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Long-time step methods for oscillatory differential equations

Abstract We consider numerical methods for nondissipative dynamical system with multiple time scales. It is assumed that the computation of the faster forces present in the problem is cheap so that the overall cost of the integration is primarily determined by the step size used to sample the slow forces, a situation that arises e.g. in molecular dynamics and partial differential equations. The aim is to construct algorithms that sample the slow forces at time intervals not restricted by the periods of the fast oscillations. An existing method, sometimes used for the problems we have in mind, is the impulse method; however this algorithm is far from optimal and we discuss some of its shortcomings. An alternative algorithm, the mollified impulse method has been suggested by the present authors and is studied here. Numerical experiments are reported.

1 Introduction

In this paper we study numerical methods for the integration in time of differential equations with fast oscillatory solutions. Let us begin by describing three examples of the types of problems we are interested in.

Molecule. A molecule can be modelled as a set of N point masses (the atoms) moving under Newton's second law

$$m_i \frac{d^2 x_i}{dt^2} = F_i, \qquad i = 1, \ldots, N. \tag{1.1}$$

In applications of interest, say in the modelling of proteins, N is a very large number. The net force F_i on the i-th atom comprises several contributions; for the sake of simplicity let us mention only two of them. (1) Strong forces exerted on i by those atoms (typically less than, say, five) chemically bonded to i. (2) Weaker forces, including electrostatic forces, exerted on i by *every other* atom in the molecule. If we collect all position vectors x_i in a $3N$-vector q, then the system of differential equations to be integrated is

$$M \frac{d^2 q}{dt^2} = F_{(1)}(q) + F_{(2)}(q), \tag{1.2}$$

where M is the diagonal matrix of the masses, $F_{(1)}$ comprises the bond forces and $F_{(2)}$ the other forces. Thus $F_{(2)}$ is a soft force whose evaluation is expensive (the complexity is $O(N^2)$: each atom interacts with every other). On the other hand, $F_{(1)}$,

while much stronger, is cheaply computed (the complexity is only $O(N)$). Also note that in a parallel implementation the part $F_{(2)}$, which is not localized in space, is likely to require much communication.

Planets. Consider now a planetary system with a large star and N planets. Assume for simplicity that the star is so massive that it does not move significantly; then the system is described by the positions x_i of the planets relative to the star and these satisfy Newton's law (1.1). The force F_i on the i-th planet consists of the large attraction of the star and the much weaker attractions of the remaining planets. The system to be integrated is of the form (1.2), with $F_{(1)}$ corresponding to the star-planet forces and $F_{(2)}$ comprising the planet-planet attractions. Here $F_{(1)}$ is strong but mathematically not very challenging: the *reduced problem*

$$M\frac{d^2q}{dt^2} = F_{(1)}(q) \tag{1.3}$$

consists of N uncoupled Kepler problems and can be solved in closed form. It is the weak force $F_{(2)}$ that may make the solution of (1.2) difficult.

Partial differential equation. In the interest of brevity we just consider here a simple problem, but many other cases can be treated similarly. Our nonlinear wave problem is (f is 2π-periodic in x)

$$u_{tt}(x,t) = u_{xx}(x,t) + f(x,u), \qquad u(x,t) \equiv u(x+2\pi,t). \tag{1.4}$$

Once more the right hand-side comprises two contributions. The first u_{xx} is the strongest because the operator ∂_{xx} has eigenvalues of arbitrarily large modulus leading to arbitrarily small time-scales. Nevertheless, the problem $u_{tt} = u_{xx}$ with periodic boundary conditions is not difficult: it may be numerically integrated with negligible errors via Fourier techniques. It is the softer term $f(x,u)$ that makes the integration nontrivial. After space discretization by a Fourier pseudospectral method, the system to be integrated in time is again of the form (1.2) with $F_{(1)}$ strong, $F_{(2)}$ weak and (1.3) solvable in closed form; q is a vector of grid values of u.

In general we will be concerned with problems (1.2) with q a D-dimensional vector and M a diagonal mass matrix. The following three assumptions are supposed to hold.

- The reduced problem (1.3) can be integrated "exactly" over any time interval $[t, t+h]$. We saw that in the examples Planets and Partial Differential Equation, the reduced problem is solvable in closed form. In the example Molecule the reduced problem has to be integrated numerically; however the cost of evaluating $F_{(1)}$ is negligible with respect to the cost of evaluating $F_{(2)}$ and, by using a very small step size h_{red}, we can very accurately integrate the reduced problem over $[t, t+h]$ with a moderate computational effort.

- The forces $F_{(1)}$ have some strong components that cause the reduced problem to have fast oscillatory motions. Note that $F_{(1)}$ may in addition have weak components leading to slow modes in the reduced problem.

- The forces $F_{(2)}$ are soft.

Our *task* is to construct an algorithm that integrates the full problem (1.2) by using (i) exact solutions of the reduced problem (1.3) over intervals $[t, t+h]$ and (ii) evaluations of $F_{(2)}$. We aim at an algorithm that uses *as few as possible* evaluations of the soft force $F_{(2)}$. This economy in $F_{(2)}$ evaluations may be motivated by either or both of the following reasons.

- The evaluation of the slow force $F_{(2)}$ is expensive. This is the situation in the examples Molecule and Planets if N is large.

- The cost of integrating the reduced system over a long interval $[t, t+h]$ does not depend heavily on the interval length h (this is the case for examples Planets and Partial Differential Equations). It is then of interest to maximize h so as to minimize the number of steps needed to cover the interval $[0, T]$ on which we wish (1.2) integrated.

We would like to sample $F_{(2)}$ at intervals *longer* (hopefully much longer) than the shortest period of the motions present in the problem. Ideally $F_{(2)}$ would be sampled at a rate governed by $F_{(2)}$ but independent of the reduced problem. We define a *long-time-step method* to be one that samples the slow force at time increments larger than half the period of the fastest oscillation in the system.

Two comments are in order. First, in the examples above, the division of forces in fast and slow occurs naturally; this need not be the case and the splitting could be made artificially [6], [8]. Second, if the reduced problem is solved with a numerical scheme using step sizes shorter than those being employed for the main problem (1.2), then the overall method is a two-time-step method. This idea might, of course, be applied recursively—the forces in reduced problem itself may be partitioned into strong and not so strong and so on, resulting in a hierarchy of step sizes.

A potential candidate for long-time-step integration is the *impulse method,* that has been used several times in the past. We discuss this method in section 2 bel ow and show that it suffers from important shortcomings. In section 3, we discuss a nontrivial improvement of the impulse method that we have called the *mollified impulse method* [1]. A numerical example is presented in the final section.

2 The Impulse Method

For simplicity we consider hereafter only the case where the mass matrix M is the unit matrix (any other case can be reduced to this by a change of variables). We denote by p the velocities/momenta dq/dt. A step $n \to n+1$ of the impulse method can be described as follows:

- **Kick.** Add $(h/2)F_{(2)}(q_n)$ to p_n to get p_n^+.
- **Oscillate.** Use the h-flow of $(d/dt)p = F_{(1)}$, $(d/dt)q = p$ to advance from (p_n^+, q_n) to (p_{n+1}^-, q_{n+1}).
- **Kick.** Add $(h/2)F_{(2)}(q_{n+1})$ to p_{n+1}^- to get p_{n+1}.

Even though there are two kicks per step, the number of evaluations of $F_{(2)}$ per step is only one: the second $F_{(2)}$ vector of the current step provides the first force to be used at the next step. If $F_{(1)} \equiv 0$ then the oscillation substep keeps p constant while q drifts according to $q_{n+1} = q_n + hp_n^+$; thus the impulse method coincides with the Verlet/Störmer/leapfrog method often used in molecular dynamics. If the forces are conservative, $F_{(1)}(q) = -\nabla W(q)$, $F_{(2)}(q) = -\nabla V(q)$ (W and V are scalar potentials), then the impulse method is symplectic [5]: this follows trivially from the observation that kick and oscillate are respectively the flows of the Hamiltonian flows with Hamiltonian functions $V(q)$, $(1/2)p^T p + W(q)$.

The impulse method is of course a particular instance of the celebrated Strang splitting [7]. In celestial mechanics it has been used successfully by Wisdom and his coworkers in several instances, going back at least to [9]; Wisdom derives this algorithm via Dirac delta functions [10]. The impulse method is derived as a multiple-time-step method in [2], [3] but these writings express little appreciation for the method because of the possibility of resonance to be studied below. Further discussion of the application of the impulse method in molecular dynamics has been provided in [1].

Let us discuss, by means of examples, some of the shortcomings of the impulse method. The scalar differential equation

$$\frac{d^2q}{dt^2} = -\Omega^2 q + F_{(2)}, \tag{2.1}$$

where $\Omega \gg 1$ describes the displacement of a unit mass subject to the pull of a stiff spring held fixed at the other end and to the pull of a constant force $F_{(2)}$. For simplicity assume initial values $q(0) = 0$ and $p(0) = 1$, so that the total energy is $1/2$ regardless of the values of Ω and $F_{(2)}$. Numerical integration by the impulse method with step size h incorporates the slow force $F_{(2)}$ by adding a term $(h/2)F_{(2)}$ to the momentum at the beginning and at the end of every step. Suppose though that h has been chosen so that $h\Omega = 2\pi$. Between the impulses the reduced problem $d^2q/dt^2 = -\Omega^2 q$ is integrated exactly; and because any solution of this problem has period $h = 2\pi/\Omega$, the result of integrating will be to leave the value of p and q exactly unchanged. Hence each complete step adds $hF_{(2)}$ to p and leaves q unchanged, so that

$$p_n = 1 + nh, \qquad q_n = 0. \tag{2.2}$$

This happens to be exact for q

$$q(t) = \Omega^{-1} \sin t\Omega + \Omega^{-2}(1 - \cos t\Omega)F_{(2)}$$

($q(nh) = 0$) but *utterly wrong* for p. The correct solution is

$$p(t) = \cos t\Omega \cdot 1 + \Omega^{-1} \sin t\Omega \cdot F_{(2)} \tag{2.3}$$

and has the constant value 1 at integer multiples nh of h. Hence the impulse method cannot successfully operate in this problem if $h\Omega = 2\pi$. We conclude that a restriction is required on the size of $h\Omega$; the step size must be chosen in accordance to the fast frequencies in spite of the fact that the impulse method would be exact if the slow forces were absent.

Additional examples where the impulse method performs badly due to lack of accuracy (rather than due to instability) can be found in [1].

A further difficulty with the impulse method stems from the resonances mentioned above. Consider now the one-degree-of-freedom oscillator

$$\frac{d^2q}{dt^2} = -\Omega^2 q - q, \tag{2.4}$$

where again $\Omega \gg 1$. We now have a point mass driven by a hard spring of stiffness Ω^2 and a soft spring of stiffness 1. The numerical solution satisfies

$$\begin{bmatrix} p_{n+1} \\ q_{n+1} \end{bmatrix} = \Psi_h \begin{bmatrix} p_n \\ q_n \end{bmatrix}$$

with the matrix Ψ_h given by

$$\Psi_h = \begin{bmatrix} \cos h\Omega - \frac{h}{2\Omega} \sin h\Omega & -\Omega \sin h\Omega - h \cos h\Omega + \frac{h^2}{4\Omega} \sin h\Omega \\ \frac{1}{\Omega} \sin h\Omega & \cos h\Omega - \frac{h}{2\Omega} \sin h\Omega \end{bmatrix}.$$

For fixed h, $n \to \infty$ stability, we require that both eigenvalues of Ψ_h should have modulus ≤ 1. Since Ψ_h has unit determinant (the impulse method is symplectic!), stability demands that Ψ_h has trace of modulus ≤ 2. The stability region is depicted unshaded in Figure 2.1. We see that, even for h very small, the method is unstable if $h\Omega$ is near an integer multiple of π; again a restriction is necessary that limits h in terms the fast period. Note that, for $\Omega = 0$, the stability restriction is $h < 2$; this could have been anticipated from our earlier remark that, for $F_{(1)} \equiv 0$, the impulse method reduces to the well-known Verlet algorithm. The presence of the fast oscillation reduces the stability threshold of the impulse method, in spite of the fact that the method uses the exact form of the reduced oscillations.

It is perhaps useful to note that the linear problem

$$\frac{d^2q}{dt^2} = -\Omega_{(1)}^2 q - \Omega_{(2)}^2 q,$$

where $\Omega_{(1)}$ and $\Omega_{(2)}$ are symmetric positive semidefinite stiffness matrices that commute, essentially reduces to (2.4) after a simultaneous diagonalization of $\Omega_{(1)}$ and $\Omega_{(2)}$.

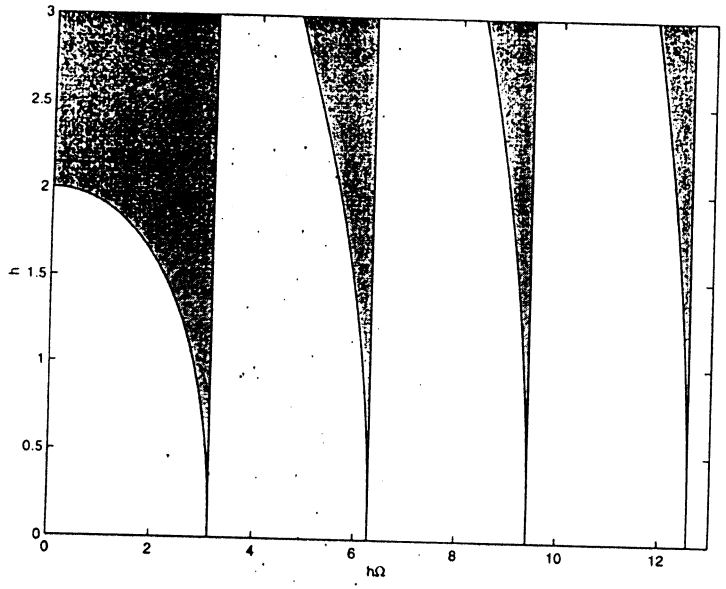

Figure 2.1: Instability region (shaded) of the impulse method for a model problem. The vertical axis corresponds to the step size h and the horizontal axis to $h\Omega$, where Ω is the fast frequency

3 The Mollified Impulse Method

The enhancement suggested in [1] for the impulse method requires the modification of the strength of the impulses $F_{(2)}(q_n)$ to become

$$\tilde{F}_{(2)}(h;q_n) = \mathcal{A}_q(h;q_n)^T F_{(2)}(\mathcal{A}(h;q_n)). \tag{3.1}$$

Evaluation of $F_{(2)}$ at $\mathcal{A}(h;q_n)$ represents an averaging; $F_{(2)}(\mathcal{A}(h;q_n)$ is expected to be a better description of the quickly varying $F_{(2)}(t)$ than the values of $F_{(2)}$ at step points used by the impulse method. Different choices of the averaging operator $\mathcal{A}(h;q_n)$ are possible and lead to different numerical methods. The transpose Jacobian $\mathcal{A}_q(h;q_n)^T$ has a mollifying effect: equation (2.3) shows that, in the true dynamics of (2.1), the effect of $F_{(2)}$ is mollified by multiplication by $\Omega^{-1}\sin t\Omega$. The action of $\mathcal{A}_q(h;q_n)^T$ on the force can be seen not only as a mollification but also as a filter damping some components of the force. Different averaging procedures give rise to different filters. This point of view is taken up below.

In the case of conservative forces, $F_{(1)} = -\nabla W$, $F_{(2)} = -\nabla V$, the mollified force $\tilde{F}_{(2)}$ is the negative gradient of $\tilde{V}(q) = V(\mathcal{A}(h,q))$ and this leads to the sy mplecticness of the mollified impulse method (use the argument that was outlined above to show the symplecticness of the impulse method).

In order to find the average $\mathcal{A}(h;q_n)$, we use an interpolation, and there is flexibility in how this is done. Let ϕ be a basis function for interpolation on a mesh consisting of all integers so that

$$\sum_n \phi(\frac{t-nh}{h})g_n$$

is the interpolant of data g_n on a mesh of spacing h. Consistency requires that

$$\sum_n \phi(s-n) \equiv 1,$$

which, by standard Fourier analysis techniques, can be easily shown to imply

$$\int_{-\infty}^{+\infty} \phi(s)\,ds = 1.$$

There are three interesting simple choices of ϕ:

1. the ShortAverage $\quad \phi(s) = \begin{cases} 1, & |s| < \frac{1}{2}, \\ \frac{1}{2}, & |s| = \frac{1}{2}, \\ 0, & |s| > \frac{1}{2}. \end{cases}$

2. the LongAverage $\quad \phi(s) = \begin{cases} \frac{1}{2}, & |s| < 1, \\ \frac{1}{4}, & |s| = 1, \\ 0, & |s| > 1. \end{cases}$

3. the LinearAverage $\quad \phi(s) = \begin{cases} 1-|s|, & |s| \le 1, \\ 0, & |s| \ge 1. \end{cases}$

The average $\mathcal{A}(h;q_n)$ is defined in terms of the solution $p(t;q_n)$, $q(t;q_n)$, $b(t;q_n)$ of an auxiliary initial value problem

$$\frac{dp}{dt} = F_{(1)}(q), \quad \frac{dq}{dt} = p, \quad \frac{db}{dt} = \phi\left(\frac{t}{h}\right) q,$$

with initial conditions $p(0) = 0$, $q(0) = q_n$, $b(0) = 0$. Note that the initial momentum is zero and that only fast forces are integrated, so that we are in fact integrating the reduced problem while simultaneously computing the integral of $\phi(t/h)q$. We define

$$\mathcal{A}(h;q_n) = \frac{1}{h}(b(+\infty;q_n) - b(-\infty;q_n))$$

so that

$$\mathcal{A}(h;q_n) = \frac{1}{h}\int_{-\infty}^{\infty} \phi(\frac{t}{h})q(t)\,dt = \int_{-\infty}^{\infty} \phi(s)q(hs)\,ds.$$

In Short, Long and LinearAverage and in other potentially useful choices, ϕ is an even function and the average reduces to $(2/h)b(+\infty;q_n)$. If furthermore, $\phi(s)$ vanishes for $|s| > \mu$, then the average is simply $(2/h)b(\mu h;q_n)$ and the integration of the auxiliary

problem is required only on a bounded t-interval. An infinite integration may be possible if the auxiliary problem can be integrated analytically in closed form. Otherwise, ϕ should be chosen to have bounded support.

The mollified method also requires the Jacobian matrix $\mathcal{A}_q(h;q_n) = (2/h)b_q(\mu h;q_n)$ formed by differentiating $(2/h)b(\mu h;q_n)$ with respect to q_n. This means that at the same time we compute the average we have to compute derivatives of the average [1].

We emphasize that, at each value of n, the auxiliary integration is used only to compute the mollified impulse. Once the impulse has been added to the momentum, the averaged position and its Jacobian matrix are discarded and the main integration is continued from q_n, which has not changed at all during the auxiliary integration.

To solve the auxiliary averaging problem, we should use exactly the same method, analytical or numerical, as that used to integrate the reduced problem (between evaluations of the slow force). Further details can be found in [1].

In the case of linear fast forces $F_{(1)}(q) = -\Omega^2 q$ (Ω a symmetric matrix) it is easy to check that the average is given by

$$\mathcal{A}(h;q) = \Phi q$$

where Φ is the matrix

$$\Phi = \frac{1}{h}\int_{-\infty}^{+\infty} \phi(\frac{t}{h}) \cos t\Omega \, dt = \int_{-\infty}^{+\infty} \phi(s) \cos sh\Omega \, ds.$$

This leads, according to (3.1) to a mollified force $\Phi F_{(2)}(\Phi q)$.

For the methods studied, the "filters" Φ are as follows:

Impulse	$\Phi = I$
ShortAverage	$\Phi = \frac{\sin \frac{h}{2}\Omega}{\frac{h}{2}\Omega}$
LongAverage	$\Phi = \frac{\sin h\Omega}{h\Omega} = \frac{\sin \frac{h}{2}\Omega}{\frac{h}{2}\Omega} \cos \frac{h}{2}\Omega$
LinearAverage	$\Phi = \left(\frac{\sin \frac{h}{2}\Omega}{\frac{h}{2}\Omega}\right)^2$

We observe that, for the mollified methods, the filter is ≈ 1 in those eigendirections of Ω whose eigenvalue ω is such that $h\omega$ is small. However the filter kills components in those eigendirections for which $h\omega$ is near an integer multiple of 2π.

It is proved in [1] that, in the case of fast linear forces, the three mollified methods possess error bounds of the form

$$\|p_n - p(t_n)\| \leq Ch, \qquad \|q_n - q(t_n)\| \leq Ch^2, \tag{3.2}$$

where the constant C depends only on bounds for $F_{(2)}$ and its first and second derivative, on t_n and on the reduced energy of the solution

$$\hat{H} = \max_{0 \leq t \leq nh} (\frac{1}{2}p(t)^T p(t) + \frac{1}{2}q(t)^T \Omega^2 q(t)).$$

The independence of the bounds on derivatives of $F_{(1)}(q)$ implies that, provided that the reduced energy is kept bounded, it is possible to apply the method with a given time-step h to faster and faster problems without impairing the accuracy. A bound for p and q in terms of the energy implies less *relative* accuracy for higher frequencies, because, for a given value of energy, the amplitudes of high frequency modes must get closer to zero as the frequency gets higher. For frequencies of order $O(h^{-1})$ only first-order relative accuracy is attained by the suggested methods and for frequencies of order $O(h^{-2})$ or greater no relative accuracy is attained. Hence, for high enough frequencies, the suggested methods do not resolve their contributions. If such frequencies are present, we might call the problem "stiff-oscillatory;" the suggested methods are then "stiff-oscillatory" solvers in the sense that they only resolve the oscillations that contribute with significant amplitudes.

If bounds for the impulse method are required that, like (3.2), are uniform over the choice of fast forces, then the order of convergence for p is 0 and the order of convergence for q is only one.

Figure 3.1 corresponds to a molecular dynamics simulation and plots energy versus time. The energy is a constant in the true solution and the advantages of the Long-Average method over the impulse method are evident. The simulation is for a 10 angstrom radius sphere of 125 flexible TIP3P water molecules at 377 K. The value of h is 5 fs. and the reduced problem is integrated by the Verlet method with $h_{\text{red}} = 1$ fs.

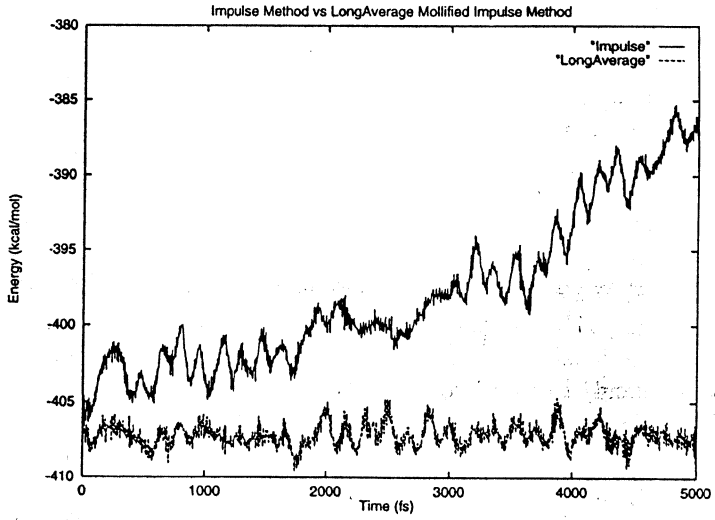

Figure 3.1: The Impulse and LongAverage methods in a large molecular dynamics problem. The horizontal axis is time. The vertical axis is energy; this is constant in the true solution

Unfortunately [1] the mollified methods also suffer from instability due to resonance. This instability is not nearly as pronounced as that of the impulse method.

4 A Partial Differential Equation Example

In this section we prove that the impulse method suffers from an order reduction when integrating the problem (1.4). It is enough to look at the simple case where $f = f(x)$ is independent of u. If the forcing term f is an odd function $f(x) \equiv -f(-x)$, then we have the sine expansions

$$u(x,t) = \sum_{m=1}^{\infty} a_m(t) \sin mx, \qquad f(x) = \sum_{m=1}^{\infty} f_m \sin mx,$$

and substitution in the differential equation shows that the Fourier coefficients are governed by the following set of uncoupled equations

$$\frac{d^2 a_m}{dt^2} = -m^2 a_m + f_m, \quad m = 1, 2, \ldots.$$

These are of the form (2.1) with arbit rarily high stiffness $-m^2$. The solution is readily found to be (a dot represents differentiation with respect to t)

$$\begin{aligned} a_m(t) &= \left(a_m(0) - \frac{f_m}{m^2}\right) \cos mt + \frac{\dot{a}_m(0)}{m} \sin mt + \frac{f_m}{m^2}, \\ \dot{a}_m(t) &= -m \left(a_m(0) - \frac{f_m}{m^2}\right) \sin mt + \dot{a}_m(0) \cos mt. \end{aligned} \tag{4.1}$$

¿From here we infer, via Parseval's formula, that a forcing term in the Sobolev space H^{r-2} and initial data $u(\cdot,0) \in H^r$, $u_t(\cdot,0) \in H^{r-1}$ yield a solution with $u(\cdot,t) \in H^r$, $u_t(\cdot,0) \in H^{r-1}$.

We now apply the impulse method to (1.4) with $h = 2\pi/M_0$, M_0 a large integer. Then, in a time step, for $m = \nu M_0$, ν integer, the m-th mode of the reduced system undergoes ν full cycles, and at $t = nh$ the numerical approximation of u_t has a coefficient (use the same argument that we used to derive (2.2))

$$\dot{A}_{\nu M_0}(nh) = \dot{a}_{\nu M_0}(0) + nh f_{\nu M_0}.$$

On the other hand, according to (4.1), the exact solution has

$$\dot{a}_{\nu M_0}(nh) = \dot{a}_{\nu M_0}(0).$$

Hence the νM_0 mode in u_t is in error by $nh f_{\nu M_0} = t f_{2\pi\nu/h}$ for each integer ν. By summing in ν we derive, via Parseval's formula, a lower bound for the spatial L_2 error in u_t proportional to

$$\text{lb} = t \left(\sum_{\nu=1}^{\infty} \left| f_{2\pi\nu/h} \right|^2 \right)^{1/2}.$$

	Impulse		LongAverage	
h	u_t	u	u_t	u
1/10	1.08×10^{-1}	3.82×10^{-3}	2.22×10^{-2}	1.07×10^{-2}
1/20	6.48×10^{-2}	9.24×10^{-4}	7.32×10^{-3}	2.71×10^{-3}
1/40	2.07×10^{-2}	2.45×10^{-4}	2.16×10^{-3}	6.82×10^{-4}
1/80	1.43×10^{-2}	5.87×10^{-5}	7.15×10^{-4}	1.71×10^{-4}
1/160	6.70×10^{-3}	1.47×10^{-5}	2.52×10^{-4}	4.27×10^{-5}
1/320	3.56×10^{-3}	3.66×10^{-6}	8.94×10^{-5}	1.07×10^{-5}

Table 4.1: Maximum errors over $0 \le t \le 2$ of the spatial L_2 norm of u_t, u when integrating a wave equation.

If f_m decays as $m^{-\alpha}$, $\alpha > 1/2$, then

$$\text{lb} \approx t \left(\frac{h}{2\pi}\right)^{\alpha} \left(\sum_{\nu=1}^{\infty} \frac{1}{\nu^{2\alpha}} \right)^{1/2}.$$

and the *L_2-order of convergence in u_t is at best α*. For piecewise smooth forcing terms with jump discontinuities, one has for each $\epsilon > 0$, $f \in H^{1/2-\epsilon}$, $u \in H^{5/2-\epsilon}$, $\alpha = 1$ and the impulse method cannot be any better than first order accurate.

We have numerically integrated from $t = 0$ to $t = 2$ the case where $u(x,0) \equiv 0$, $u_t(x,0) \equiv 0$, f odd, $f(x) = 1$ for $0 < x < \pi/2$, $f(x) = -1$, for $\pi/2 < x < \pi$. The spatial discretization is carried out with a pseudospectral Fourier (sine) method with a high number of modes, so that all errors shown are due to the discretization in time. The numerical results are displayed in Table 4.1 where the order reduction in u_t of the impulse method is apparent. For comparison we have also included the results corresponding to the LongAverage mollified method; the order of convergence in u_t is now 1.5 (the convergence of the mollified methods can be analyzed as in [1], section 6).

The example in this section is a translation to a partial differential equation setting of the ordinary differential equation example (2.1). The example of poor performance of the impulse method given in section 6 of [1] can be adapted in a similar way to yield examples of order reduction of the impulse method when applied to partial differential equations. The exact amount of order reduction for a given partial differential equation is governed by the errors in integrating the different modes and by the rate of decay of the Fourier coefficients a_m as a function of the wave number m, see the discussion in [4], section 6.3.

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