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MOLLIFIED IMPULSE METHODS FOR HIGHLY OSCILLATORY DIFFERENTIAL EQUATIONS*

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Abstract. We introduce a family of impulselike methods for the integration of highly oscillatory second-order differential equations whose forces can be split into a fast part and a slow part. Methods of this family are specified by two weight functions ϕ, ψ; one is used to average positions and the other to mollify the force. When the fast forces are conservative and $\phi = \psi$, the methods here coincide with the mollified impulse methods introduced by García-Archilla, Sanz-Serna, and Skeel. On the other hand, the methods here extend to nonlinear situations a well-known class of exponential integrators introduced by Hairer and Lubich for cases of linear fast forces. A convergence analysis is presented that provides insight into the role played by the processes of mollification and averaging in avoiding order reduction. A simple condition on the weight functions is shown to be both necessary and sufficient to avoid order reduction.

Key words. impulse methods, highly oscillatory problem, Fourier analysis

AMS subject classifications. 65L20, 65M12, 70F10, 70H05

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1. Introduction.

We consider numerical methods for the integration of multiple-time-scale problems of the form

$$M\frac{d^2}{dt^2}q = f(q) + g(q), \tag{1}$$

where M is a symmetric positive-definite mass matrix and the forces are split into a *soft* or *slow* part g that does not contribute any fast modes to the solution and a *strong* or *fast* part f such that the *reduced* problem

$$M\frac{d^2}{dt^2}q = f(q)$$

possesses highly oscillatory modes (and possibly slow modes as well). These problems arise in many situations including molecular dynamics, astronomy, and the time integration of partial differential equations describing wave phenomena. The fast/slow splitting is of interest in situations where the computational cost of integrating the reduced system is much smaller than that of integrating the full system. For instance, in an N-body problem, the evaluation of the fast force is cheaper than that of the slow force if the former is composed only of next-neighbor interactions and the latter includes interactions between all particles. A second example is provided by cases where the reduced problem can be solved analytically with a cost that is independent (or almost independent) of the step length. In such situations the aim is to sample the slow forces as sparingly as possible and, certainly, at a rate that is not determined by the periods of the fast motions, i.e., by the stiffness of the reduced problem.

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The impulse method was devised to cater to these situations. The time stepping of the impulse method intersperses evaluations of the slow forces at intervals of length h with integrations of the reduced system that are taken to be exact, either because an analytic integration is feasible or because, in a multiple time-step approach [7], [8], [17], a numerical integration is performed with a time step much smaller than h. Unfortunately, the impulse method, which is formally of second-order accuracy, leads only to errors that behave $O(h^2)$ if h is small as compared with the smallest period of the reduced system. An alternative family of methods, the mollified impulse methods, was introduced in [5]; there is one mollified impulse method for each choice of a so-called weight function. Proved in [5] is the fact that, for several choices of weight functions, the mollified impulse method yields errors in q that behave as $O(h^2)$, where the implied constant is independent of the size of the fast forces and depends only on the energy of the solution and on bounds for g and its derivatives. It is then possible to apply the mollified impulse methods with a given time step h to faster and faster problems without impairing the accuracy. This is feasible because, for a given oscillation amplitude, the energy grows with the frequency; therefore, in solutions of limited energy, fast oscillations are present with small amplitudes and need not be accurately resolved. In conclusion, for problems with fast oscillations, the scenario here is then similar to that found in the development of stiff solvers [3], [12] for problems with fast rates of decay: Good stiff solvers perform satisfactorily with step lengths independent of the stiffness of the problem and determined only by the smoothness of the solution, and this is possible because they need not accurately resolve fast components. As in the (nonoscillatory) stiff situation [3], [12], methods for highly oscillatory problems have a conventional order that is brought out in simulations where the step length h is small when compared to the stiffness of the problem and a *stiff order* that manifests itself in the cases where h is not small. In general the stiff order is smaller than the conventional order, and one speaks of an *order reduction*.

In this paper we reconsider the ideas behind the mollified impulse method. In section 2 we introduce a large family of methods, the (ϕ, ψ)-methods, which extends in two ways the family in [5]. In the first place, (ϕ, ψ)-methods are specified by *two* independent weight functions: one, ψ, that defines the so-called mollification and one, ϕ, that is employed in an averaging. On the other hand, our description here of the mollification process depends on the Alekseev–Groebner formula [11] and applies to cases where the fast forces are nonconservative. This should be compared with the methods in [5] that depend on one weight function and apply only to conservative fast forces (Hamiltonian reduced problems). In section 3, it is shown that, if ϕ and ψ are taken to coincide and the reduced problem is Hamiltonian, the family of methods considered here coincides with the mollified methods of [5].

When the fast forces are linear, the reduced problem may in principle be integrated analytically, and we show in section 4 that the (ϕ, ψ)-method can be implemented in terms of two *filters* defined in terms of the Fourier transforms of the weights ϕ and ψ. In this case of linear fast forces, the family of (ϕ, ψ)-methods essentially mimics a by now well known family of exponential integrators first described by Hairer and Lubich [9] (see also, among others, [2] and Chapter XIII in the monograph [10]; an error analysis has been provided in [6]). The relation between weights and filters is explored in further detail in section 7, where filters are characterized via a classical Fourier analysis result of Paley and Wiener.

Sections 5 and 6 contain an analysis of the accuracy of (ϕ, ψ)-methods as applied to problems with linear fast forces. The approach here resembles in a way that in [5], because it is based on the weight functions rather than on the corresponding filters.

The analysis here is then completely different from those in the convergence proofs presented in [6] and (for a particular model problem with only one fast frequency) in Chapter XIII of [10]; both proofs are carried out in terms of the filters. We show how a study in terms of weights makes it possible to identify in a natural way simple conditions on the methods that are both necessary and sufficient to ensure that no order reduction takes place. Essentially, no order reduction is equivalent to the requirement that the translation of the weight function are a basis set for a consistent interpolation scheme. On the other hand, our analysis differs from that in [5] in a number of points that we believe to be of some importance. We cater here to weight functions of arbitrary bounded support; in [5] the support had to be contained in $[-1, 1]$. Our analysis applies to cases where the mollification filter ψ is different from the averaging filter ϕ; this not only means that more methods are covered but also tells apart the effects of the averaging from those of the mollifier. We finally mention that section XIV.2.4 of [10] presents an analysis for the long-average mollified impulse method that covers fast forces more general than those considered by us.

Extensive numerical experiments based on the new methods will be provided in a forthcoming paper.

2. Description of the methods. For numerical work, we rewrite the system (1) in the first-order format

$$\frac{d}{dt}p = f(q) + g(q), \qquad \frac{d}{dt}q = M^{-1}p, \tag{2}$$

with the reduced version

$$\frac{d}{dt}p = f(q), \qquad \frac{d}{dt}q = M^{-1}p. \tag{3}$$

If we denote by P_n and Q_n the numerical approximations to the true solution values of the momenta $p_n = p(t_n)$ and coordinates $q_n = q(t_n)$, respectively, at the step point $t_n = nh$, a step $n \to n + 1$ of any of the methods considered in this paper may be fit into the following composition or split-step pattern.

Kick. Compute an approximation $\bar{G}_n$ to the value of the slow force $g(q_n)$, and then set $P_n^+ = P_n + \frac{h}{2}\bar{G}_n$.

Oscillation. Use the h-flow of the reduced problem (3) to advance from (P_n^+, Q_n) to (P_{n+1}^-, Q_{n+1}). In other words, (P_{n+1}^-, Q_{n+1}) is obtained by integrating, over a time interval of length h, the system (3) with initial conditions (P_n^+, Q_n).

Kick. Set $P_{n+1} = P_{n+1}^- + \frac{h}{2}\bar{G}_{n+1}$.

Of course, the force $\bar{G}_{n+1}$ at the second kick of the current step coincides with the force at the first kick of the next step, so that the methods essentially consist of a sequence of oscillations $(P_n^+, Q_n) \to (P_{n+1}^-, Q_{n+1})$ followed by kicks $P_{n+1}^- = P_{n+1}^+ + h\bar{G}_{n+1}$; it is not necessary to compute the vector P_{n+1} unless output at t_{n+1} is required.

Different methods within the class considered here differ in the way in which the forces $\bar{G}_n$ are computed. The simplest and earliest choice, that of the original impulse method, is given by $\bar{G}_n = g(Q_n)$ and, unfortunately, suffers from an order reduction in p from 2 to 0 and in q from 2 to 1 in the stiff oscillatory situations considered here [5]. An improvement that may ensure (stiff) order 1 in p and (stiff) order 2 in q was presented in [5]. The family of mollified impulse methods introduced there have

$$\bar{G}_n = \mathcal{M}(Q_n, h)g(\mathcal{A}(Q_n, h)), \tag{4}$$

where, given Q_n and h, $\mathcal{A}(Q_n, h)$ represents an average of values of q and $\mathcal{M}$ is a so-called mollifier matrix. The use of $\mathcal{A}$ avoids [5] the dangers associated with sampling at grid points a quickly varying $g(q(t))$, and the role of $\mathcal{M}$ is to mimic the way in which extra external forces contribute to build up the momentum in highly oscillatory problems (see the analysis and counterexamples in sections 5 and 6 below).

As discussed in [5], there is much freedom within the class of mollified impulse methods, both in how $\mathcal{M}$ and $\mathcal{A}$ may be mathematically specified and in the analytic or numerical technique employed to actually compute them. Here we add to this freedom by further enlarging the class of possible choices in (4).

Before we proceed, we need some notation. We denote by $\mathcal{P}(p, q, t)$, $\mathcal{Q}(p, q, t)$ the flow of the reduced system (3), so that $p(t) = \mathcal{P}(p_0, q_0, t)$, $q(t) = \mathcal{Q}(p_0, q_0, t)$ is the value at time t of the solution of (3) with initial conditions $p(0) = p_0$, $q(0) = q_0$. Thus $P_{n+1}^- = \mathcal{P}(P_n^+, Q_n, h)$, and $Q_{n+1} = \mathcal{Q}(P_n^+, Q_n, h)$. For compactness, it is useful to combine P_n and Q_n into a single vector $Y_n = (P_n, Q_n)$ and similarly write $y(t) = (p(t), q(t))$, $\mathcal{Y} = (\mathcal{P}, \mathcal{Q})$, etc. If d represents the number of degrees of freedom in the problem, we will also use the $(2d) \times (2d)$ Jacobian matrix $\mathcal{Y}'(\alpha, t)$ of $\mathcal{Y}(\alpha, t)$ with respect to its argument α, which can be found by integrating the variational equation

$$\frac{\partial}{\partial t}\mathcal{Y}'(\alpha, t) = \begin{bmatrix} 0 & f'(\mathcal{Q}(\alpha, t)) \\ M^{-1} & 0 \end{bmatrix} \mathcal{Y}'(\alpha, t), \tag{5}$$

with initial condition $\mathcal{Y}'(\alpha, 0) = I_{2d}$. It is clear that $\mathcal{Y}'$ possesses a natural block structure corresponding to the partition of y:

$$\mathcal{Y}' = \begin{bmatrix} \mathcal{P}_p & \mathcal{P}_q \\ \mathcal{Q}_p & \mathcal{Q}_q \end{bmatrix}.$$

Each of the methods considered here is defined by two *weight* functions. For the purpose of this paper, a weight function is a bounded, integrable real-valued function $\chi(t)$ that is assumed to be even $\chi(-t) \equiv \chi(t)$ and to satisfy

$$\int_{-\infty}^{\infty} \chi(s) ds = 1. \tag{6}$$

(Note that we do not require $\chi \geq 0$.)

We may now describe the new methods. As in [5], to construct $\mathcal{A}$, we start by choosing a weight function ϕ and then define

$$\mathcal{A}(Q_n, h) = \frac{1}{h} \int_{-\infty}^{\infty} q^*(t) \phi\left(\frac{t}{h}\right) dt = \int_{-\infty}^{\infty} q^*(hs) \phi(s)\, ds, \tag{7}$$

where $q^*(t)$ is obtained by solving the reduced problem (3) with initial conditions $q = Q_n$, $p = 0$, i.e., $q^*(t) = \mathcal{Q}(0, Q_n, t)$. Since q^* is an even function of t, the integrals in (7) are in practice replaced by twice their value over $(0, \infty)$.

To define the mollifier, we choose a second weight function ψ, and, at each time step, we find a matrix-valued function Y' of the independent variable t

$$Y'(t) = \begin{bmatrix} P_p(t) & P_q(t) \\ Q_p(t) & Q_q(t) \end{bmatrix}$$

by integrating the variational problem ($q^*(t)$ is as above)

$$\frac{d}{dt}Y' = \begin{bmatrix} 0 & f'(q^*(t)) \\ M^{-1} & 0 \end{bmatrix} Y', \tag{8}$$

with initial condition $Y'(0) = I_{2d}$, and then set

$$\mathcal{M}(Q_n, h) = \frac{1}{h}\int_{-\infty}^{\infty} R(t)\psi\left(\frac{t}{h}\right)\,dt = \int_{-\infty}^{\infty} R(hs)\psi(s)\,ds, \tag{9}$$

where $R(t)$ is the upper left $d \times d$ block of the inverse matrix $Y'(t)^{-1}$, i.e.,

$$R(t) = [I_d, 0_d]Y'(t)^{-1}[I_d, 0_d]^T.$$

Note that q^*, Y', R depend on Q_n, but this dependence is not reflected in the notation, and that again, in practice, the required integrals may be replaced by twice their value over $(0, \infty)$. (Reversing the sign of t in (8) shows that the $(1,1)$ and $(2,2)$ diagonal blocks of $Y'(t)$ are even functions of t, while the off-diagonal blocks are odd functions of t. The inverse $Y'(t)^{-1}$ inherits this odd/even structure, and therefore $R(t)$ is even.)

To sum up, for any pair of weight functions ϕ and ψ, we have introduced a numerical scheme, to be referred to as the (ϕ, ψ)-*method*, that uses the kick/oscillation/kick structure with kicking forces $\bar{G}_n$ given by (4) and $\mathcal{A}$ and $\mathcal{M}$ defined in (7) and (9). We will stretch somehow the notation and understand that (δ, ψ), with δ the standard Dirac function, refers to a method with mollification but no averaging; (ϕ, δ) refers to a method with averaging but no mollification, and (δ, δ) is the original impulse method. All methods are symmetric or time-reversible [16], [10] and therefore convergent of the second order (in nonstiff situations). Furthermore, since individual kicks and oscillations preserve volume in phase space, all methods are volume-preserving.

The methods require at each step two integrations of the reduced problem: one to carry out the oscillation $(P_n^+, Q_n) \to (P_{n+1}^-, Q_{n+1})$ and one to compute the auxiliary $q^*(t)$ that features in (7) and (9). Furthermore the latter is to be carried out in tandem with the integration of the variational problem (8); see [5]. In some applications (see section 4 below) these integrations may be performed analytically, and in other cases one has to resort to a numerical technique with a small time step. If numerical integration is used, the weight functions ϕ and ψ have to possess bounded support so that the auxiliary problems are integrated only over a bounded time interval. The integrals in (7) and (9) can be computed along the integrations for q^* and Y' if one appends extra unknown functions b, c that evolve in time according to $db/dt = \phi(t/h)q^*(t)$ and $dc/dt = \psi(t/h)R(t)$; cf. [5].

We end this section by presenting the motivation for the definition of the mollifier. The original impulse method can be expressed [18] in terms of the Dirac delta function as an exact integration of the approximation

$$\frac{d^2}{dt^2}q = f(q) + \sum_n \delta\left(\frac{t - t_n}{h}\right) g(Q_n),$$

and the idea behind the mollification is to employ less abrupt versions [5]

$$\frac{d^2}{dt^2}q = f(q) + \sum_n \psi\left(\frac{t - t_n}{h}\right) G_n^*, \tag{10}$$

where G_n^* is the force $g(\mathcal{A}(Q_n, h))$ to be mollified.

In order to incorporate the forces $\psi((t-t_n)/h)G_n^*$ into the solution of the reduced problem, we use here the Alekseev–Groebner (AG)/nonlinear variation of constants formula [11] as distinct from the approach used in section 5 of [5], which is limited

to the case where the reduced system is Hamiltonian. According to the AG formula, solutions of (2) can be expressed in terms of the reduced flow $\mathcal{Y}$ as

$$y(t_b) = \mathcal{Y}(y(t_a), t_b - t_a) + \int_{t_a}^{t_b} \mathcal{Y}'(y(s), t_b - s) \begin{bmatrix} g(y(s)) \\ 0 \end{bmatrix} ds.$$

Assume then that, at the step $n-1 \to n$, we have performed the corresponding oscillation and we wish to additionally incorporate the effect of $\psi((t-t_n)/h)G_n^*$, acting while $t \le t_n$. (The effect of the force acting in the interval $t \ge t_n$ is incorporated at the first kick of the next step in a symmetric way.) We set $t_b = t_n$ and let $t_a \downarrow -\infty$, to conclude that

$$\left(\int_{-\infty}^{t_n} \mathcal{Y}'(y(s), t_n - s) \psi \left(\frac{s - t_n}{h} \right) ds \right) \begin{bmatrix} G_n^* \\ 0 \end{bmatrix} \tag{11}$$

is the change in solution caused by the extra force. Therefore, the extra momentum is

$$\left(\int_{-\infty}^{t_n} \mathcal{P}_p(y(s), t_n - s) \psi \left(\frac{s - t_n}{h} \right) ds \right) G_n^*,$$

and we would like to add this expression to P_n^- to obtain P_n. There are two difficulties to be tackled. The first stems from the fact that (11) contains the solution $y(t)$ being sought; it is readily circumvented by using an approximation to $y(t)$. The second is that present in (11) is a *family* of Jacobian matrices, one for each vector $y(s)$, so that, in principle, we may fear that, for each s, in order to find $\mathcal{Y}'(y(s), t_n - s)$ we would have to solve a different initial value problem for (5). However, differentiation of the identity $\mathcal{Y}(\mathcal{Y}(\alpha, t), -t) \equiv \alpha$ (group property of the flow) yields for the corresponding Jacobian matrices the well-known relation

$$\mathcal{Y}'(\mathcal{Y}(\alpha, t), -t) = \mathcal{Y}'(\alpha, t)^{-1}. \tag{12}$$

We then approximate the unknown $y(s)$ by $\mathcal{Y}((0, Q_n), s - t_n)$, use the relation (12) with $\alpha = (0, Q_n)$, $t = s - t_n$), and rewrite (11) as

$$\left(\int_{-\infty}^{t_n} \mathcal{Y}'((0, Q_n), s - t_n)^{-1} \psi \left(\frac{s - t_n}{h} \right) ds \right) \begin{bmatrix} G_n^* \\ 0 \end{bmatrix},$$

an expression that, after shifting the integration variable and multiplying by 2 to account for the effect of ψG_n^* acting while $t \ge t_n$, leads to (9).

3. Conservative fast forces. When the fast forces are conservative, $f(q) = -\nabla W(q)$, with W a scalar potential function, the system (3) is Hamiltonian [16], [10], [14], and the symmetries associated with Hamiltonian flows allow a simplification of the mollification procedure. The key observation is as follows.

LEMMA 1. *Assume that the reduced problem* (3) *is Hamiltonian. Then*

$$\mathcal{Y}'(\alpha, t)^{-1} = J^{-1} \mathcal{Y}'(\alpha, t)^T J,$$

where J is the matrix that defines the canonical symplectic form of the Hamiltonian formalism. In particular, the upper left block of the inverse of $\mathcal{Y}'(\alpha, t)$ coincides with $\mathcal{Q}_q(\alpha, t)^T$ (transposed lower right block).

Proof. Due to the symplecticness of Hamiltonian flows, $K = \mathcal{Y}'(\alpha, t)$ satisfies the relation $K^T J K = J$, or $K^{-1} = J^{-1} K^T J$. ∎

After this result, in the Hamiltonian case, the matrix R averaged in (9) can be found without inverting the $(2d) \times (2d)$ Jacobian Y'; instead we set

$$R(t) = Q_q(t)^T, \tag{13}$$

with Q_q found from solving

$$\frac{d}{dt}\begin{bmatrix} Q_p(t) \\ Q_q(t) \end{bmatrix} = \begin{bmatrix} 0 & f'(q^*(t)) \\ M^{-1} & 0 \end{bmatrix} \begin{bmatrix} Q_p(t) \\ Q_q(t) \end{bmatrix},$$

with initial condition $Q_p(t) = 0_d$, $Q_q(t) = I_d$. The left upper and lower blocks of Y' have been discarded from the variational equation (8) as they are not coupled to the lower right block Q_q to be used in (13).

The mollified impulse method was conceived by Skeel [5] in a context where much relevance was attached to the symplectic character [16], [10], [14] of the numerical schemes considered, and, for this reason, the paper [5] deals only with the case of conservative fast forces. In [5] the weight function ϕ may be freely chosen, but the mollifier is determined by

$$\mathcal{M}(Q_n, h) = \mathcal{A}'(Q_n, h)^T \tag{14}$$

(a prime denotes differentiation with respect to Q), a choice that ensures that, whenever the force g is conservative with $g(q) = -\nabla U(q)$, the force $\bar{G}_n$ used in the kicks is itself conservative as the negative gradient of the averaged potential $U(\mathcal{A}(Q_{n+1}, h))$. In the present work, fast forces need not be conservative, and there are two weight functions ϕ and ψ to be chosen. Nevertheless, if the fast forces are conservative and if ψ is chosen to coincide with ϕ, the (ϕ, ϕ)-methods defined here coincide with the methods introduced in [5]: Differentiating the average of q^* and transposing as in (14) is equivalent to averaging the transposed of the corresponding Jacobian as in (9) and (13).

4. Linear fast forces. We now address the case where the fast forces are linear: $f(q) = -Sq$, with S a stiffness matrix. We do not assume S to be symmetric, but, in order to deal with oscillatory problems, we suppose that $M^{-1/2} S M^{-1/2}$ possesses only real nonnegative eigenvalues and can be diagonalized. The material below would remain valid even if the conditions on S may be relaxed considerably; for instance, $M^{-1/2} S M^{-1/2}$ could be allowed to have complex eigenvalues close to the positive real axis. An abstract situation where S is the generator of a cosine operator [1] in a Banach space could also be catered to, but we will not concern ourselves with such extensions.

Under the hypothesis above, there exists a unique (in general, nonsymmetric) matrix Ω such that $\Omega^2 = M^{-1/2} S M^{-1/2}$ and all eigenvalues of Ω are nonnegative; the solution flow of the reduced problem is given in terms of Ω by $y(t) = \mathcal{R}(t) y(0)$, where $\mathcal{R}(t)$ is the rotation matrix

$$\mathcal{R}(t) = \begin{bmatrix} M^{1/2} \cos t\Omega \, M^{-1/2} & -M^{1/2} \Omega \sin t\Omega \, M^{1/2} \\ M^{-1/2} \Omega^{-1} \sin t\Omega \; M^{-1/2} & M^{-1/2} \cos t\Omega \, M^{1/2} \end{bmatrix}$$

or, in the spirit of the theory of cosine operators [1],

$$\mathcal{R}(t) = \begin{bmatrix} M^{1/2} C(t) M^{-1/2} & M^{1/2} \frac{d}{dt} C(t) M^{1/2} \\ M^{-1/2} \int_0^t C(s) ds \; M^{-1/2} & M^{-1/2} C(t) M^{1/2} \end{bmatrix},$$

with $C(t) = \cos t\Omega$. The second formula for $\mathcal{R}$ possesses the merit of deemphasizing the dependence of the material presented here on special properties of the trigonometric functions; the occurrence of the derivative and the integral is a direct consequence of the fact that p is essentially the time derivative of q. The upper left block of $\mathcal{R}(t)$ is bounded by a constant, and therefore the lower left block possesses an estimate of the form $O(t)$; the analysis below is based on these facts. On the other hand, from the group properties of the flow, $\mathcal{R}(t)\mathcal{R}(s) = \mathcal{R}(t+s)$, so that, in particular, $\mathcal{R}(-t)$ is the inverse of $\mathcal{R}(t)$; these properties are not contingent on trigonometric identities and will also be crucial below. It is perhaps of some interest to point out that, in agreement with section 3, if the problem is Hamiltonian, then Ω is symmetric and the upper left block of $\mathcal{R}(-t)$ coincides with the transpose of the lower right block of $\mathcal{R}(t)$.

The definition (7) now yields, since $\mathcal{R}(t)^{-1} = \mathcal{R}(-t)$,

$$\begin{aligned}\mathcal{A}(Q_n, h) &= M^{-1/2}\left(\frac{1}{h}\int_{-\infty}^{\infty}\cos t\Omega\,\phi\left(\frac{t}{h}\right)\,dt\right)M^{1/2}\,Q_n\\ &= M^{-1/2}\left(\int_{-\infty}^{\infty}\cos sh\Omega\,\phi(s)\,ds\right)M^{1/2}\,Q_n,\end{aligned}$$

an expression that, after introducing the Fourier transform of the even function ϕ

$$\hat{\phi}(\omega) = \int_{-\infty}^{\infty}\exp(-i\omega t)\phi(t)\,dt = \int_{-\infty}^{\infty}\cos\omega t\phi(t)\,dt, \tag{15}$$

can be rewritten as

$$\mathcal{A}(Q_n, h) = \mathcal{A}_h Q_n = \left(M^{-1/2}\hat{\phi}(h\Omega)M^{1/2}\right)Q_n.$$

Similarly, (9) now reads

$$\begin{aligned}\mathcal{M}_h &= M^{-1/2}\left(\frac{1}{h}\int_{-\infty}^{\infty}\cos t\Omega\,\psi\left(\frac{t}{h}\right)\,dt\right)M^{1/2}\\ &= M^{-1/2}\left(\int_{-\infty}^{\infty}\cos sh\Omega\,\psi(s)\,ds\right)M^{1/2}\end{aligned}$$

or

$$\mathcal{M}_h = M^{-1/2}\hat{\psi}(h\Omega)M^{1/2},$$

with

$$\hat{\psi}(\omega) = \int_{-\infty}^{\infty}\exp(-i\omega t)\psi(t)\,dt = \int_{-\infty}^{\infty}\cos\omega t\psi(t)\,dt, \tag{16}$$

and we conclude that the kicking force is given by

$$\bar{G}_n = M^{-1/2}\hat{\psi}(h\Omega)M^{1/2}g\left(M^{-1/2}\hat{\phi}(h\Omega)M^{1/2}Q_n\right). \tag{17}$$

For cases of linear fast forces where the stiffness matrix S is symmetric, a number of recent contributions starting from [9] have considered a family of kick-oscillate-kick algorithms whose kicking force includes *four* independent filtering functions (see

Chapter XIII of [10], [6], and references therein). If the attention is restricted to symmetric (time reversible) methods within that family, then the number of independent filters is reduced to two and the format for the kicking force is precisely (17) (see section 7).

Some final remarks: The real filter functions $\hat{\phi}$, $\hat{\psi}$ are even. Since weight functions are assumed throughout to satisfy the normalizing condition (6), we have $\hat{\phi}(0) = \hat{\psi}(0) = 1$. Furthermore the integrability of the weights implies that $\hat{\phi}$ and $\hat{\psi}$ are continuous, vanish at ∞, and possess the estimates $\|\hat{\phi}\|_\infty \leq \|\phi\|_1$, $\|\hat{\psi}\|_\infty \leq \|\psi\|_1$. If in particular ϕ or ψ are nonnegative, then $\|\hat{\phi}\|_\infty = 1$ or $\|\hat{\psi}\|_\infty = 1$. When ϕ or ψ are the Dirac function, then the Fourier transform is the unit function and the average or mollification filters become the identity, as they should.

5. Analysis: Mollification. Throughout this section and the next, we assume that the mass matrix M is the identity. What follows may easily be extended to the case $M \neq I$ (but the formulas soon become cluttered with powers of M); alternatively, a problem with $M \neq I$ may be reduced to the case $M = I$ by a linear change of variables [5]. Similarly, we assume that the stiffness matrix S is symmetric and positive-semidefinite, so that, in the Euclidean norm, $\|\cos t\Omega\| \leq 1$; again the analysis below may be easily extended to cover the more relaxed hypotheses on S considered in section 4, but this brings a bound for $\|\cos t\Omega\|$ as an additional constant in many of the formulas.

The analysis begins with the following result, which is Lemma 3 of [5] (but there is a square root missing from some formulas in that paper). To simplify the writing, we denote by $\bar{g}(\cdot) = \mathcal{M}_h g(\mathcal{A}_h \cdot)$ the function that provides the kicking force and furthermore set $\bar{g}_n = \bar{g}(q_n)$. Similarly we set $g^*(\cdot) = g(\mathcal{A}_h \cdot)$ and $g_n^* = g^*(q_n)$. Furthermore we denote by L_0, L_1, and L_2 a bound for g, a Lipschitz constant for g, and a Lipschitz constant for the derivative of g, respectively, when they exist; it follows from the boundedness of the filters that, if g is Lipschitz continuous, $\bar{g}$ and g^* are then also Lipschitz continuous with constants $\bar{L}_1 = \|\psi\|_1 L_1 \|\phi\|_1$ and $L^* = L_1 \|\phi\|_1$, respectively.

THEOREM 1. *Assume that the problem* (2) *with linear fast forces satisfies the hypotheses above, with g Lipschitz continuous, and is solved with $P_0 = p(0)$ and $Q_0 = q(0)$ by means of a (ϕ, ψ)-method (ϕ and/or ψ may be taken to be δ). Then the global error satisfies*

$$\|Q_n - q_n\| \leq \cosh(t_n \sqrt{\bar{L}_1}) \cdot \max_{1 \leq j \leq n} \|\sigma_{q,j}\|$$

and

$$\|P_n - p_n\| \leq \|\sigma_{p,n}\| + \bar{L}_1 t_n \cosh(t_n \sqrt{\bar{L}_1}) \cdot \max_{1 \leq j \leq n} \|\sigma_{q,j}\|,$$

where $\sigma_{p,n}$ $\sigma_{q,n}$ are the quadrature errors

$$\begin{bmatrix} \sigma_{p,n} \\ \sigma_{q,n} \end{bmatrix} = \sum_{j=0}^{n} h 1_j \begin{bmatrix} \cos(t_n - t_j)\Omega \\ \Omega^{-1} \sin(t_n - t_j)\Omega \end{bmatrix} \bar{g}_j - \int_0^{t_n} \begin{bmatrix} \cos(t_n - t)\Omega \\ \Omega^{-1} \sin(t_n - t)\Omega \end{bmatrix} g(q(t))\, dt \tag{18}$$

(1_j is defined to be 1 except for $1_0 = 1_n = 1/2$).

This theorem, based on a Gronwall lemma argument, provides a basic stability result for all of the methods in the class considered in this paper. To be noted is

the fact that the truncation error perpetrated at each step does not explicitly feature in the global error bound; instead the stepwise truncation errors up to t_n have been compounded into a single quadrature error σ_n. Integrated forms of the truncation error may lead to sharper error bounds than a stepwise approach whenever error cancellations are to be expected. This is an old theme in the analysis of numerical methods that, for ordinary differential equations, goes back at least to Spijker's thesis (see the discussion in [15]).

If $\bar{g}_n = g(Q_n)$ (original impulse method), σ coincides with the error in the trapezoidal quadrature rule. In the highly oscillatory scenario considered here where $h\Omega$ is not assumed to be small, the function $\cos(t_n - t)\Omega$ has an unbounded first derivative, and one cannot expect to derive $O(h)$ error bounds for σ_p that are uniform in Ω. A counterexample is provided by the case of a scalar harmonic oscillator of frequency ω subject to a constant external force g with $h\omega = 2\pi$ (the situation presented in [5] to prove that the global error—not the quadrature error—of the impulse method has stiff order 0 in the p variables). In the p component, the integral in (18) vanishes, while the trapezoidal quadrature rule takes the $O(1)$ value $t_n g$. For the q component the situation is not as bad: $\Omega^{-1}\sin(t_n - t)\Omega$ has a bounded first derivative, and standard theory leads to $O(h)$ error bounds for σ_q and hence for $Q_n - q_n$ in the application of the original impulse method to stiff oscillatory situations.

The proof of the next lemma essentially reverses the construction of the mollifier in section 2: There we incorporated into the kicking force $\bar{G}_n$ the "distributed" force $\psi((t - t_n)/h)G_n^*$ (see (10)) by way of the mollification matrix; we now recover the distributed force from the mollification matrix. The meaning of the lemma is clear: While the impulse method approximates the oscillatory integral in (18) by interpolation of the whole integrand, mollified methods interpolate only the soft force $g(q(t))$. This is precisely the idea behind Filon-type methods for the quadrature of oscillatory functions; see, e.g., [13].

LEMMA 2. *The quadrature error* (18) *may be rewritten as*

$$\begin{aligned}\begin{bmatrix}\sigma_{p,n}\\ \sigma_{q,n}\end{bmatrix} &= \int_{-\infty}^{\infty}\begin{bmatrix}\cos(t_n - t)\Omega\\ \Omega^{-1}\sin(t_n - t)\Omega\end{bmatrix}\sum_{j=0}^{n} 1_j\psi\left(\frac{t - t_j}{h}\right) g_j^*\, dt\\ &\quad - \int_0^{t_n}\begin{bmatrix}\cos(t_n - t)\Omega\\ \Omega^{-1}\sin(t_n - t)\Omega\end{bmatrix} g(q(t))\, dt.\end{aligned} \tag{19}$$

Furthermore, for a mollified method (ϕ, ψ) (ϕ may be the Dirac function) in which ψ has bounded support and vanishes for $|\ t\ | > \mu > 0$, the quadrature error is of the form

$$\begin{bmatrix}\sigma_{p,n}\\ \sigma_{q,n}\end{bmatrix} = \int_0^{t_n}\begin{bmatrix}\cos(t_n - t)\Omega\\ \Omega^{-1}\sin(t_n - t)\Omega\end{bmatrix} I(t)\, dt + \beta_n, \tag{20}$$

where $I(t)$ is the interpolation error

$$I(t) = \left(\sum_{j=0}^{n}\psi\left(\frac{t - t_j}{h}\right) g_j^*\right) - g(q(t)) \tag{21}$$

and β_n represents boundary effects and can be estimated as

$$\|\beta_n\| \le 2\mu(1 + t_n^2)^{1/2}\|\psi\|_1 L_0 h.$$

Proof. By the definition of the mollifier and since the integral of $\sin(t_j - t)\Omega\psi((t - t_j)/h)$ vanishes, the jth term T_j of the sum in (18) can be written as

$$\begin{aligned} h1_j\mathcal{R}(t_n - t_j) &\begin{bmatrix} \hat{\psi}(h\Omega)g_j^* \\ 0 \end{bmatrix} \\ &= 1_j \int_{-\infty}^{\infty} \mathcal{R}(t_n - t_j) \begin{bmatrix} \cos(t_j - t)\Omega \\ \Omega^{-1}\sin(t_j - t)\Omega \end{bmatrix} \psi\left(\frac{t - t_j}{h}\right) g_j^*\, dt \\ &= 1_j \int_{-\infty}^{\infty} \begin{bmatrix} \cos(t_n - t)\Omega \\ \Omega^{-1}\sin(t_n - t)\Omega \end{bmatrix} \psi\left(\frac{t - t_j}{h}\right) g_j^*. \end{aligned}$$

Away from the boundary, when j is such that $0 \le t_j - \mu h$, $t_j + \mu h \le t_n$, the last integral may be taken between the limits 0 and t_n and incorporated into the integral in (18). There are at most 2μ boundary values of j (μ near 0 and μ near t_n). For those values, the corresponding term T_j is incorporated only in part to the integral. The lemma follows after noticing that each T_j can be bounded by $h(1 + t_n^2)^{1/2}\|\psi\|_1 L_0$. ∎

After Theorem 1 and Lemma 2, global error estimates depend on bounds for the interpolation error (21), and we now turn to these. It is well known that a minimum requirement for any linear interpolation scheme is that it reproduces with no error the constant functions:

$$\sum_{j=-\infty}^{\infty} \psi(t - j) \equiv 1, \tag{22}$$

a condition that was featured in [5]. We recall from the standard theory behind the Poisson summation formula that the 1-periodic function

$$\Psi(t) = \sum_{j=-\infty}^{\infty} \psi(t - j)$$

(the sum is well defined if ψ has bounded support) has a Fourier series

$$\Psi(t) = \sum_n c_n \exp(i2\pi nt)$$

whose coefficients are values of the Fourier transform of ψ:

$$c_n = \int_0^1 \exp(-i2\pi nt)\Psi(t)\, dt = \int_{-\infty}^{\infty} \exp(-i2\pi nt)\psi(t)\, dt = \hat{\psi}(2\pi n).$$

Therefore (22) is equivalent to the condition

$$\hat{\psi}(2\pi n) = 0, \quad n = \pm 1, \pm 2, \ldots \tag{23}$$

that appears in the analysis of [10], [6]. We now prove that these conditions are essentially necessary and sufficient to achieve stiff order of convergence 1.

THEOREM 2. *With the hypotheses of Theorem* 1, *assume that* g *has a bounded derivative and that the weight function* ψ *has bounded support and satisfies* (22) *or* (23) *(*ϕ *may be the Dirac function). Then the global error possesses a bound*

$$\|P_n - p_n\| + \|Q_n - q_n\| \le Ch,$$

where the constant C depends on ψ, ϕ, t_n, L_0, and L_1 and also on a bound E for the reduced energy of the true solution

$$E = \max_{-\mu h \le t \le t_n + \mu h} \left(\frac{1}{2}\|p(t)\|^2 + \frac{1}{2}\|\Omega q(t)\|^2 \right).$$

Conversely, if the (ψ, ϕ)-method, where ψ is boundedly supported and ϕ may be δ, possesses a global error bound of this form, then (22) *and* (23) *hold true.*

Proof. Consider a method such that $\hat{\psi}(2k\pi) \neq 0$ for $k \neq 0$ an integer. In the case of a scalar harmonic oscillator with frequency $\omega = 2k\pi/h$ forced by a constant g, the global errors can be found explicitly, and $P_n - p_n$ turns out to possess an $O(1)$ behavior as $h \to 0$.

Let us next derive the error bound when $\phi = \delta$. It is standard to show (by approximating $m(t)$ by a constant) that, when interpolating a function m, the interpolation error

$$\left(\sum_{j=\infty}^{\infty} \psi\left(\frac{t - t_j}{h} \right) m(t_j) \right) - m(t)$$

can be bounded by $K_\psi K_1 h$, where K_ψ depends only on ψ and K_1 is a bound for the derivative $(d/dt)m(t)$. In our situation, where $m(t) = g(q(t))$ and $(d/dt)m(t) = g'p$, this yields an upper bound of the form $K_\psi L_1 \sqrt{E} h$ for the interpolation error in (21) for t away from the boundary $\mu h \le t \le t_n - \mu h$. The remaining intervals $0 \le t \le \mu h$ and $t_n - \mu h \le t \le t_n$ have length $O(h)$, and in them $I(t)$ is bounded. This, along with Lemma 2 and Theorem 1, yields the error bound for the global error.

The effect of an averaging operation with $\phi \neq \delta$ is to perturb the interpolation by bringing in approximate values $g_n^* = g(\mathcal{A}_h q_n)$ for the function values $g_n = g(q_n)$. Since $(I - \mathcal{A}_h)(h\Omega)^{-1}$ can be bounded independently of h and Ω (see the proof of (28) below), the differences $g_n^* - g_n$ are $O(h)$, with the implied constant depending on L_1, ϕ, and a bound for $\|\Omega q_n\|$. Then a global error bound $O(h^2)$ also holds in the presence of averaging. ∎

6. Analysis: Averaging. In this section we prove that, for suitable averaging operators, the (ϕ, ψ)-method yields $O(h^2)$ errors in q uniformly in the stiffness of the problem. After Theorem 2, we consider only situations where ψ is of bounded support and (22) holds.

The analysis begins by observing that, from the Alekseev–Groebner variation of constants formula:

$$p(t) = \mathcal{P}(p(0), q(0)) + \int_0^t \cos s\Omega \, g(q(s))\, ds,$$

and

$$q(t) = \mathcal{Q}(p(0), q(0)) + \int_0^t \Omega^{-1} \sin s\Omega \, g(q(s))\, ds,$$

or, after integration by parts,

$$q(t) = \mathcal{Q}(p(0), q(0)) + \int_0^t \cos s\Omega \int_s^t g(q(u))\, du\, ds.$$

Thus, there is one quadrature of the force to build up the momentum and *two* in the evolution of q. In numerical methods, global errors are built up from local errors in a way analogous to that in which forcing terms build up the true solution. We showed in section 5 how the global error for p and q is obtained after one quadrature, and we shall presently show how the global error for q may be obtained by two quadratures. To avoid order reduction, each of these quadratures has to employ a weight function, and this essentially explains why methods that include mollification but no averaging cannot achieve stiff order 2 in q.

Led by the preceding insight, the idea now is to integrate by parts in (19) (note that (20) is of no use because the boundary terms β_n are $O(h)$). The analysis is straightforward except for problems with the boundary, and to soften these we proceed as follows. The functions $\psi((t-t_j)/h)$, $0 \le j \le n$, do not add up to 1 near the boundaries of the interval $I_n = [0, t_n]$ (this is because, for t_j near the boundary, $\psi((t-t_j)/h)$ "spreads" out of I_n, and, correspondingly, there are basis functions $\psi((t-t_j)/h)$, with $t_j < 0$ or $t_j > t_n$, that "intrude" into I_n). For fixed h and t_n, a system of $n+1$ functions λ_j with the partition of unity property

$$\sum_{j=0}^{n} \lambda_j(t) = 1, \quad 0 \le t \le t_n,$$

is easily constructed by setting, for $0 \le t \le t_n$,

$$\begin{aligned}
\lambda_0(t) &= \psi\left(\frac{t-t_0}{h}\right),\\
\lambda_j(t) &= \psi\left(\frac{t-t_j}{h}\right) + \psi\left(\frac{-t-t_j}{h}\right), \quad 0 < j < \mu,\\
\lambda_j(t) &= \psi\left(\frac{t-t_j}{h}\right), \qquad \mu \le j \le n-\mu,\\
\lambda_j(t) &= \psi\left(\frac{t-t_j}{h}\right) + \psi\left(\frac{-t+2t_n-t_j}{h}\right), \quad n-\mu < j < n,\\
\lambda_n(t) &= \psi\left(\frac{t-t_n}{h}\right).
\end{aligned}$$

(Near the boundaries the basis function $\psi((t-t_j)/h)$ have been "reflected" about 0 or t_n to compensate for the functions with $j = -1, -2, \ldots$ or $j = n+1, n+2, \ldots$ missing from the new basis.) The introduction of this corrected set of basis functions makes it possible to extend to the common interval $0 \le t \le t_n$ the integrals in (19).

LEMMA 3. *If ψ is of bounded support as in Lemma 2, the quadrature error $\sigma_{q,n}$ satisfies*

$$\begin{aligned}
\sigma_{q,n} = &\int_0^{t_n} \Omega^{-1} \sin(t_n - t)\Omega \sum_{j=0}^{n} \lambda_j(t) g_j^* \, dt\\
&- \int_0^{t_n} \Omega^{-1} \sin(t_n - t)\Omega \, g(q(t)) \, dt + \beta_n^*,
\end{aligned} \tag{24}$$

where β_n^* represent boundary contributions, with

$$\|\beta_n^*\| \le 2\mu^2 \|\psi\|_1 L_0 h^2,$$

so that, after integration by parts,

$$\sigma_{q,n} = \int_0^{t_n} \cos(t_n - t)\Omega\, I^*(t)\, dt + \beta_n^*,$$

with I^* equal to the integrated interpolation error

$$I^*(t) = \int_0^t \left[\left(\sum_{j=0}^{n} \lambda_j(s) g_j^* \right) - g(q(ts)) \right] ds. \tag{25}$$

Proof. The q-component of the first integral in (19) differs from the first integral in (24) only because of the contributions of values of j in the summation corresponding to t_j near the boundary. For $0 \le j < \mu$ there is a difference

$$1_j \int_{t_j - \mu h}^{0} \Omega^{-1} \sin(t_n - t)\Omega\ \psi\left(\frac{t - t_j}{h}\right) g_j^*\, dt$$
$$-1_j \int_{0}^{\mu h - t_j} \Omega^{-1} \sin(t_n - t)\Omega\ \psi\left(\frac{-t - t_j}{h}\right) g_j^*\, dt$$

or

$$1_j \int_{t_j - \mu h}^{0} \left[\Omega^{-1} \sin(t_n - t)\Omega - \Omega^{-1} \sin(t_n + t)\Omega\right]\ \psi\left(\frac{t - t_j}{h}\right) g_j^*\, dt,$$

whose Euclidean norm is $\le 2\mu h \times (h/2)\|\psi\|_1 \times L_0$ (note that $\Omega^{-1}\sin(t_n - t)\Omega$ is Lipschitz continuous in t with Lipschitz constant 1 so that the term in square brackets has norm $\le 2\mu h$). The estimate for β_n^* follows readily by summing over the contributions of j near the boundary at 0 and by treating in a similar way the boundary at t_n. ∎

In particular, at $t = t_n$,

$$I^*(t_n) = \sum_{j=0}^{n} h 1_j g_j^* - \int_0^{t_n} g(q(s))\, ds, \tag{26}$$

and we find once more the trapezoidal quadrature rule. For methods without averaging, $g_n^* = g(q_n)$ and second-order accuracy cannot be achieved in stiff cases where g oscillates with periods of the order of h. A simple counterexample is as follows. We take $d = 2$ and (the subindex refers to the components of the vectors)

$$\frac{d^2}{dt^2} q_{(1)} = -\omega^2 q_{(1)}, \quad \frac{d^2}{dt^2} q_{(2)} = -q_{(1)}; \tag{27}$$

the force $-\omega^2 q_{(1)}$ driving the first component is taken to be fast, and the force $q_{(1)}$ driving the second component is taken to be soft. We focus on the initial data $q_{(1)}(0) = \omega^{-1}$, $q_{(2)}(0) = \omega^{-3}$, $p_{(1)}(0) = 0$, $p_{(2)}(0) = 0$, leading to the solution $q_{(1)}(t) = \omega^{-1}\cos\omega t$, $q_{(2)}(t) = \omega^{-3}\cos\omega t$, that has reduced energy bounded independently of $\omega \ge 1$. If $h\omega = 2\pi$, then, in (26), the integral vanishes, while the value of the quadrature rule is the $O(h)$ vector $[0, \omega^{-1}t_n]$. Computation of the actual global error shows that in this instance $Q_n - q_n$ is also $O(h)$ and not $O(h^2)$.

The next and last lemma is relevant in understanding why averaging works: While g_j^* is only an $O(h)$ approximation to the true value $g(q(t_j))$ of the function being integrated in (25) or (26), hg_j^* provides a higher-order approximation to the integral

of $g(q(t))$ in the neighborhood of t_j. Note that below we use, without loss of generality, the same upper bound μ for the supports of ϕ and ψ.

LEMMA 4. *Under the hypotheses of Theorem* 2*, the following estimate holds:*

$$\|q(t) - \mathcal{A}_h q_j\| \leq (\mid t - t_j \mid + \|\phi\|_1)\sqrt{2E}\, h, \quad -\mu h \leq t \leq t_n + \mu h, \tag{28}$$

so that, in particular,

$$\|g_j - g_j^*\| = \|g(q(t_j)) - g(\mathcal{A}_h q(t_j))\| \leq L_1 \|\phi\|_1 \sqrt{2E}\, h.$$

Furthermore, if g possesses a Lipschitz continuous derivative and ϕ is boundedly supported with $\phi = 0$ for $\mid t \mid > \mu > 0$, then

$$h g_j^* = \int_{t_j - \mu h}^{t_j + \mu h} \phi\left(\frac{t - t_j}{h}\right) g(q(t))\, dt + h r_j, \tag{29}$$

where r_j can be estimated as

$$\|r_j\| \leq \|\phi\|_1 \left[L_2(\mu + \|\phi\|_1)^2 E + \frac{1}{2}\mu^2 L_0 L_1 \right] h^2.$$

Proof. To bound $q(t) - \mathcal{A}_h q_j$, add and subtract q_j. Then $q(t) - q_j$ may be written as the integral of p, and $(I - \mathcal{A}_h)q_j$ is given, by the definition of $\mathcal{A}_h$, as an integral involving the expression $(1 - \cos t\Omega)q_j$, which can be bounded by $\|h\Omega q_j\|$.

Next, by expanding g around $\mathcal{A}_h q_j$ we get

$$g(q(t)) = g_j^* + J_j[q(t) - \mathcal{A}_h q_j] + d_j, \quad t_j - \mu h \leq t \leq t_j + \mu h,$$

where J_j is the relevant Jacobian and the residual d_j may be bounded, according to (28) as $(1/2)L_2[(\mu + \|\phi\|_1)\sqrt{2E}\, h]^2$. Integration yields

$$-r_j = J_j \frac{1}{h} \int_{t_j - \mu h}^{t_j + \mu h} \phi\left(\frac{t - t_j}{h}\right) [q(t) - \mathcal{A}_h q_j]\, dt + e_j,$$

where the integrated residual e_j is bounded by $\|\phi\|_1$ times the bound for d_j. We are therefore left with the task of estimating the last integral. We note that, by the definition of averaging,

$$\frac{1}{h} \int_{t_j - \mu h}^{t_j + \mu h} \phi\left(\frac{t - t_j}{h}\right) \mathcal{A}_h q_j\, dt = \mathcal{A}_h q_j = \frac{1}{h} \int_{t_j - \mu h}^{t_j + \mu h} \phi\left(\frac{t - t_j}{h}\right) \cos(t - t_j)\Omega\, q_j dt,$$

while, by using the form of the true flow,

$$\frac{1}{h}\int_{t_j-\mu h}^{t_j+\mu h}\phi\left(\frac{t-t_j}{h}\right)q(t)\,dt = \frac{1}{h}\int_{t_j-\mu h}^{t_j+\mu h}\phi\left(\frac{t-t_j}{h}\right)[\cos(t-t_j)\Omega q_j+\sin(t-t_j)\Omega p_j+\Delta_j]\,dt, \tag{30}$$

where $\Delta_j=\Delta_j(t)$ is the integral contribution from the variation of constant formula

$$\Delta_j(t)=\int_{t_j}^{t}\Omega^{-1}\sin(t-s)\Omega\, g(q(s))\,ds.$$

In (30) the integral of the sine term vanishes by symmetry and that of the cosine term is cancelled with the same contribution from $\mathcal{A}_h$. This leaves us the term with Δ_j, and we note that, for $t_j-\mu h\le t\le t_j+\mu h$,

$$\|\Delta_j\|\le\int_{t_j}^{t}\mid t-s\mid L_0\,ds\le\frac{1}{2}\mu^2L_0h^2.$$

After combining all of these estimates, we obtain the bound being sought. ∎

Equipped with (29), we return to (25). Away from the integration limits, the integral of $\lambda_j(s)$ is h so that the jth term in the summation matches, except for an $O(h^3)$ residual, the integral of $\phi((s-t_j)/h)g(q(s))$. Therefore it is appropriate to impose the condition

$$\sum_{j=-\infty}^{\infty}\phi(t-j)\equiv 1, \tag{31}$$

as this would ensure that, except for boundary effects, the sum matches the whole integral. This leads us to the next theorem, where, for completeness, we refer to the equivalent formulation

$$\hat{\phi}(2\pi n)=0,\quad n=\pm1,\pm2,\ldots \tag{32}$$

of the last condition.

THEOREM 3. *With the hypotheses of Theorem* 1*, assume that g has a bounded, Lipschitz continuous derivative and that the weight functions ϕ and ψ have bounded support and satisfy* (22)–(23) *and* (31)–(32)*. Then the global error possesses a bound*

$$h\|P_n-p_n\|+\|Q_n-q_n\|\le Ch^2,$$

where the constant C depends on ψ, ϕ, t_n, L_0, L_1, L_2, and E.

Conversely, if the (ψ,ϕ)-method with boundedly supported ϕ and ψ possesses a bound of this form, then (22)–(23) *and* (31)–(32) *hold.*

Proof. The necessity of the condition for ϕ is proved by considering the counterexample (27).

To prove the bound we construct a set of interpolation basis functions κ_j, $j=0,1,\ldots,n$, by applying to the functions $\phi((t-t_j)/h)$ the construction that was used to derive the λ_j's from the $\psi((t-t_j)/h)$'s. Then, the κ_j's add to 1 and

$$I^*(t)=\sum_{j=0}^{n}\left[\int_0^t\lambda_j(s)g_j^*\,ds-\int_0^t\kappa(s)g(q(ts))\,ds\right].$$

If k is the largest j such that $t_j \le t$, we split I^* as $I^* = I_1^* + I_2^*$, with

$$I_1^* = \sum_{j=0}^{n} \left[\int_0^{t_k} \lambda_j(s) g_j^* \, ds - \int_0^{t_k} \kappa(s) g(q(ts)) \, ds \right],$$
$$I_2^* = \sum_{j=0}^{n} \left(\int_{t_k}^{t} \lambda_j(s) \right) g_j^* - \int_{t_k}^{t} g(q(s)) \, ds.$$

Both expressions being subtracted in I_2^* can be approximated with $O(h^2)$ errors by $(t - t_k)g_k$. For I_1^*, and as noted above, if t_j is away from the integration limits, the jth term in the sum is $O(h^3)$. For $j < \mu$, the term is only $O(h^2)$, because there κ_j does not quite match $\phi((t - t_j)/h)$. The terms with t_j near t can be dealt with in a similar way. ∎

7. Filters and weights. As discussed in section 4, when applied to cases with linear fast forces, the methods in this paper can be specified and implemented in terms of the two filter functions $\hat{\phi}$ and $\hat{\psi}$ in (17). However, both the implementation of the methods in nonlinear cases and the analysis in sections 5 and 6 require the weight functions themselves ϕ and ψ. Let us then address the question of whether given two real, even filter functions there exist corresponding weight functions that generate them as in (15)–(16). We furthermore recall that weights are assumed to be bounded and that the interest should be restricted to weights with bounded support if one is to compute numerically the averaging and mollifier operators.

The answer to our question is well known in Fourier analysis: According to a classical result by Paley and Wiener, a square integrable function $\hat{\chi}(\omega)$ of the real variable ω is the Fourier transform of a square integrable function χ supported in $[-\nu, \nu]$, $\nu > 0$, if and only if $\hat{\chi}$ can be extended to a holomorphic function of ω in the whole complex plane such that for all complex ω

$$| \hat{\chi}(\omega) | \le C \exp(\nu \, | \, \omega \, |).$$

For given ν, the space of all such $\hat{\chi}$ of *exponential type* is referred to as the Paley–Wiener space $PW_{[-\nu,\nu]}$. Hence any reversible method for linear fast forces of the family considered in [10], [6] for which the filter functions belong to some $PW_{[-\nu,\nu]}$ space can be extended to a (ϕ, ψ)-method applicable to nonlinear fast forces simply by taking as weights the inverse Fourier transforms of the filters. An example will be provided at the end of this section.

From the classical theorems of Weierstraß and Hadamard, it is well known that entire functions (functions holomorphic in the whole complex plane) are not determined by their zeros. However, a result by Titchmarsh (see, e.g., [4]) implies that any function $\hat{\chi}$ in $PW_{[-\nu,\nu]}$ can be expressed in terms of its infinitely many zeros ω_n as

$$\hat{\chi}(\omega) = \hat{\chi}(0) \prod_n \left(1 - \frac{\omega}{\omega_n} \right);$$

for the optimal convergence of the numerical method, $\hat{\chi}(0) = 1$ and the set of zeros must at least contain all nonzero even multiples of π. In this sense, the choice called *short* in [5],

$$\hat{\chi}_s(\omega) = \prod_{k=1} \left(1 - \frac{\omega^2}{4k^2\pi^2} \right) = \frac{\sin(\omega/2)}{\omega/2},$$

appears as a *minimal* filter: Filters of all potentially useful (ϕ, ψ)-methods can be obtained by multiplying $\hat{\chi}_s$ by suitable factors that bring in additional zeros. The corresponding weight function χ_s equals 1 for $-1/2 \le t \le 1/2$ and vanishes elsewhere. Obviously, no weight function may have support smaller than $[-1/2, 1/2]$ if its translations are to add to 1 (see (22), (31)).

Two other weight functions were explicitly discussed in [5]. The *long* weight χ_l, with value $1/2$ for $-1 \le t \le 1$ and 0 elsewhere, is a dilation of the short weight: $\chi_l(t) = (1/2)\chi_s(t/2)$. The *linear* weight function is the convolution of the short weight with itself, $\chi_{lin} = \chi_s * \chi_s$; it is the well-known hat basis function for piecewise linear interpolation with $\chi_{lin}(0) = 1$ and $\chi_{lin}(t) = 0$ for $| t | \ge 1$. The filter functions are, respectively, given by $\hat{\chi}_l(\omega) = \hat{\chi}_s(2\omega)$ (zeros at $k\pi$, $k \ne 0$) and $\hat{\chi}_{lin}(\omega) = \hat{\chi}_s(\omega)^2$ (double zeros at $2k\pi$, $k \ne 0$). Of course, convolution of the weights means product of the filters, and dilations translate into rescalings of ω.

The way to further generalizations by using convolutions and dilations is clear; these generalizations include the spline weights $\chi_s * \cdots * \chi_s$ (or $\chi_l * \cdots * \chi_l$) obtained by iterating the convolution of χ_s (or χ_l) with itself; the filters are the powers of $\hat{\chi}_s$ (or $\hat{\chi}_l$). More factors in the convolution mean higher-order zeros in the filter, and hopefully a better filtering, at the price of a longer support that entails higher computational work. The uncertainty principle implies that there is a limit on how much one can simultaneously concentrate near $t = 0$ the mass of χ and near $\omega = 0$ the mass of $\hat{\chi}$: Thus low computational cost and the drastic suppression of high frequencies are contradictory goals.

It is not our purpose here to settle the question as to the best choice of weight functions. We feel that the answer would very much depend both on the problem being solved and on the relation between the computational costs of integrating the reduced problem and of sampling the soft forces.

We shall finish the paper by presenting an example that illustrates how methods for linear fast forces based on filters can be extended to nonlinear fast forces by using weights. Grimm and Hochbruck have suggested [6] the filters $\omega^{-1} \sin \omega$ for the average and $\omega^{-2} \sin^2 \omega$ for the mollifier. These functions have exponential type 1 and 2, respectively, and, via the Paley–Wiener theorem, the method introduced in [6] can be extended to nonlinear fast forces by the (ϕ, ψ)-method that uses as weights the corresponding inverse Fourier transforms with supports $[-1, 1]$ and $[-2, 2]$. In fact, the weights are readily seen to be $\phi = \chi_l$ and $\psi = \chi_l * \chi_l$.

For a numerical test of this method, we use the nonlinear fast forces problem in section 4 of [5] and consider a system consisting of two unit point masses in the plane. The first mass is attached to one end of a (potentially strong) spring of unit length with stiffness ω^2 (in the experiments $0 \le \omega^2 \le 900$). The other end of this spring is fixed at the origin. The second mass is attached to the first through a (soft) spring of unit length and stiffness $1/2$. Initially the first mass is at $(1, 0)$ and the second at $(2, 0)$ so that the potential energy of the system is 0. The corresponding initial velocities are $(\sqrt{2}/4, \sqrt{2}/4)$ and $(-\sqrt{2}/4, \sqrt{2}/4)$, and the integration takes place for $0 \le t \le 16$, with step lengths $h = 1/2$ and $h = 1/4$.

Numerical results are presented for the $(\chi_l, \chi_l * \chi_l)$-method and, for comparison, also for the original impulse (δ, δ)-method and for the short filter (χ_s, χ_s)-method of [5]. The figure plots as a function of ω, $0 \le \omega \le 30$, the maximum over $0 \le t \le 16$ of the Euclidean norm of the error in the 4-dimensional vector of positions of the masses. For small values of ω the first spring is not really strong, and $(\chi_l, \chi_l * \chi_l)$ performs worse than the other two methods. For ω larger than, say, 10, the results of the original impulse method are clearly inferior to those of the methods that use

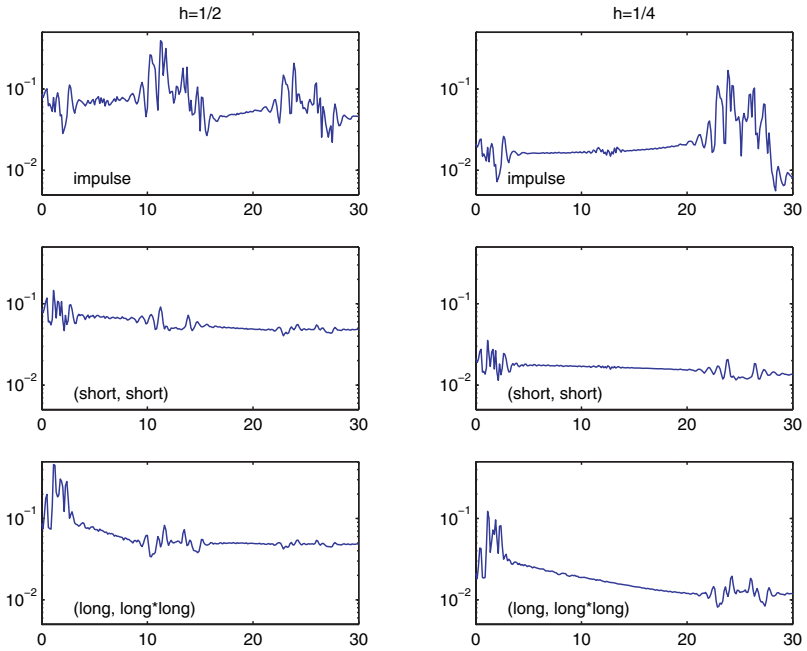

FIG. 7.1. *Two spring nonlinear problem: error in positions against* ω.

averaging and mollification. For the (χ_s, χ_s)-method the maximum over ω of the error is 0.1461 when $h = 1/2$ and 0.0354 when $h = 1/4$; for $(\chi_l, \chi_l * \chi_l)$ the corresponding figures are 0.4618 and 0.1227; thus both methods show in this nonlinear problem an $O(h^2)$ error behavior (as that ensured by Theorem 3 for the linear case). For the impulse method halving h brings down the error from 0.3931 to 0.1686, so that an order reduction manifests itself. In Figure 7.1 it is apparent that the order reduction is more pronounced if the attention is restricted to ω larger than, say, 20: Near $\omega = 8\pi$ the errors for $h = 1/4$ are hardly smaller than those for $h = 1/2$.

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REFERENCES

[1] W. Arendt, Ch. J. K. Batty, M. Hieber, and F. Neubrander, *Vector-Valued Laplace Transforms and Cauchy Problems*, Birkhäuser, Basel, 2001.
[2] D. Cohen, E. Hairer, and Ch. Lubich, *Numerical energy conservation for multi-frequency oscillatory differential equations*, BIT, 45 (2005), pp. 287–305.
[3] K. Dekker and J. G. Verwer, *Stability of Runge-Kutta Methods for Stiff Nonlinear Differential Equations*, North-Holland, Amsterdam, 1984.
[4] A. G. García, *A brief walk through sampling theory*, Adv. Imag. Electron Phys., 124 (2002), pp. 63–137.
[5] B. García-Archilla, J. M. Sanz-Serna, and R. D. Skeel, *Long-time-step methods for oscillatory differential equations*, SIAM J. Sci. Comput., 20 (1998), pp. 930–963.
[6] V. Grimm and M. Hochbruck, *Error analysis of exponential integrators for oscillatory second-order differential equations*, J. Phys. A, 39 (2006), pp. 5495–5507.
[7] H. Grubmüller, *Dynamiksimulation sehr großer Makromoleküle auf einem Parallelrechner*, Master's thesis, Physik-Dept. der Tech. Univ. München, Munich, 1989.

[8] H. Grubmüller, H. Heller, A. Windemuth, and K. Schulten, *Generalized Verlet algorithm for efficient molecular dynamics simulations with long-range intereactions*, Mol. Sim., 6 (1991), pp. 121–142.

[9] E. Hairer and Ch. Lubich, *Long-time energy conservation of numerical methods for oscillatory differential equations*, SIAM J. Numer. Anal., 38 (2000), pp. 414–441.

[10] E. Hairer, Ch. Lubich, and G. Wanner, *Geometric Numerical Integration*, 2nd ed., Springer, Berlin, 2006.

[11] E. Hairer, S. P. Nørsett, and G. Wanner, *Solving Ordinary Differential Equations* I*, Nonstiff Problems*, 2nd. ed., Springer, Berlin, 1993.

[12] E. Hairer and G. Wanner, *Solving Ordinary Differential Equations* II*, Stiff and Differential-Algebraic Problems*, 2nd ed., Springer, Berlin, 1996.

[13] A. Iserles, *On the numerical quadrature of highly-oscillating integrals* I: *Fourier transforms,* IMA J. Numer. Anal., 24 (2004), pp. 365–391.

[14] B. Leimkuhler and S. Reich, *Simulating Hamiltonian Dynamics*, Cambridge University Press, Cambridge, 2005.

[15] J. M. Sanz-Serna, *Stability and convergence in numerical analysis* I: *Linear problems, a simple, comprehensive account*, in Nonlinear Differential Equations, J. K. Hale and P. Martínez-Amores, eds., Pitman, Boston, 1985, pp. 64–113.

[16] J. M. Sanz-Serna and M. P. Calvo, *Numerical Hamiltonian Problems*, Chapman and Hall, London, 1994.

[17] M. Tuckerman, B. J. Berne, and G. J. Martyna, *Reversible multiple time scale molecular dynamics,* J. Phys. Chem., 99 (1995), pp. 1990–2001.

[18] J. Wisdom, *The origin of the Kirkwood gaps: A mapping for asteroidal motion near the* 3/1 *commensurability*, Astrophysics J., 87 (1982), pp. 577–593.