Mollified impulse methods revisited

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(I) INTRODUCTION
The problem: Multiple-time scale second-order ODEs

\[
\frac{d}{dt}p = f(q) + g(q), \quad \frac{d}{dt}q = M^{-1}p.
\]

- \( M \) symmetric, positive-definite \( d \times d \).

- \( g \) soft/slow, no fast modes.

- \( f \) strong/fast, gives fast modes (and possibly slow).
Assumption: The integration of the reduced problem
\[
\frac{dp}{dt} = f(q), \quad \frac{dq}{dt} = M^{-1}p.
\]
is cheaper than the integration of the full system. ($N$-body problems, analytic integration of reduced problem, PDEs, . . .)

Aim: Integrate using $g$ sparingly and at rate independent of the stiffness of reduced problem.
Method format: Step $n \rightarrow n + 1$, from $t_n = nh$, consists of

- **Kick:** $P_n^+ = P_n + \frac{h}{2} \tilde{G}_n$, with $\tilde{G}_n \approx g(q_n)$.

- **Oscillation:** Advance from $(P_n^+, Q_n)$ to $(P_{n+1}^-, Q_{n+1})$ with reduced flow.

- **Kick:** $P_{n+1} = P_{n+1}^- + \frac{h}{2} \tilde{G}_{n+1}$. 

**Impulse method:** Simplest choice, $\tilde{G}_n = g(Q_n)$ (Grubmüller and coworkers, Tuckermann/Berne/Martyna, multiple time-step Verlet).

Errors behave as $O(h^2)$ only if $h$ small with respect to fast periods. (Counterexamples in García-Archilla/SS/Skeel 98.)

**Mollified impulse methods (GA/SS/S):** Errors in $q/p$ are $O(h^2)/O(h)$ uniformly in stiffness; constants depend on energy of solution and bounds for $g$.

**Stiff Order/Order reduction:** Only $1/0$ for $q/p$ in impulse, $2/1$ in mollified.
**Scope:** GA/SS/98 restrict attention to conservative fast forces. They introduce a mollified impulse method for each choice of a so-called *weight* function. Their methods were constructed to be symplectic.

Here fast forces need not be conservative. Free choice of *two* weight functions. We may recover methods of a well-known family of exponential integrators.

Analysis based on weight functions (not filters). Simple necessary and sufficient condition for no order reduction.
(II) DESCRIPTION OF THE NEW METHODS
Some notation:

Denote by $\mathcal{P}(p,q,t)$, $\mathcal{Q}(p,q,t)$ the flow of the reduced system.

Combine $P_n$ and $Q_n$ into $Y_n = (P_n, Q_n)$ (similarly write $y(t) = (p(t), q(t))$, $\mathcal{Y} = (\mathcal{P}, \mathcal{Q})$, etc.).

Variational equation for Jacobian $\mathcal{Y}'(\alpha, t)$ of $\mathcal{Y}(\alpha, t)$

$$\frac{\partial}{\partial t} \mathcal{Y}'(\alpha, t) = \begin{bmatrix} 0 & f'(Q(\alpha, t)) \\ M^{-1} & 0 \end{bmatrix} \mathcal{Y}'(\alpha, t); \quad \mathcal{Y}' = \begin{bmatrix} \mathcal{P}_p & \mathcal{P}_q \\ \mathcal{Q}_p & \mathcal{Q}_q \end{bmatrix}.$$
Force format for kicks: Rather than $\bar{Q}_n = g(Q_n)$, use

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

$A(Q_n, h)$ is an average of values of $q$ and $M$ is a so-called mollifier matrix.

Weight functions: A wf is a bounded, integrable real-valued function $\chi(t)$ assumed even $\chi(-t) \equiv \chi(t)$ and to satisfy

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

(Note $\chi \geq 0$ not required.) Two wf used to specify each method, one $\phi$ defines the averaging, the other $\psi$ the mollifier.
Averaging: (\(\phi\) wf for averaging)

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

where \(q^*(t)\) is obtained by solving the reduced problem with initial conditions \(q = Q_n, p = 0\).

Since \(q^*\) is an even function of \(t\), the integrals are in practice replaced by twice their value over \((0, \infty)\).
**Mollification:** Find a matrix-valued function $Y'$ by integrating the variational problem ($q^*(t)$ as above)

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

with initial condition $Y'(0) = I_{2d}$.

Set ($\psi$ wf for averaging)

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

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

$$R(t) = [I_d, 0_d]Y'(t)^{-1}[I_d, 0_d]^T.$$
Motivation for mollifier: Impulse method equivalent to exact integration of

\[ \frac{d^2}{dt^2}q = f(q) + \sum_n \delta(t - t_n)g(Q_n), \]

where \( \delta \) is standard Dirac’s function.

Rather employ less abrupt versions

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

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

Forces \( \psi\left(\frac{(t - t_n)}{h}\right)G_n^* \) are incorporated into the solution of the reduced problem via Alekseev-Groebner (AG)/nonlinear variation of constants formula.
Since
\[ y(t_b) = \mathcal{V}(y(t_a), t_b - t_a) + \int_{t_a}^{t_b} \mathcal{V}'(y(s), t_b - s) \left[ g(y(s)) \right] ds, \]

the effect of \( \psi((t - t_n)/h)G^*_n \), acting while \( t \leq t_n \), is to add to the solution
\[
\left( \int_{-\infty}^{t_n} \mathcal{V}'(y(s), t_n - s)\psi\left(\frac{s - t_n}{h}\right) ds \right) \begin{bmatrix} G^*_n \\ 0 \end{bmatrix},
\]

which, using properties of flows, may be rewritten as
\[
\left( \int_{-\infty}^{t_n} \mathcal{V}'((0, Q_n), s - t_n)^{-1}\psi\left(\frac{s - t_n}{h}\right) ds \right) \begin{bmatrix} G^*_n \\ 0 \end{bmatrix},
\]

hence the recipe for the mollifier.
(III) PARTICULAR CASES
Conservative fast forces: \( f(q) = -\nabla W(q) \). Geometry of Hamiltonian flows imply \( \gamma'(\alpha, t)^{-1} = J^{-1} \gamma'(\alpha, t)^T J \). No need for inverting \((2d) \times (2d)\) Jacobian \( Y'\): instead mollify with

\[ R(t) = Q_q(t)^T, \]

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 \( Q_p(t) = 0_d, Q_q(t) = I_d \).

Hence if \( \psi = \phi \), we have as in GA/SS/S

\[ \mathcal{M}(Q_n, h) = A'(Q_n, h)^T. \]

If slow forces are also conservative \( g(q) = -\nabla U(q) \), then kicking force is \( \bar{G}_n = U(A(Q_{n+1}, h)) \), and method is symplectic.
**Linear fast forces:** \( f(q) = -Sq \), with \( S \) a stiffness matrix. Suppose that \( M^{-1/2}SM^{-1/2} \) possesses only real eigenvalues \( \geq 0 \) and can be diagonalized.

There exists a unique (in general, nonsymmetric) \( \Omega \) such that \( \Omega^2 = M^{-1/2}SM^{-1/2} \) and spectrum of \( \Omega \) is \( \geq 0 \). Reduced flow is rotation with matrix

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

with \( C(t) = \cos t\Omega \). (Trig. functions are deemphasized here.)
Averaging/Mollification in linear case: By definition

\[ A(Q_n, h) = M^{1/2} \left( \int_{-\infty}^{\infty} \cos sh\Omega \phi(s) \, ds \right) M^{-1/2} Q_n. \]

Introducing the Fourier transform of the even function \( \phi \)

\[ \hat{\phi}(\omega) = \int_{-\infty}^{\infty} \exp(-i\omega t) \phi(t) \, dt = \int_{-\infty}^{\infty} \cos \omega t \phi(t) \, dt, \]

average becomes

\[ A(Q_n, h) = A_h Q_n = \left( M^{1/2} \hat{\phi}(h\Omega) M^{-1/2} \right) Q_n. \]

Similarly

\[ M_h = M^{1/2} \hat{\psi}(h\Omega) M^{-1/2}. \]
**Filters:** Therefore for linear fast forces, methods can be described by/implemented through the associated filters $\hat{\phi}$ and $\hat{\psi}$, rather than in terms of the defining weights $\phi$ and $\psi$.

Methods here essentially reproduce a well-known family of exponential integrators (Hairer/Lubich). (Convergence studied by Hairer/Lubich/Wanner, Grimm/Hochbruck.)
(III) ANALYSIS: MOLLIFICATION

(From now, fast forces are linear, $M = I$.)

Notation:

• Function for kicking force: \( \bar{g}(\cdot) = \mathcal{M}_h g(A_h \cdot) \). At true solution: \( \bar{g}_n = \bar{g}(q_n) \).

• Averaged but unmollified force: \( g^*(\cdot) = g(A_h \cdot) \). At true solution: \( g^*_n = g^*(q_n) \).

• \( L_0, L_1, L_2 \) resp denote a bound for \( g \), a Lipschitz constant for \( g \) and a Lipschitz constant for the derivative of \( g \), when they exist.

• If \( g \) is Lipschitz continuous, then so are \( \bar{g} \) and \( g^* \) with constants \( \bar{L}_1 = \|\psi\|_1 L_1 \) and \( L^* = \|\psi\|_1 L_1 \|\phi\|_1 \).
Global errors bounded by quadrature errors: (Gronwall.)

Theorem 1. \( g \) Lipschitz continuous, \( P_0 = p(0) \) and \( Q_0 = q(0) \).

Employ a \((\phi, \psi)\)-method (\( \phi \) and/or \( \psi \) may be taken to be \( \delta \)).

Then global errors satisfies

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

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

where the quadrature errors \( \sigma_{p,n} \) \( \sigma_{q,n} \) are the first and second components of

\[
\sum_{j=0}^{n} h_{1_j} \left[ \frac{\cos(t_n - t_j)\Omega}{\Omega^{-1} \sin(t_n - t_j)\Omega} \right] \bar{g}_j - \int_0^{t_n} \left[ \frac{\cos(t_n - t)\Omega}{\Omega^{-1} \sin(t_n - t)\Omega} \right] g(q(t)) \, dt
\]

(\( 1_j \) is defined to be \( 1 \) except for \( 1_0 = 1_n = 1/2 \)).
• For *impulse method* $\sigma$ is error in trapezoidal rule!

• Since $h\Omega$ is not assumed small, $\cos(t_n-t)\Omega$ has an unbounded first derivative. Cannot expect to derive $O(h)$ error bounds for $\sigma_p$ that are uniform in $\Omega$.

• Possible to construct counterexample that shows that for $p$ quadrature error (and global error) is only $O(1)$.

• For $q$ component situation is better: $\Omega^{-1}\sin(t_n-t)\Omega$ has a bounded first derivative and standard theory leads to $O(h)$ error bounds for $\sigma_q$ and therefore for $Q_n - q_n$. 
When mollified forces are used, the quadrature error may be rewritten (invert the argument used to motivate the mollification formula) as

\[
\begin{bmatrix}
\sigma_{p,n} \\
\sigma_{q,n}
\end{bmatrix} = \int_{-\infty}^{\infty} \left[ \frac{\cos(t_n - t) \Omega}{\Omega^{-1} \sin(t_n - t) \Omega} \right] \sum_{j=0}^{n} 1_j \psi \left( \frac{t - t_j}{h} \right) g^*_j \, dt \\
- \int_{0}^{t_n} \left[ \frac{\cos(t_n - t) \Omega}{\Omega^{-1} \sin(t_n - t) \Omega} \right] g(q(t)) \, dt.
\]

As in Filon quadrature, now trig. functions are not interpolated!

Discrepancy in integration limits above eliminated in next lemma, which leaves us with an interpolation problem.
Lemma 1. For a mollified method $(\phi, \psi)$ (\(\phi\) may be the Dirac function) in which $\psi$ has bounded support and vanishes for $|t| > \mu > 0$, the quadrature error is of the form

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

where $I(t)$ is the interpolation error

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

and $\beta_n$ represents boundary effects and can be estimated as

\[
\|\beta_n\| \leq 2\mu(1 + t_n^2)^{1/2}\|\psi\|_1 L_0 h.
\]
The interpolation problem: Minimum requirement is to interpolate with no error the constant functions:

\[(*) \quad \sum_{j=-\infty}^{\infty} \psi(t-j) \equiv 1.\]

From the theory behind the Poisson summation formula, the rhs in (*) is a 1-periodic function \(\Psi\) whose Fourier series

\[\psi(t) = \sum_{n} c_n \exp(i2\pi nt)\]

has coefficients given by values of the Fourier transform of \(\psi\):

\[c_n = \int_{0}^{1} \exp(-i2\pi nt)\psi(t) dt = \int_{-\infty}^{\infty} \exp(-i2\pi nt)\psi(t) dt = \hat{\psi}(2\pi n).\]

Therefore (*) is equivalent to the condition

\[(**) \quad \hat{\psi}(2\pi n) = 0, \quad n = \pm 1, \pm 2, \ldots\]
Theorem 2. With the hypotheses of Theorem 1, assume that $g$ has a bounded derivative and that $\psi$ has bounded support and satisfies (*) or (**) ($\phi$ may be the Dirac function). Then the global error possesses a bound

$$\|P_n - p_n\| + \|Q_n - q_n\| \leq Ch$$

where the constant $C$ depends on $\psi$, $\phi$, $t_n$, $L_0$, $L_1$ and also on a bound $E$ for the reduced energy of the true solution

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

Conversely, if the $\psi, \phi$-method, where $\psi$ is boundedly supported and $\phi$ may be $\delta$, possesses a global error bound of this form, then (*) and (**) hold true.
(V) ANALYSIS: AVERAGING
From the variation AG formula:

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

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

or, after integration by parts,

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

Thus, one quadrature of the force builds up the momentum and two make \( q \) evolve. Hence expect that global error for \( q \) may be expressed by two quadratures. This is the subject of the next result.
Lemma 2. If $\psi$ is of bounded support, the quadrature error $\sigma_{q,n}$ satisfies

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

with $I^*$ equal to the integrated interpolation error

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

$\beta_n^*$ represent boundary contributions with

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

and, away from the boundaries, $\lambda_j(t) = \psi((t - t_j)/h)$. 

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To gain insight, look at integrated interpolation error at \( t = t_n \)

\[
I^*(t_n) = \sum_{j=0}^{n} h_1 j g^*_j - \int_{0}^{t_n} g(q(s)) \, ds.
\]

Again the trapezoidal quadrature if \( g^*_j = g(q_j) \). Idea: choose \( q^*_j \) so that

\[
h g^*_j \approx \int_{0}^{t_n} \phi\left(\frac{t - t_j}{h}\right) g(q(t)) \, dt
\]

Consistency again demands

\[
(†) \sum_{j=-\infty}^{\infty} \phi(t - j) \equiv 1, \quad \text{i.e.} \quad (††) \hat{\phi}(2\pi n) = 0, \quad n = \pm 1, \pm 2, \ldots
\]
Theorem 3. With the hypotheses of Theorem 1, assume that $g$ has a bounded, Lipschitz continuous derivative and that the weight functions $\phi$ and $\psi$ have bounded support and satisfy (*)-(**), (†)-(††). Then the global error possesses a bound

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

where the constant $C$ depends on $\psi$, $\phi$, $t_n$, $L_0$, $L_1$, $L_2$ and $E$.

Conversely, if the $(\psi, \phi)$-method with boundedly supported $\phi$ and $\psi$, has a bound of this form, then (*)-(**) and (†)-(††) hold.
(VI) WEIGHTS AND FILTERS
**Question:** If the filters (used for linear problems) are known, can we find weight functions that generated then?

**Paley–Wiener:** square integrable fnctn. \( \hat{\chi}(\omega) \) is the Fourier transform of a square integrable function \( \chi \) supported in \([-\nu, \nu]\), \( \nu > 0 \) if and only if \( \hat{\chi} \) can be extended to a holomorphic function of \( \omega \) in the whole complex plane with

\[
| \hat{\chi}(\omega) | \leq C \exp(\nu |\omega|).
\]

**Paley–Wiener space:** \( PW_{[-\nu,\nu]} \)
**Titchmarsh:** \( \hat{\chi} \) in \( PW_{[-\nu,\nu]} \) can be written in terms of its infinitely many zeros \( \omega_n \) as

\[
\hat{\chi}(\omega) = \hat{\chi}(0) \prod_n \left(1 - \frac{\omega}{\omega_n}\right).
\]

**Short filter:** Hence the choice in GA/SS/S

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

is the *minimal* filter. (\( \chi \) is 1 for \(-1/2 \leq t \leq 1/2\).) Other suggested choices: multiply the filter/take convolution of the weight.