

Comparison of integrators for the Fermi-Pasta-Ulam problem.

R.I. McLachlan, D.R.J. O’Neale
(*Institute of Fundamental Sciences, Massey University*)
{r.mclachlan, d.r.oneale}@massey.ac.nz

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1 Overview and Introduction

We look at the Fermi-Pasta-Ulam problem with three stiff (fast) and three soft (slow) springs as it is given in [HLW06] (**I.5.1**).

$$H = \frac{1}{2} \sum_{i=1}^3 (y_{0,i}^2 + y_{1,i}^2) + \frac{1}{2} \omega^2 \sum_{i=1}^3 x_{1,i}^2 + \frac{1}{4} \left((x_{0,1} - x_{1,1})^4 + \sum_{i=1}^2 (x_{0,i+1} - x_{1,i+1} - x_{0,1} - x_{1,i})^4 + (x_{0,3} + x_{1,3})^4 \right)$$

- $x_{0,i}$: Scaled displacement of i th stiff spring.
- $x_{1,i}$: Scaled expansion (or compression) of the i th stiff spring.
- $y_{0,i}$ and $y_{1,i}$: The conjugate momenta of the above.

As in [HLW06], we use initial conditions: $x_{0,1}(0) = 1$, $x_{1,1}(0) = \omega^{-1}$, $y_{0,1}(0) = 1$, $y_{1,1}(0) = 1$ and all other entries are zero. I.e.

$$z(0) = [1, 0, 0, \omega^{-1}, 0, 0, 1, 0, 0, 1, 0, 0]^T.$$

The energy of the i th stiff spring is

$$I_j = \frac{1}{2} (y_{1,j}^2 + \omega^2 x_{1,j}^2)$$

and the total oscillatory energy $I = \sum_j I_j$ is an adiabatic invariant.

Here we look at the leap-frog method, the mid-point rule and trigonometric integrators in their symmetric¹ one-step formulation of eqns (2.7) and (2.8) of [HLW06] (**XIII.2.2**). The methods are then characterised entirely by their filter functions which we give below (Table 1); (A)-(E) are from [HLW06] (**XIII.2.2**), (G) is from [GH06].

	$\psi(\xi)$	$\phi(\xi)$	
(A)	$\text{sinc}^2(\frac{1}{2}\xi)$	1	Gautschi (1961)
(B)	$\text{sinc}(\xi)$	1	Deuffhard (1979)
(C)	$\text{sinc}^2(\xi)$	$\text{sinc}(\xi)$	García-Archilla et al. (1999)
(D)	$\text{sinc}^2(\frac{1}{2}\xi)$	$\text{sinc}(\xi)(1 + \frac{1}{3}\sin^2(\frac{1}{2}\xi))$	Hochbruck and Lubich (1999)
(E)	$\text{sinc}^2(\xi)$	1	Hairer and Lubich (2000)
(G)	$\text{sinc}^3(\xi)$	$\text{sinc}(\xi)$	Grimm and Hochbruck (2006)

Table 1: Filter functions for the various trig integrators

The methods are symplectic if and only if $\psi(\xi) = \text{sinc}(\xi)\phi(\xi)$, methods (B) and (C) are therefore the only symplectic trig integrators on our list. although the trig methods are not symplectic in general, one can show that they preserve a modified symplectic form [HLW06] (**XIII.11-(3)**). For short (i.e. $T = 1$) time periods and small (i.e $h \rightarrow 0$) step size all the methods are second order accurate in position; see [HLW06] (**XIII.2.3**). Beyond the small step size regime this changes, but since the system is chaotic, global errors are, perhaps, not sensible quantities to study. For this reason we use quantities such as the change in the Hamiltonian to quantify the accuracy of the methods.

One of the notable features of the trig methods is that they can suffer from resonances at integer multiples of π causing large errors in various quantities. One can try to use the filter functions to prevent this, possibly at the expense of causing other unwanted phenomena.

2 Resonances for a planar problem

The problem of resonances for numerical integrators can be most easily and dramatically illustrated for a planar Hamiltonian system.

The resonances which affect the trig integrators at odd and even multiples of π are order two and one resonances respectively. These resonances are typically unstable (result in unbounded growth with time). The trig integrators can also suffer from order three resonances; these are also typically unstable but are slower to increase than the lower order resonances. The order three resonance occurs at $h\omega/\pi = 2/3$ for the trig integrators and at $h\omega/\pi = 2\sqrt{3}/\pi \simeq 1.1$ for the mid-point rule. Order four resonances (at $h\omega/\pi = \frac{1}{2}$ for the trig methods, $h\omega/\pi = 2/\pi \simeq 0.64$ for the mid-point rule) can be either stable or unstable but typically have smaller magnitude/growth than the lower order resonances. Higher order resonances are generally stable[Arn89].

The analysis in [SS00] shows that for a planar Hamiltonian system

$$H(q, p) = \frac{1}{2}p^2 + \frac{1}{2}\omega^2 q^2 + \frac{1}{3}Bq^3 + \frac{1}{4}Cq^4 + \mathcal{O}(q^5) \quad (1)$$

¹The method is symmetric $\Leftrightarrow \psi(\xi) = \text{sinc}(\xi)\psi_1(\xi)$, $\psi_0(\xi) = \cos(\xi)\psi_1(\xi)$

the order three and four resonances of the midpoint rule occur for $h = \frac{2}{\omega}\sqrt{3}$ and $h = \frac{2}{\omega}$ respectively. The order three resonances are unstable at equilibrium whenever the potential has a cubic term ($B \neq 0$) while the order four resonances are unstable at equilibrium when $(\omega^2 C - B^2)(\omega^2 C - 2B^2) < 0$.

We take the system given by (1) with $B = C = -1$ and, fixing the step size at $h = 0.02$ we vary ω such that $0 < h\omega/\pi \leq 4.5$. Figure 1 shows the maximum deviation in the Hamiltonian for integration over the interval $[0, 1000]$.

The widths of the resonant bands for the symplectic trigonometric method (B) appear to render it unusable. Method (A) fares slightly better due to the absence of the wide resonant spikes at even multiples of π . Methods (C) and (G) seem to give excellent results, though we will see later that this is not the case in general.

The mid-point rule is not affected by resonances of order lower than three because its eigenvalues are limited to $\exp(i\theta)$, $\theta \in (0, \pi)$.

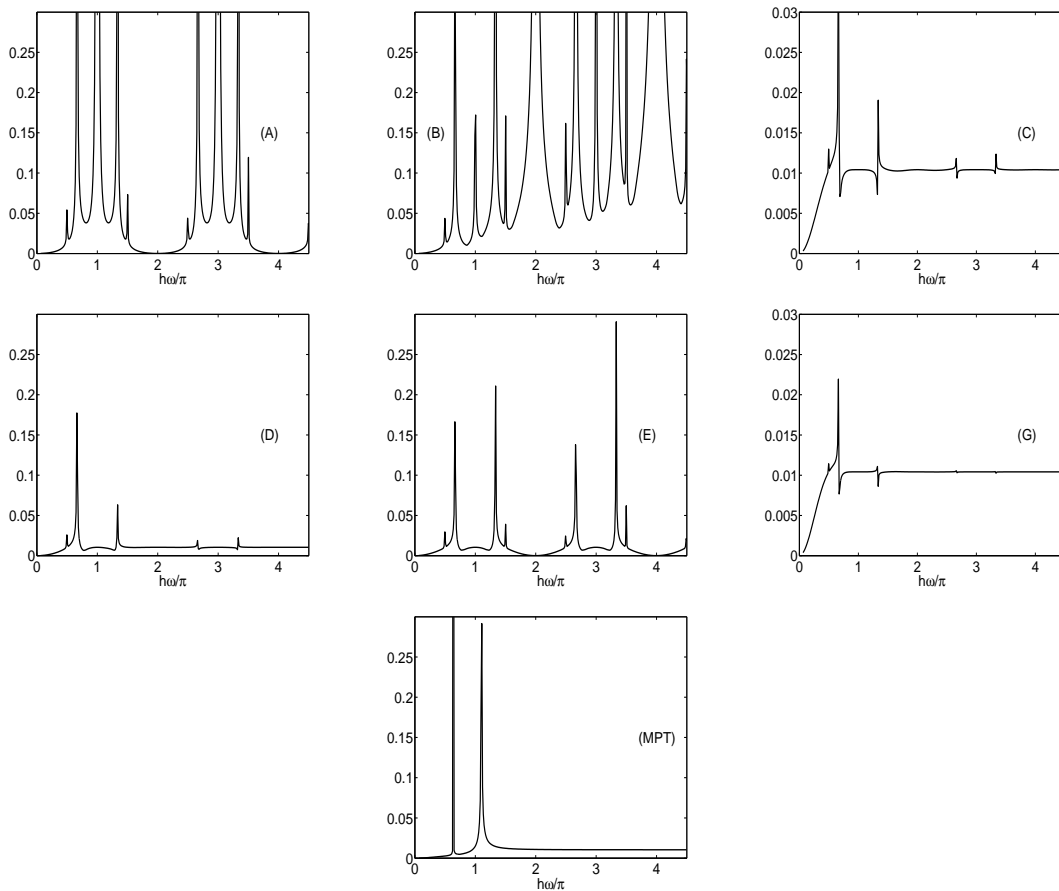


Figure 1: Maximum error of total energy on the interval $[0, 1000]$ as a function of $h\omega/\pi$ for the Hamiltonian $H(q, p) = \frac{1}{2}p^2 + \frac{1}{2}\omega^2 q^2 - \frac{1}{3}q^3 - \frac{1}{4}q^4$, (step size $h = 0.02$). Note the different vertical axis for methods (C) and (G).

3 Energy Deviation: Fixed Step Size

The FPU problem is Hamiltonian — its energy is an invariant quantity. Since the system is chaotic it doesn't make sense to look at the global error (in position) of an individual orbit, except for very short integration lengths. Therefore, to illustrate the effect of resonances on the numerical solutions we look at the errors in the energy of a numerical solutions for fixed step size and integration length. In figure 2 we plot the maximum deviation in the energy over the interval $[0, 1000]$ as a function of $h\omega/\pi$ for fixed $h = 0.02$.

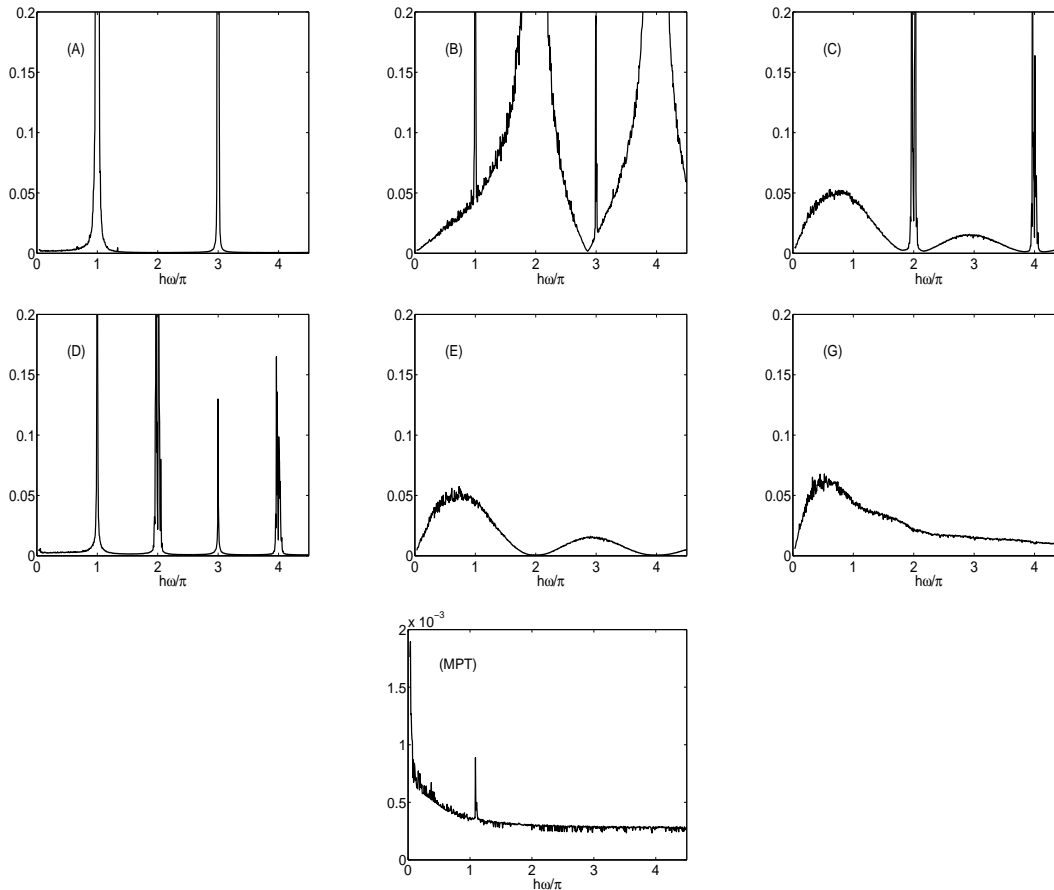


Figure 2: Maximum error of total energy on the interval $[0, 1000]$ as a function of $h\omega/\pi$, (step size $h = 0.02$). Note the different vertical axis for (MPT).

In figure 2 the trig methods don't appear to show any of the order three and four resonances that were so clear for the planar system. This is due to relatively slow growth of these higher order resonances combined with the relatively short integration length. For longer integration times these resonances become apparent. We illustrate this in figure 3 by plotting the value of the Hamiltonian for three choices of step size using method (A) with an integration time roughly ten times longer than those used in figure 2. We take one step size $h = 2\pi/(3\omega) \simeq 0.0419$ on the order three resonance and two step sizes immediately either side of the resonant value; $h = 0.044$ and $h = 0.04$.

We observe that the maximum energy error is no longer bounded for the resonant step size.

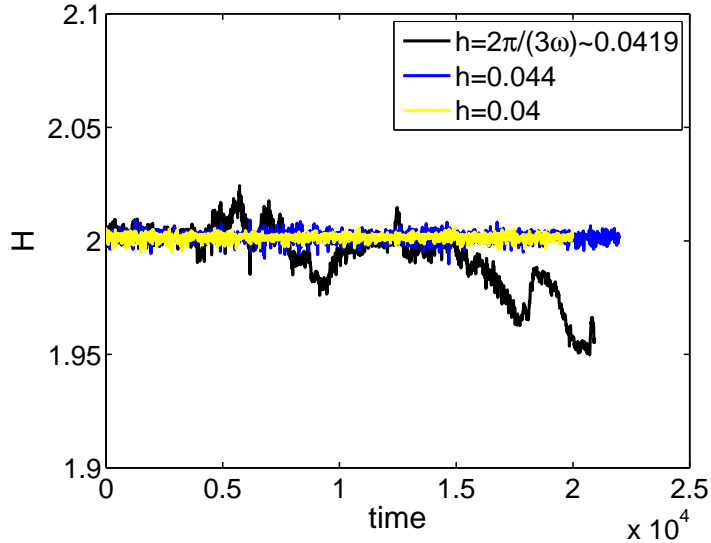


Figure 3: Total energy of solutions calculated with method (A) for step sizes slightly below ($h = 0.04$), on ($h = 2\pi/(3\omega) \simeq 0.0419$, $\omega = 50$), and slightly greater than ($h = 0.044$) the resonant value.

4 Oscillatory Energy Deviation: Fixed Step Size

The oscillatory energy $I = \sum_j I_j$ of the FPU system is not a conserved quantity but, rather, an adiabatic invariant: a nearly conserved quantity which oscillates about its mean value with some standard deviation. The standard deviation of I is therefore possibly a better characterisation of the oscillatory energy than the maximum deviation. We show both in figure 4 in order to compare the trig methods and the mid-point rule. All the methods with the exception of the trig integrator (G) and the mid-point rule can be seen to be severely affected by resonances.

The exact solution of the FPU problem has $I(t) = Const. + \mathcal{O}(\omega^{-1})$. That is, the standard deviation of the total oscillatory energy as a function of ω should look like $C\omega^{-1}$. In most of the examples of figure 4 this general pattern can be seen away from the resonant frequencies.

We used a very long ($T = 1 \times 10^6$) integration period and a small ($h = 0.002$) time step which resolved all the fast oscillations (for $\omega = 50$) to calculate, σI , the standard deviation of the oscillatory energy. This allowed us to determine the value of coefficient ($C = 0.75$) and give a reference solution for the behaviour of $\sigma I(\omega)$. Figure 5 shows $\sigma I/\omega$ minus the reference solution, that is we plot $\sigma I\omega - 0.75$ against $h\omega/\pi$, again, for fixed step size $h = 0.02$. We can see that for the trig method (G), the cost of preventing resonances is to also prevent the correct behaviour of the oscillatory energy. The only methods which manages to approximate the correct behaviour, (a horizontal line at zero), is the mid-point rule. The trig methods (A) and (D) show the correct behaviour away from resonant values of ω .

For fixed $h\omega$ the value of $\omega\sigma I$ does not converge to the correct value as $h \rightarrow 0$.

5 Energy Conservation: Fixed $h\omega$

Results for symplectic integrators concerning approximate energy conservation and preservation of a modified Hamiltonian hold in the limit of small step size. As the step size increases, one see the difference between the modified Hamiltonian and the original one grow — the energy

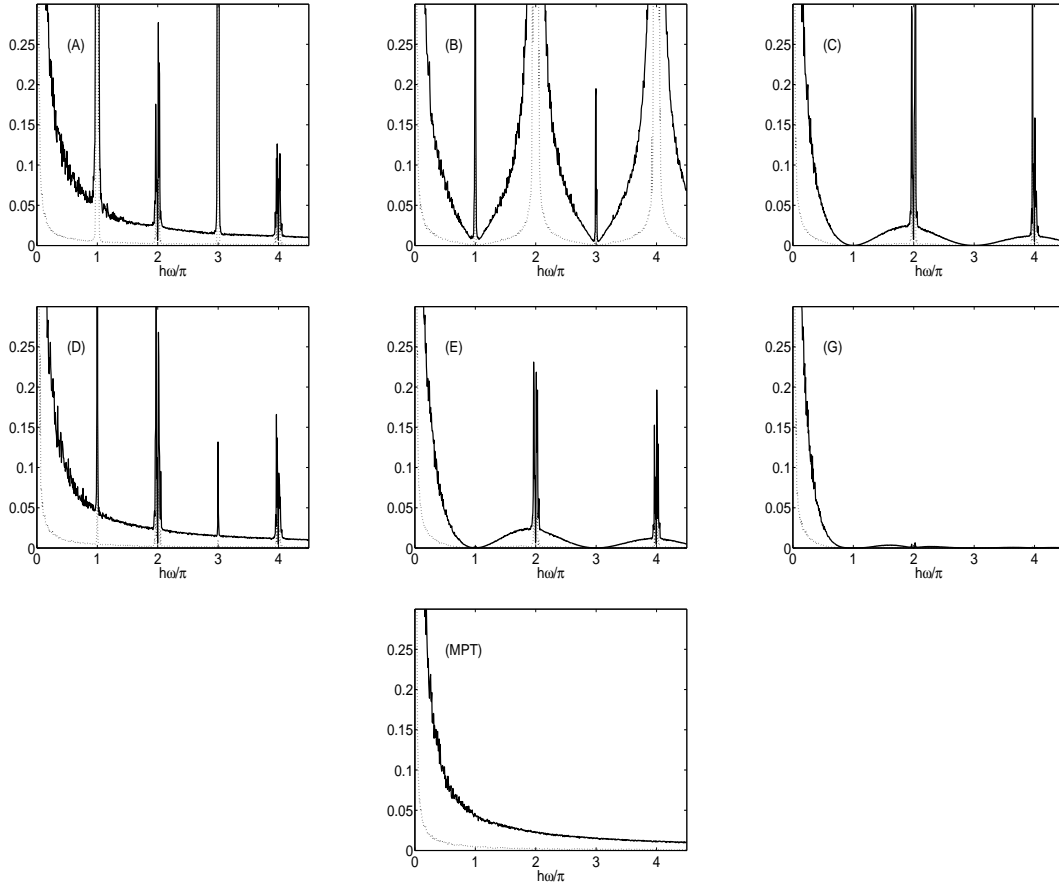


Figure 4: Maximum (*solid*) and standard (*dotted*) deviation of the oscillatory energy on the interval $[0, 1000]$ as a function of $h\omega/\pi$, (step size $h = 0.02$).

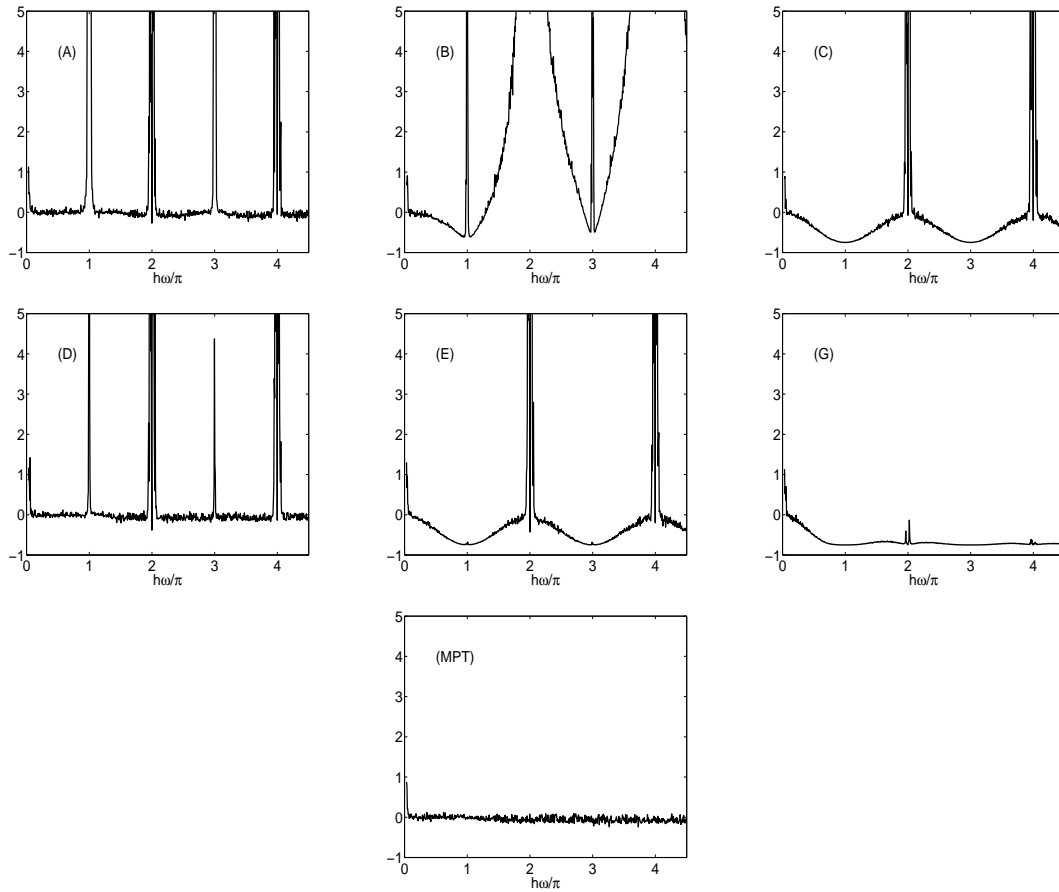


Figure 5: Standard deviation of oscillatory energy, on the interval $[0, 1000]$, scaled by ω and shifted by a reference solution, (i.e. $\sigma I(\omega)\omega - 0.75$) as a function of $h\omega/\pi$, (step size $h = 0.02$).

of the numerical solution oscillates with greater amplitude as step size increases and backward error analysis — the usual tool for showing near-conservation of energy — no longer holds.

For linear systems $f(z) = Az$, the condition (on the filter functions ϕ and ψ) for a numerical (trig) method to conserve total energy up to $\mathcal{O}(h)$, independent of $h\omega$, is incompatible with the condition for a (trig) method to be symplectic. Since symplectic methods are not exactly energy conserving either, a fair question to ask is how well a particular numerical method is able to approximately conserve the total energy and how much extra work is needed in order to get better conservation of energy. That is, what is the order of the numerical scheme with respect to energy conservation.

In figure 6 we fix $h\omega = 0.5, 1.5$ and 5 and let h (and ω) vary. We plot the maximum deviation in the total energy on the interval $[0, 1000]$ against the step size h and use this to show the orders of the schemes with respect to energy conservation. The trig methods (E) and (G) satisfy a condition

$$\phi(\xi) = \text{sinc}^2(\xi)\phi(\xi) \tag{2}$$

necessary for the methods to conserve total energy up to $\mathcal{O}(h)$ independent of $h\omega$ for *linear* problems [GH06], [HL00]. Methods (B), (C) and, of course, the mid-point rule are symplectic.

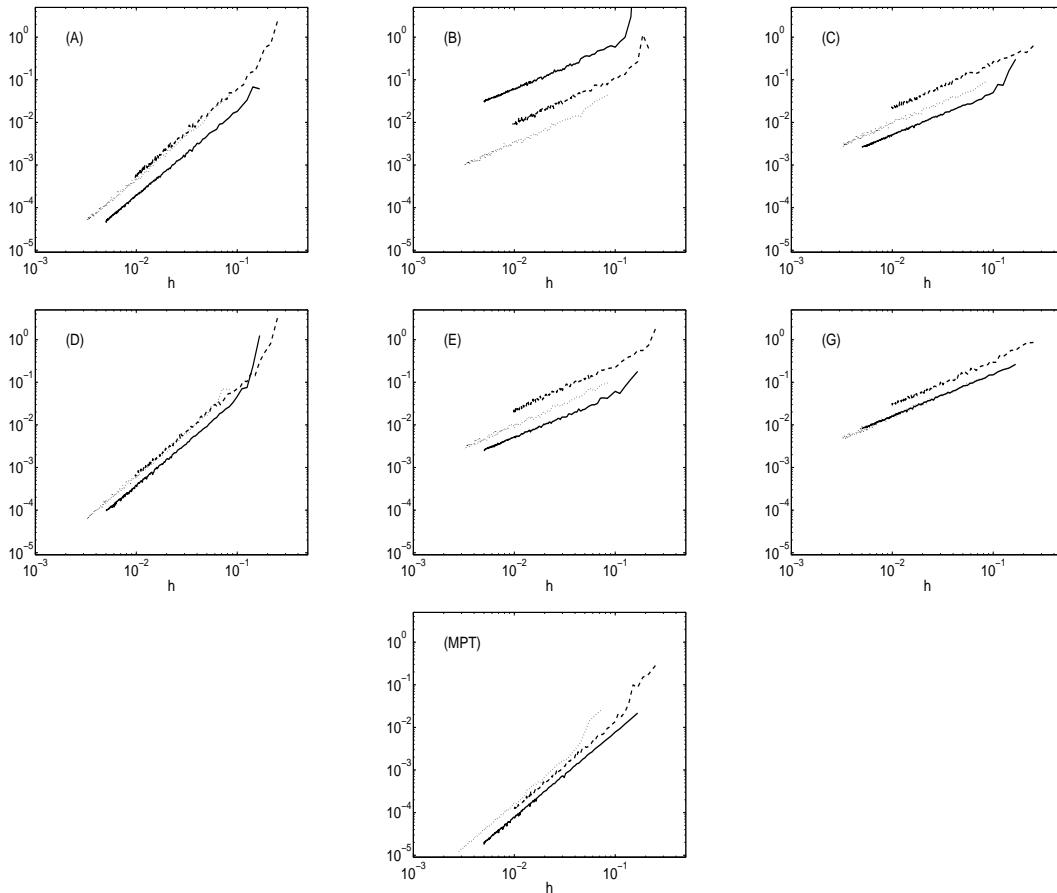


Figure 6: Maximum deviation in the total energy on the interval $[0, 1000]$ as a function of h for fixed $h\omega = 0.5$ (dotted), $h\omega = 1.5$ (dashed) and $h\omega = 5$ (solid).

Curiously, apart from the mid-point rule, the only other methods which are second order

for energy conservation are methods (A) and (D) which are not symplectic and do not satisfy the above condition (2) for finite-energy of linear problems. However, these are precisely the methods which correctly captured the ω^{-1} behaviour for the oscillatory energy deviation (away from resonances) in figures 4 and 5. They also satisfy a condition necessary for $\mathcal{O}(h^2)$ energy conservation [HLW06] (XIII.11-(8))

6 Slow Exchange of Oscillatory Energy

The FPU problem exhibits a slow exchange of energy between the stiff springs, that is, the distribution of I between I_1 , I_2 and I_3 changes with time. These effects take place on a time scale $t = \mathcal{O}(\omega)$. A good numerical method should capture the rate of the slow exchange and should give correct statistics for the mean distribution of energy between the stiff springs. For the trig integrators to correctly approximate the slow exchange it is necessary that their filter functions satisfy

$$\psi(h\omega)\phi(h\omega) = \text{sinc}(h\omega), \quad (3)$$

[HLW06] (XIII.4.2).

Here we show the oscillatory energy in the stiff springs and the total oscillatory (figure 7) energy on the interval $[0, 200]$ for the trig integrators and the mid-point rule for $\omega = 50$ with step size $h = 0.03$. For comparison we include the same results computed using the leap-frog integrator using a smaller step size ($h=0.001$) so that all the fast oscillations are resolved.

Of the trig methods, only method (B) satisfies the slow exchange condition (3). For the values used here, $h\omega = 1.5$, method (D) almost satisfies (3) with $\psi(1.5)\phi(1.5) \simeq 0.95\text{sinc}(1.5)$ which accounts for its good behaviour. Method (A) gets the energy exchange slightly too fast while method (E) and the mid-point rule get the exchange slightly too slow, methods (C) and (G) get the exchange slower still.

Although it doesn't get the rate of exchange correct for the oscillatory energy, the mid-point rule is the only method for which the energy in I_1 decreases all the way to zero before increasing again — the behaviour seen in the reference solution. The trig methods transfer only a portion of the oscillatory energy between springs for this value of $h\omega$.

The condition for correctly approximating the slow exchange depends on $h\omega$. That is, for fixed ω the methods will give different rates of slow exchange for different step sizes — a purely numerical property since the rate of exchange should depend only on the parameters of the FPU problem itself. In figure 8 we plot I_1 , the energy in the first stiff spring on the interval $[0, 200]$ and with $\omega = 50$. We use three different step sizes so that $h\omega$ takes in the values 0.5, 1.5 and 5.

Getting the slow exchange correct independent of $h\omega$ is a much tougher requirement for a numerical method with all the methods apart from (B) performing badly when $h\omega$ is large. It might be sensible to ask questions about how quickly the behaviour for the slow exchange converges to the correct behaviour as $h\omega$ decreases. Since the point of the trig integrators is to be able to take step sizes larger than those allowed by traditional restrictions on $h\omega$ (most M.D. calculations use a rule-of-thumb of $h\omega = 0.1$) one could ask 'What is the slow exchange behaviour for $h\omega$ small but above the traditional limits?'

We also note that the amount of oscillatory energy transferred between springs is a function of $h\omega$. For example, method (B) has the correct *rate* of oscillatory energy transfer independent of $h\omega$ but transfers the correct *amount* of oscillatory energy only as $h\omega \rightarrow$.

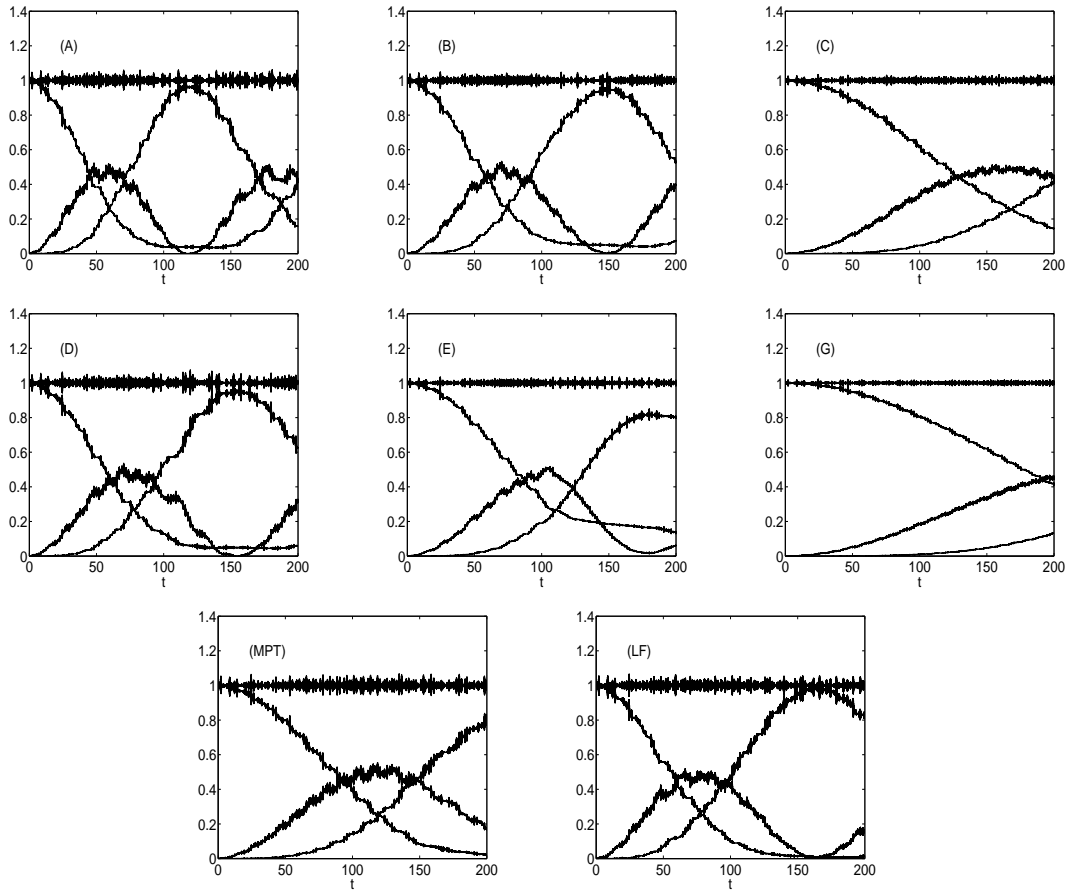


Figure 7: Oscillatory energy exchange between stiff spring on the interval $[0, 200]$ for fixed step size $h = 0.03$ and with $\omega = 50$. The solution for the leapfrog method, (LF), was computed with step size $h = 0.001$, resolving all oscillations (i.e. $h\omega = 0.05$.)

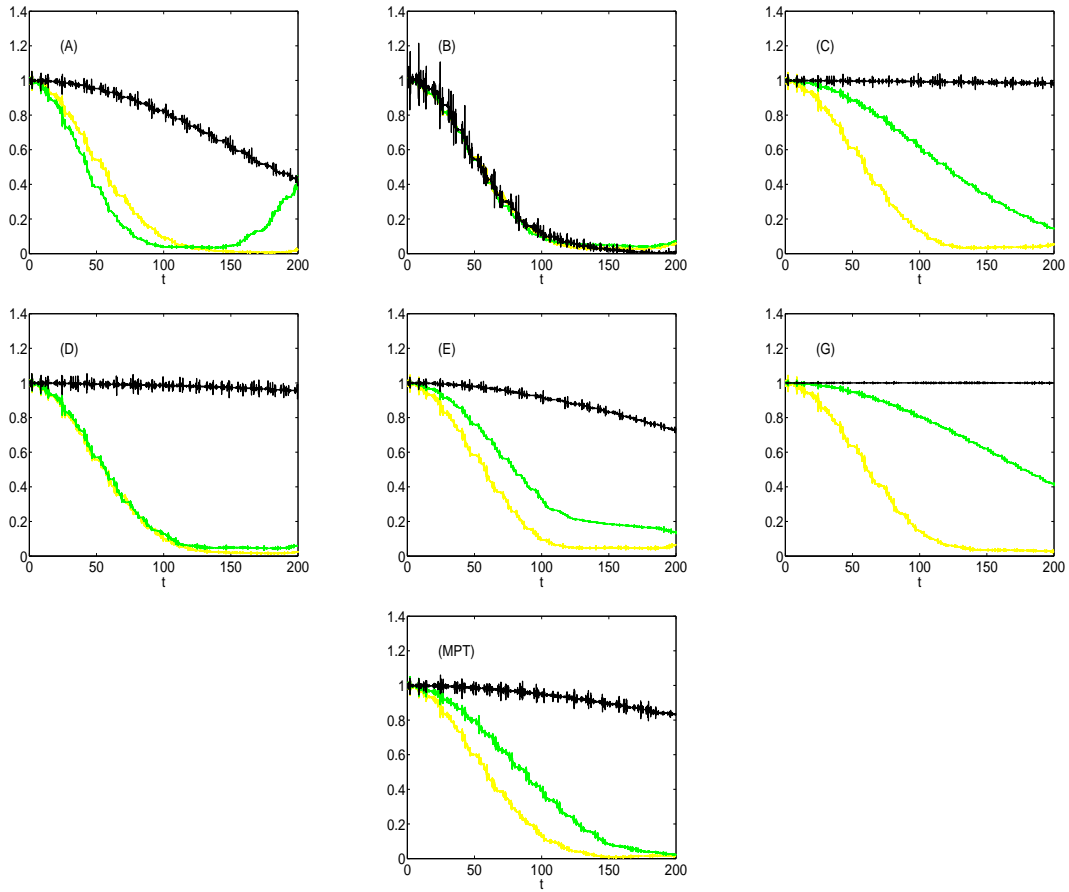


Figure 8: Oscillatory energy in the first stiff spring, on the interval $[0, 200]$ and with $\omega = 50$ for step sizes $h = 0.01$ (*yellow/lightest*, $h\omega = 0.5$), $h = 0.03$ (*green*, $h\omega = 1.5$) and $h = 0.1$ (*black/darkest*, $h\omega = 5$).

7 Long-time/Statistical Properties

We saw in section 6 that the slow exchange of energy between the stiff springs is a difficult property to capture for numerical methods. Here we give some long-time results for the FPU problem. That is, we ask whether the numerical schemes get the correct mean values and distributions for the energy in the stiff springs. We used an integration interval of $[0, 1 \times 10^6]$ and frequency $\omega = 50$ for the fast oscillation. The step size was fixed at $h = 0.02$ for the trig methods and the mid-point rule. As a reference solution, we use the leap-frog method with $h = 0.002$, a step size small enough to resolve the fast oscillations. We saved every 100th data point for the trig methods and mid-point rule and every 1000th for the leap-frog method. We present, in table 2, the average values of the oscillatory energy in each of the stiff springs, the standard deviation in the total oscillatory energy and the relative maximum deviation in the Hamiltonian for each of the methods.

It is worth noting that for these calculations $h\omega = 1$ is only moderately large; $h\omega = 2.5$, for example, would give dramatically different results.

	\bar{I}_1	\bar{I}_2	\bar{I}_3	σI	$\Delta_{max} H/H^{ref}(0)$
(A)	3.367e-01	3.279e-01	3.360e-01	1.475e-02	1.290e-03
(B)	3.273e-01	3.466e-01	3.266e-01	1.312e-02	7.800e-03
(C)	3.341e-01	3.300e-01	3.363e-01	1.137e-02	2.221e-02
(D)	3.378e-01	3.262e-01	3.366e-01	1.477e-02	1.616e-03
(E)	3.319e-01	3.373e-01	3.311e-01	1.123e-02	2.188e-02
(G)	3.207e-01	3.597e-01	3.199e-01	9.198e-03	3.280e-02
mid-pt	3.400e-01	3.197e-01	3.408e-01	1.468e-02	3.789e-04
leap-frog	3.377e-01	3.243e-01	3.385e-01	1.496e-02	2.514e-03

Table 2: Mean values of I_1 , I_2 and I_3 , standard deviation in the total oscillatory energy and maximum deviation of the total energy for the trig methods, the mid-point rule and the leap-frog method calculated on the interval $[0, 1 \times 10^6]$ with $\omega = 50$. The calculations with the trig methods and the mid-point rule used a step size of $h = 0.02$ and saved every 100th point for the statistics. The calculation with the leap-frog method used $h = 0.002$ which resolves all the fast oscillations to give a reference solution. For the leap-frog method, every 1000th point was saved.

Another way to look at the data in table 2 is to subtract the leap-frog reference values from each row and then look at the absolute mean $\frac{1}{3} \sum |\bar{I}_j - \bar{I}_j^{ref}|$ of the differences. We present this data in table 3 along with the relative differences between the standard deviations of the total oscillatory energy and the reference value and the relative errors in each of the I_j .

The methods which give the best results for the long-time statistics for the mean difference in the oscillatory energy with respect to the reference solution are the trig methods (A) and (D) and the mid-point rule — the same methods which did well at capturing the total oscillatory energy (see section 4).

In addition to getting the average values I_j , $j = 1, 2, 3$ correct, a numerical method should give the correct distribution of I_j values, that is, it should visit the appropriate parts of the I_j phase space for the correct amounts of time. We try to visualise this for the various methods by plotting contours of the probability distribution functions for I_1 and I_2 . For clarity we show only the contours higher than the average values of the reference solution. The reference solution shows quite a lot of structure with certain regions of the $I_1 - I_2$ plane preferred over other regions. None of the methods considered here manage to capture all of the structure correctly.

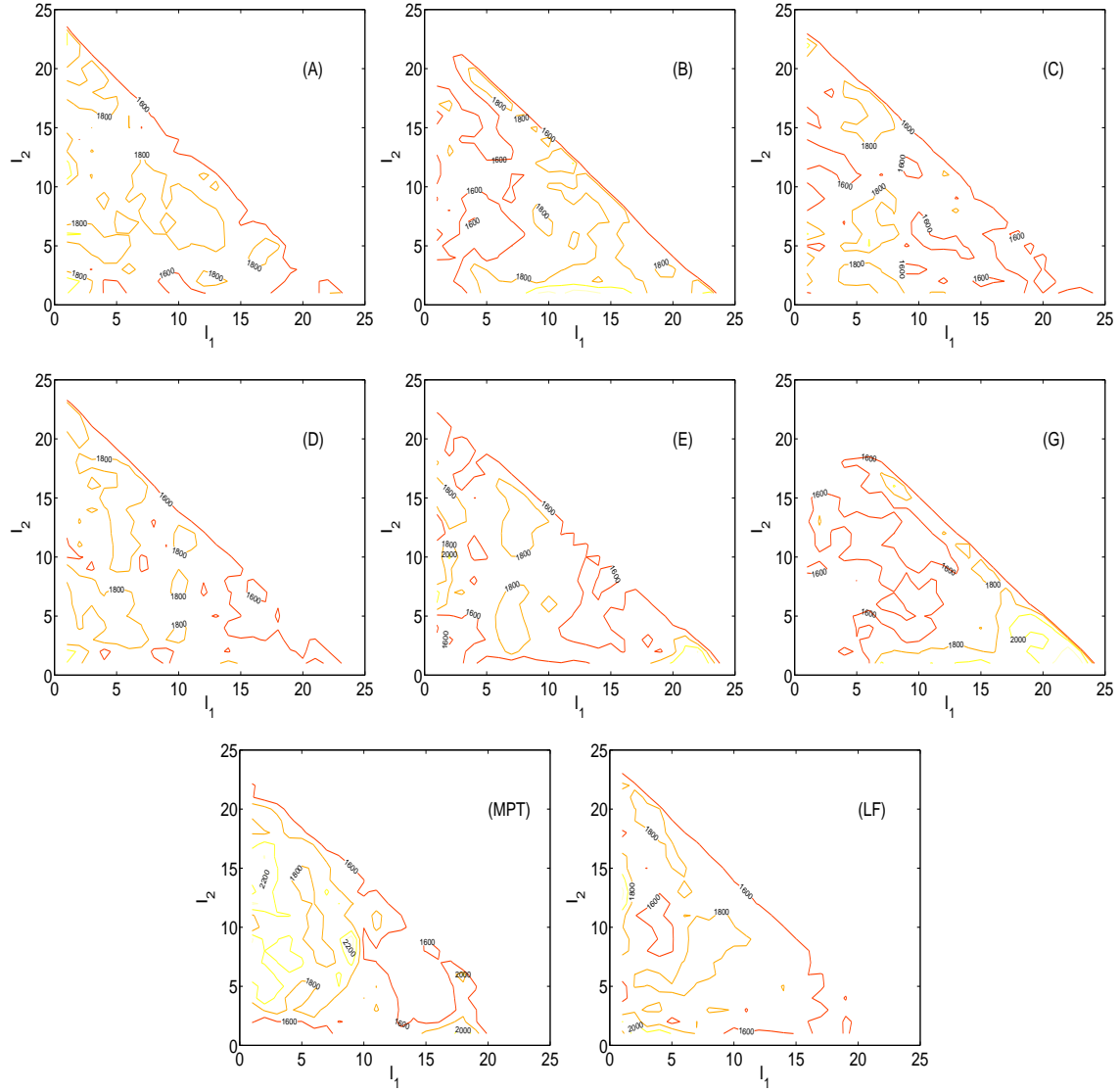


Figure 9: Contour plots of the upper portion of the probability distribution functions of I_1 and I_2 for solutions on the interval $[0, 1 \times 10^6]$ with $\omega = 50$ and $h = 0.02$ (every 100th point saved), except for the leap-frog solution which used $h = 0.002$, to resolve all oscillations and saved every 1000th point. Lighter shading corresponds to higher frequency count.

	$\frac{\bar{I}_1 - \bar{I}_1^{ref}}{\bar{I}_1^{ref}}$	$\frac{\bar{I}_2 - \bar{I}_2^{ref}}{\bar{I}_2^{ref}}$	$\frac{\bar{I}_3 - \bar{I}_3^{ref}}{\bar{I}_3^{ref}}$	$\frac{\sigma I - \sigma I^{ref}}{\sigma I^{ref}}$	$\frac{1}{3} \sum \bar{I}_j - \bar{I}_j^{ref} $
(A)	-3.11e-03	1.10e-02	-7.40e-03	-1.46e-02	2.37e-03
(B)	-3.09e-02	6.86e-02	-3.51e-02	-1.23e-01	1.49e-02
(C)	-1.07e-02	1.73e-02	-6.61e-03	-2.40e-01	3.82e-03
(D)	1.76e-04	5.88e-03	-5.78e-03	-1.27e-02	1.31e-03
(E)	-1.72e-02	4.01e-02	-2.18e-02	-2.50e-01	8.74e-03
(G)	-5.04e-02	1.09e-01	-5.51e-02	-3.85e-01	2.37e-02
mid-pt	6.65e-03	-1.41e-02	6.84e-03	-1.92e-02	3.05e-03

Table 3: Differences between the I_j and σI of table 2 and the reference solutions computed using leap-frog, along with the absolute mean of the differences in I_j .

8 Conclusions

1. Order three resonances are generally unstable and cannot be avoided, as a consequence the trig integrators are unstable for $3h\omega = 2n\pi$, $n \in \mathbb{Z}$.
2. It is not enough to have, for example ΔI bounded; one also wants the correct distribution of I .
3. None of the trig methods manage to capture all properties and some perform worse than the mid-point rule.

Table 4 gives a comparison of the trig methods and the midpoint rule for a selection of criteria. It is far from exhaustive. Other sensible measures of performance might include long time averages, e.g. Lyapunov exponents.

	(A)	(B)	(C)	(D)	(E)	(G)	(MPT)
$H(h\omega)$	✓	×	✓	✓	✓	✓	✓✓
$H(h)$	$\mathcal{O}(h^2)$	$\mathcal{O}(h)$	$\mathcal{O}(h)$	$\mathcal{O}(h^2)$	$\mathcal{O}(h)$	$\mathcal{O}(h)$	$\mathcal{O}(h^2)$
I	✓	×	×	✓	×	×	✓
dI_j/dt	×	✓	×	×	×	×	×
I_j stats	×	×	×	×	×	×	×

Table 4: A quick comparison of the performance of various methods.

It is also sensible to ask if there are trig integrators of a wider class which may get more properties correct. One possibility may be to use more force evaluations allowing more free parameters which can be chosen to capture more properties.

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