Modified trigonometric integrators

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$$H(q,p) = \underbrace{\frac{1}{2}\|p\|^2 + \frac{1}{2}\|\Omega q\|^2}_{\text{fast, linear}} + \underbrace{W(q)}_{\text{slow, nonlinear}} \iff \begin{pmatrix} \Omega \dot{q} \\ \dot{p} \end{pmatrix} = \begin{pmatrix} 0 & \Omega \\ -\Omega & 0 \end{pmatrix} \begin{pmatrix} \Omega q \\ p \end{pmatrix} + \begin{pmatrix} 0 \\ -\nabla W(q) \end{pmatrix}$$

The matrix Ω is symmetric positive-semidefinite, e.g., $\Omega = \left(\begin{smallmatrix} 0 & 0 \\ 0 & \omega I \end{smallmatrix}\right)$ with $\omega \gg 1$.

$$p_n^+ = p_n - \frac{h}{2}\nabla W(q_n) \qquad\qquad p_n^+ = p_n - \frac{h}{2}\nabla W\left(\widetilde{\Phi}\widetilde{q}_n\right)$$

$$\begin{pmatrix} \Omega q_{n+1} \\ p_{n+1}^- \end{pmatrix} = \begin{pmatrix} \cos h\widetilde{\Omega} & \sin h\widetilde{\Omega} \\ -\sin h\widetilde{\Omega} & \cos h\widetilde{\Omega} \end{pmatrix} \begin{pmatrix} \Omega q_n \\ p_n^+ \end{pmatrix} \underset{\widetilde{\Phi}\widetilde{q}=q}{\overset{\widetilde{\Omega}\widetilde{q}=\Omega q}{\iff}} \begin{pmatrix} \widetilde{\Omega}\widetilde{q}_{n+1} \\ p_{n+1}^- \end{pmatrix} = \begin{pmatrix} \cos h\widetilde{\Omega} & \sin h\widetilde{\Omega} \\ -\sin h\widetilde{\Omega} & \cos h\widetilde{\Omega} \end{pmatrix} \begin{pmatrix} \widetilde{\Omega}\widetilde{q}_n \\ p_n^+ \end{pmatrix}$$

$$p_{n+1} = p_{n+1}^- - \frac{h}{2}\nabla W(q_{n+1}) \qquad\qquad p_{n+1} = p_{n+1}^- - \frac{h}{2}\nabla W\left(\widetilde{\Phi}\widetilde{q}_{n+1}\right)$$

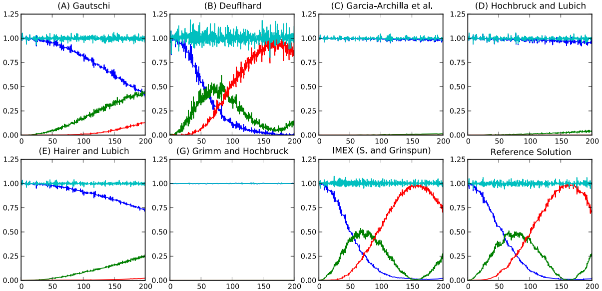
- Choosing $\widetilde{\Omega} = \Omega$ gives the **Deuflhard/impulse method**, which has problematic resonances.
- Choosing $h\widetilde{\Omega}/2 = \arctan(h\Omega/2)$ gives the **IMEX method**, which is symmetric, symplectic, consistent for slow energy exchange, and *nonresonant* (S. and Grinspun, SIAM MMS, 2009).
- Modulated Fourier expansion shows that energy exchange is dictated by three parameters, called α, β, γ. For the true solution, $\alpha = \beta = \gamma = 1$, but consistency requires only $\alpha = 1$.

Theorem (McLachlan and S.)

1. *Given $\widetilde{\Omega}$, there is a unique choice of filters giving a symmetric, symplectic method with $\alpha = 1$.*
2. *Deuflhard/impulse is the unique method with $\alpha = \beta = 1$.*
3. *IMEX is the unique method with $\alpha = \gamma = 1$.*

Fermi–Pasta–Ulam energy exchange comparison

$\omega = 50, \quad T = 200, \quad h = 0.1$:



Maximum deviation of adiabatic invariant $I_1 + I_2 + I_3$, scaled by ω

$h\omega/\pi \in (0, 4.5], \quad T = 1000, \quad h = 0.02$: