non-linear wave equations.* An extension to infinite dimension with arbitrarily large frequencies permits to treat the long-time behaviour of one-dimensional semi-linear wave equations. Long-time conservation of harmonic actions along the analytic solution is studied in [Bou96, Bam03]. The technique of modulated Fourier expansion yields new insight into the long-time behaviour of the analytic solution [CHL08b], of pseudo-spectral semi-discretizations [HL08], and of full discretizations [CHL08a]. This is discussed in Sect. 4.

In Sect. 5, an interesting analogy between highly oscillatory differential equations and linear multistep methods for non-stiff problems $\ddot{q} = -\nabla U(q)$ is established (see [HL04]). The inverse of the step size plays the role of ω, and the parasitic solutions of the multistep method correspond to high oscillations in the solution of (1.1). The near conservation of the harmonic actions thus yields the bounded-ness of the parasitic solutions over long times, and permits to prove that special linear multistep methods are suitable for the long-time integration of Hamiltonian systems (like those arising in the computation of planetary motion).

2 Backward error analysis

An important tool for a better understanding of the long-time behaviour of numerical methods for ordinary differential equations is backward error analysis. We present the main ideas, some important consequences, and also its limitations in the case of highly oscillatory problems.

2.1 General idea

The principle applies to general ordinary differential equations $\dot{y} = f(y)$ and to general (numerical) one-step methods $y_{n+1} = \Phi_h(y_n)$, such as Runge–Kutta, Taylor series, composition and splitting methods. It consists in searching for a modified differential equation

$$\dot{z} = f_h(z) = f(z) + hf_2(z) + h^2 f_3(z) + \cdots, \qquad z(0) = y_0, \tag{2.1}$$

where the vector field is written as a formal series in powers of the step size h, such that the numerical solution for the original problem is equal (in the sense of formal power series) to the exact solution of the modified differential equation (see Fig. 1).

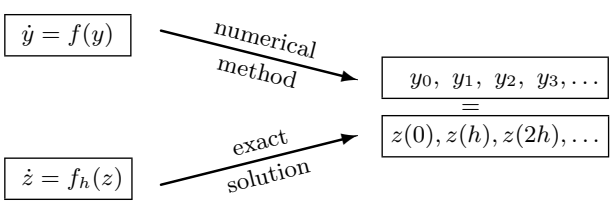

Fig. 1. Idea of backward error analysis

To obtain the coefficient functions $f_j(y)$, we note that we have the relation $z(t+h) = \Phi_h\big(z(t)\big)$ for the (formal) solution of (2.1). Expanding

both sides of this relation into a power series of h and comparing equal powers of h, permits us to compute the functions $f_j(y)$ in a recursive manner.

The importance of backward error analysis resides in the fact that for differential equations with certain structures (Hamiltonian, reversible, divergence-free, etc.) solved with suitable geometric integrators (symplectic, symmetric, volume-preserving, etc.), the modified differential equation has the same structure as the original problem. The study of the modified differential equation then gives insight into the numerical solution. The rest of this section is devoted to make these statements more precise for the important special case of the Störmer–Verlet (leapfrog) discretisation.

2.2 Störmer–Verlet discretisation

For ease of presentation we restrict our considerations to the special Hamiltonian system

$$\ddot q = f(q) \quad \text{with} \quad f(y) = -\nabla U(q), \tag{2.2}$$

where $U(q)$ is a smooth potential function. Its most obvious discretisation (augmented with an approximation to the velocity $p = \dot q$) is

$$\begin{aligned} q^{n+1} - 2q^n + q^{n-1} &= h^2 f(q^n) \\ q^{n+1} - q^{n-1} &= 2h\, p^n . \end{aligned} \tag{2.3}$$

Due to pioneering work on higher order variants by Störmer, and due to its importance in molecular dynamics simulations recognised by Verlet, it is often called Störmer–Verlet method. In the literature on partial differential equations it is known as the leapfrog discretisation.

Introducing $p^{n+1/2} := (q^{n+1} - q^n)/h$ as an intermediate slope, this method can be written as

$$\begin{aligned} p^{n+1/2} &= p^n + \frac{h}{2} f(q^n) \\ q^{n+1} &= q^n + h\, p^{n+1/2} \\ p^{n+1} &= p^{n+1/2} + \frac{h}{2} f(q^{n+1}) \end{aligned} \tag{2.4}$$

which is clearly recognised as a symmetric one-step method for (2.2). It is a geometric integrator par excellence: the numerical flow $(q^n, p^n) \mapsto (q^{n+1}, p^{n+1})$ is symplectic when $f(q) = -\nabla U(q)$, it is volume preserving in the phase space, and it is time reversible (see [HLW03]). It is also

the basic scheme for various extensions to higher order methods: composition and splitting methods, partitioned Runge–Kutta methods, and symmetric multistep methods.

2.3 Formal backward error analysis

We search for a modified differential equation such that its solution $\big(q(t), p(t)\big)$, which should not be confused with the solution of (2.2), formally interpolates the numerical solution of (2.3), i.e.,

$$\begin{aligned} q(t+h) - 2q(t) + q(t-h) &= h^2 f\big(q(t)\big) \\ q(t+h) - q(t-h) &= 2h\, p(t). \end{aligned} \tag{2.5}$$

Expanding the left hand sides into Taylor series around $h = 0$, eliminating higher derivatives by successive differentiation, and expressing the resulting differential equations in terms of q and p, yields

$$\begin{aligned} \dot p &= f(q) + \tfrac{h^2}{12}\Big(f''(q)(p,p) + f'(q)f(q)\Big) - \tfrac{h^4}{720}\Big(f''''(q)\big(p,p,p,p\big) \\ &\quad + 6\, f'''(q)\big(f(q),p,p\big) + 24\, f''(q)\big(f'(q)p,p\big) + 3\, f''(q)\big(f(q),f(q)\big) \\ &\quad + 6\, f'(q)f''(q)(p,p) + 6\, f'(q)f'(q)f(q)\Big) + \mathcal{O}(h^6) \\ \dot q &= p - \tfrac{h^2}{6}\, f'(q)p + \tfrac{h^4}{180}\Big(f'''(q)\big(p,p,p\big) + 3\, f''(q)\big(f(q),p\big) \\ &\quad + 6\, f'(q)f'(q)p\Big) + \mathcal{O}(h^6). \end{aligned} \tag{2.6}$$

Due to the symmetry of the method, the modified differential equation becomes a series in even powers of h.

For the case of a Hamiltonian system (2.2), i.e., $f(q) = -\nabla U(q)$, the modified differential equation (2.6) is also Hamiltonian

$$\dot p = -\nabla_q H_h(p,q), \qquad \dot q = \nabla_p H_h(p,q)$$

with modified Hamiltonian

$$\begin{aligned} H_h(p,q) &= \tfrac12\|p\|^2 + U(q) + \tfrac{h^2}{24}\Big(2\,U''(q)\big(p,p\big) - \|U'(q)\|^2\Big) \\ &\quad - \tfrac{h^4}{720}\Big(U^{(4)}(q)\big(p,p,p,p\big) - 6\,U'''(q)\big(U'(q),p,p\big) \\ &\qquad + 3\,U''(q)\big(U'(q),U'(q)\big) - 12\,\|U''(q)p\|^2\Big) + \mathcal{O}(h^6). \end{aligned} \tag{2.7}$$

An important consequence of this observation is the following: since the numerical solution of the Störmer–Verlet discretisation is (at least

formally) equal to the exact solution of the modified differential equation, we have that $H_h(p^n, q^n) = \text{const}$. As long as the numerical solution stays in a compact set, this implies that the energy $H(p,q) = \frac{1}{2}\|p\|^2 + U(q)$ remains close to a constant, i.e., $H(p^n, q^n) = \text{const} + \mathcal{O}(h^2)$ without any drift.

The next section shows how this statement can be made rigorous.

2.4 Rigorous backward error analysis

For a rigorous analysis, the modified differential equation constructed in the previous sections has to be truncated suitably:

$$\dot{z} = f_{h,N}(z) = f(z) + hf_2(z) + \cdots + h^{N-1} f_N(z), \qquad z(0) = y_0. \quad (2.8)$$

Obviously, equality does not hold any more in Fig. 1 and an error of size $\mathcal{O}(h^{N+1})$ is introduced. More precisely, if $y_{n+1} = \Phi_h(y_n)$ denotes the one-step method, and $\varphi_{N,t}(y)$ the flow of the truncated differential equation (2.8), we have $\|\Phi_h(y_0) - \varphi_{N,h}(y_0\| \le C_N h^{N+1}$ for arbitrary N. The freedom of choosing the truncation index N can be used to minimise this estimate. For analytic $f(y)$ and for standard numerical integrators (such as partitioned Runge–Kutta methods including the Störmer–Verlet discretisation), the choice $N \sim h^{-1}$ yields an estimate

$$\|\Phi_h(y_0) - \varphi_{N,h}(y_0\| \le h\gamma M\, \mathrm{e}^{-\alpha/\omega h}, \quad (2.9)$$

where α and γ are constants that only depend on the numerical method, M is an upper bound of $f(y)$ on a disc of radius $2R$ around the initial value y_0, and $\omega = M/R$ is related to a Lipschitz constant of $f(y)$. A detailed proof can be found in [HLW06, Chap. IX].

Notice that (2.9) yields an estimate for one step only (local error). To get estimates for the global error and information on the long-time behaviour, knowledge on the propagation of perturbations is needed.

- *Conservation of energy.* In the case of a symplectic method applied to a Hamiltonian system, the modified equation is Hamiltonian (see Section 2.3). The truncated modified Hamiltonian $H_{N,h}(p,q)$ is exactly conserved along the solution of (2.8). Therefore, local deviations in $H_{N,h}(p^n, q^n)$ are just summed up, and one obtains from (2.9) that this modified Hamiltonian is conserved along the numerical solution up to exponentially small errors $\mathcal{O}(\mathrm{e}^{-\gamma/2\omega h})$ on exponentially long time intervals $0 \le t \le \mathcal{O}(\mathrm{e}^{\gamma/2\omega h})$. This implies the absence of any drift in the numerical Hamiltonian $H(p^n, q^n)$.

- *Integrable Hamiltonian systems.* Symplectic integrators applied to a nearly integrable Hamiltonian system give raise to a modified equation that is a perturbed Hamiltonian system. The celebrated KAM theory can be used get insight into the long-time behaviour of numerical integrators, e.g., linear growth of the global error.
- *Chaotic systems.* In the presence of positive Lyapunov exponents, the numerical solution remains close to the exact solution of the truncated modified equation only on time intervals of length $\mathcal{O}(h^{-1})$. Energy is well conserved by symplectic integrators also in this situation.

2.5 Limitation in the presence of high oscillations

The estimate (2.9) does not give any useful information if the product ωh is of size one or larger. Recall that ω is a kind of Lipschitz constant of the vector field $f(y)$ which, in the case of a stable Hamiltonian system, can be interpreted as the highest frequency in the solution. This means that for highly oscillatory differential equations the step size is restricted to unrealistic small values.

From the example of the harmonic oscillator $H(p,q) = \frac{1}{2}(p^2 + \omega^2 q^2)$ it can be seen that the estimate (2.9) cannot qualitatively be improved. In fact, for all reasonable integrators, the scaled numerical solution $(\omega q^n, p^n)$ depends on the step size h only via the product ωh.

The aim of the next section is to present a theory that permits to analyse the long-time behaviour of numerical time integrators in the presence of high oscillations.

3 Modulated Fourier expansion

In this section we consider Hamiltonian systems

$$\ddot{q} + \Omega^2 q = g(q), \qquad g(q) = -\nabla U(q), \tag{3.1}$$

where, for ease of presentation, Ω is a diagonal matrix and $U(q)$ is a smooth potential function. Typically, Ω will contain diagonal entries ω with large modulus. We are interested in the long-time behaviour of numerical solutions when ω times the step size h is not small, so that classical backward error analysis cannot be applied.

3.1 Modulated Fourier expansion of the analytic solution

We start with the situation, where Ω contains only diagonal entries which are either 0 or ω, and we split the components of q accordingly, i.e., $q = (q_0, q_1)$ and $\Omega = \operatorname{diag}(0, \omega I)$. Both, q_0 and q_1 are allowed to be vectors. There are two time scales in the solution of equation (3.1):

- fast time ωt in oscillations of the form $\mathrm{e}^{\mathrm{i}\omega t}$;
- slow time t due to the zero eigenvalue and the non-linearity.

In the absence of the non-linearity $g(q)$, the solution of (3.1) is a linear combination of 1, t, and $\mathrm{e}^{\pm \mathrm{i}\omega t}$. For the general case we make the ansatz

$$q(t) = \sum_{k \in \mathbb{Z}} z^k(t)\, \mathrm{e}^{\mathrm{i}k\omega t}, \tag{3.2}$$

where $z^k(t)$ are smooth functions with derivatives bounded uniformly in ω. The function $z^0(t)$ is real-valued, and $z^{-k}(t)$ is the complex conjugate of $z^k(t)$. Inserting (3.2) into the differential equation (3.1), expanding the non-linearity into a Taylor series around z^0, and comparing coefficients of $\mathrm{e}^{\mathrm{i}k\omega t}$ yields

$$\begin{pmatrix} \ddot z_0^k + 2\mathrm{i}k\omega \dot z_0^k - k^2\omega^2 z_0^k \\ \ddot z_1^k + 2\mathrm{i}k\omega \dot z_1^k + (1-k^2)\,\omega^2 z_1^k \end{pmatrix} = \sum_{m \ge 0} \frac{1}{m!} \sum_{s(\alpha)=k} g^{(m)}(z^0)\, z^\alpha, \tag{3.3}$$

where $\alpha = (\alpha_1, \dots, \alpha_m)$ is a multi-index, $s(\alpha) = \sum_{j=1}^m \alpha_j$, and $g^{(m)}(z^0)\, z^\alpha = g^{(m)}(z^0)\big(z^{\alpha_1}, \dots, z^{\alpha_m}\big)$. The second sum is over multi-indices $\alpha = (\alpha_1, \dots, \alpha_m)$ with $\alpha_j \neq 0$.

To obtain smooth functions $z_j^k(t)$ with derivatives bounded uniformly for large ω, we separate the dominating term in the left-hand side of (3.3), and eliminate higher derivatives by iteration. This gives a second order differential equation for z_0^0, first order differential equations for z_1^1 and z_1^{-1}, and algebraic relations for all other variables. Under the "bounded energy" assumption on the initial values

$$\|\dot q(0)\|^2 + \|\Omega\, q(0)\|^2 \le E, \tag{3.4}$$

it is possible to prove that the coefficient functions are bounded (on intervals of size one) as follows: $z_0^0(t) = \mathcal{O}(1)$, $z_1^{\pm 1}(t) = \mathcal{O}(\omega^{-1})$, $\dot z_1^{\pm 1}(t) = \mathcal{O}(\omega^{-2})$, and $z_j^k(t) = \mathcal{O}(\omega^{-|k|-2})$ for the remaining indices (j,k), see [HLW06, Sect. XIII.5].

The time average of the potential $U(q)$ along the analytic solution (3.2) only depends on the smooth coefficient functions $z^k(t)$ and is (formally)

given by (with $\mathbf{z} = (\dots, z^{-1}, z^0, z^1, z^2, \dots)$)

$$\mathcal{U}(\mathbf{z}) = U(z^0) + \sum_{m\geq 1} \frac{1}{m!} \sum_{s(\alpha)=0} U^{(m)}(z^0) z^\alpha. \tag{3.5}$$

It is an interesting fact and crucial for the success of the expansion (3.2) that the functions $y^k(t) = z^k(t)\,\mathrm{e}^{\mathrm{i}k\omega t}$ are solution of the infinite dimensional Hamiltonian system

$$\ddot{y}^k + \Omega^2 y^k = -\nabla_{-k}\,\mathcal{U}(\mathbf{y}), \tag{3.6}$$

where ∇_{-k} indicates the derivative with respect to the component "$-k$" of the argument $\mathbf{y}$. Its Hamiltonian

$$\mathcal{H}(\mathbf{y}, \dot{\mathbf{y}}) = \frac{1}{2} \sum_{k\in\mathbb{Z}} \Big((\dot{y}^{-k})^T \dot{y}^k + (y^{-k})^T \Omega^2 y^k \Big) + \mathcal{U}(\mathbf{y}) \tag{3.7}$$

is therefore a conserved quantity of the system (3.6), and hence also of (3.3). Since $q_0(t) = z_0^0(t) + \mathcal{O}(\omega^{-3})$, $\dot{q}_0(t) = \dot{z}_0^0(t) + \mathcal{O}(\omega^{-2})$, $q_1(t) = z_1^1(t)\,\mathrm{e}^{\mathrm{i}\omega t} + z_1^{-1}(t)\,\mathrm{e}^{-\mathrm{i}\omega t} + \mathcal{O}(\omega^{-2}) = y_1^1(t) + y_1^{-1}(t) + \mathcal{O}(\omega^{-2})$ and $\dot{q}_1(t) = \mathrm{i}\omega\big(y_1^1(t) - y_1^{-1}(t)\big) + \mathcal{O}(\omega^{-2})$ by the estimates for z_j^k, the quantity (3.7) is $\mathcal{O}(\omega^{-1})$ close to the total energy of the system

$$H\big(q(t), \dot{q}(t)\big) = \frac{1}{2}\big(\|\dot{q}(t)\|^2 + \|\Omega q(t)\|^2\big) + U\big(q(t)\big). \tag{3.8}$$

The averaged potential $\mathcal{U}(\mathbf{y})$ is invariant under the one-parameter group of transformations $y^k \to \mathrm{e}^{\mathrm{i}k\tau} y^k$. Therefore, Noether's theorem yields the additional conserved quantity

$$\mathcal{I}(\mathbf{y}, \dot{\mathbf{y}}) = -\mathrm{i}\omega \sum_{k\in\mathbb{Z}} k\,(y^{-k})^T \dot{y}^k \tag{3.9}$$

for the system (3.6). It is $\mathcal{O}(\omega^{-1})$ close to the harmonic energy

$$I\big(q(t), \dot{q}(t)\big) = \frac{1}{2}\big(\|\dot{q}_1(t)\|^2 + \omega^2 \|q_1(t)\|^2\big) \tag{3.10}$$

of the highly oscillatory part of the system.

The analysis of this section can be made rigorous by truncating the arising series and by patching together estimates on short intervals to get information on intervals of length ω^{-N} (with arbitrary N). In this way one can prove that the harmonic energy (3.10) remains constant up to oscillations of size $\mathcal{O}(\omega^{-1})$ on intervals of length ω^{-N}, a result first obtained by [BGG87].

3.2 Exponential integrators

Since $q^{n+1} - 2\cos(h\Omega)\, q^n + q^{n-1} = 0$ is an exact discretisation of the equation $\ddot{q} + \Omega^2 q = 0$, it is natural to consider the numerical scheme

$$q^{n+1} - 2\cos(h\Omega)\, q^n + q^{n-1} = h^2 \Psi g(\Phi q^n) \tag{3.11}$$

as discretisation of (3.1). Here, $\Psi = \psi(h\Omega)$ and $\Phi = \phi(h\Omega)$, where the filter functions $\psi(\xi)$ and $\phi(\xi)$ are even, real-valued functions satisfying $\psi(0) = \phi(0) = 1$. Special cases are the following:

(A)	$\psi(h\Omega) = \operatorname{sinc}^2(\frac{1}{2}h\Omega)$	$\phi(h\Omega) = 1$	[Gau61]
(B)	$\psi(h\Omega) = \operatorname{sinc}(h\Omega)$	$\phi(h\Omega) = 1$	[Deu79]
(C)	$\psi(h\Omega) = \operatorname{sinc}^2(h\Omega)$	$\phi(h\Omega) = \operatorname{sinc}(h\Omega)$	[GASS99]

where $\operatorname{sinc}(\xi) = \sin\xi/\xi$. It is also natural to complete formula (3.11) with a derivative approximation p^n given by

$$q^{n+1} - q^{n-1} = 2h \operatorname{sinc}(h\Omega)\, p^n, \tag{3.12}$$

because, for $q(t) = \exp(\mathrm{i}\Omega t)\, q^0$, the derivative $p(t) = \dot{q}(t)$ satisfies this relation without error.

Written as a one-step method, we obtain

$$\begin{aligned} \widetilde{p}^n &= p^n + \frac{h}{2}\Psi_1 g(\Phi q^n) \\ q^{n+1} &= \cos(h\Omega)\, q^n + \Omega^{-1}\sin(h\Omega)\, \widetilde{p}^n \\ p^{n+1} &= \Omega\sin(h\Omega)\, q^n + \cos(h\Omega)\, \widetilde{p}^n + \frac{h}{2}\Psi_1 g(\Phi q^{n+1}), \end{aligned} \tag{3.13}$$

where $\Psi_1 = \psi_1(h\Omega)$ with $\psi_1(\xi) = \psi(\xi)/\operatorname{sinc}(\xi)$. Notice that, for $\Omega \to 0$, this integrator reduces to the Störmer–Verlet discretisation (2.4).

3.3 Modulated Fourier expansion of numerical solution

We are interested in the long-time behaviour of numerical approximations to the highly oscillatory Hamiltonian system (3.1). Our focus will be on the near conservation of the total energy (3.8) and of the harmonic energy (3.10) over long times.

In complete analogy to what we did in Sect. 3.1 for the analytic solution, we separate the fast and slow modes by the ansatz

$$q^n = \widetilde{q}(t_n) \qquad \text{with} \qquad \widetilde{q}(t) = \sum_{k\in\mathbb{Z}} z^k(t)\, \mathrm{e}^{\mathrm{i}k\omega t}, \tag{3.14}$$

where $t_n = nh$, and the coefficient functions are again assumed to be smooth with derivatives bounded uniformly in ω. Inserting this ansatz