Reconsidering Trigonometric Integrators

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Overview

1. Motivation: GRK with $h\omega$ large.
2. Intro to trig integrators and a planar problem.
3. Intro to the F.P.U. problem
4. Numerical results and observations. (But what to observe?)
Motivation

What is the nonlinear stability behaviour of GRK methods for $h\omega$ large?

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

Methods remain stable, even for $h\omega \gg 1$, except at resonances.

Example

<table>
<thead>
<tr>
<th>Method</th>
<th>Order Resonances</th>
</tr>
</thead>
<tbody>
<tr>
<td>GRK1/midpoint</td>
<td>3rd &amp; 4th order resonances</td>
</tr>
<tr>
<td>GRK2</td>
<td>2nd, 3rd &amp; 4th order resonances</td>
</tr>
<tr>
<td>GRK3</td>
<td>1st, 2nd, 3rd &amp; 4th order resonances</td>
</tr>
</tbody>
</table>
Resonant step sizes are determined by the (linear) stability function
\[ R(z) = \frac{P(z)}{Q(z)} = \exp(i\theta), \quad z = h\lambda \]
We get order \( n \) resonance with \( h \) such that \( \theta = \frac{2\pi}{n}, \quad n \in \mathbb{N} \)

**Example**

The midpoint rule: \[ R(Z) = \frac{1+z/2}{1-z/2}, \quad z = \pm \omega i, \text{ i.e. } \theta \to \pi \text{ as } h \to \infty \]

3rd order resonances are generically unstable (Arnold, 1989).
4th order resonances can be stable or unstable (Skeel & Srinivas, 2000).
Motivation

Resonant step sizes are determined by the (linear) stability function $R(z) = P(z)/Q(z) = \exp(i\theta)$, $z = h\lambda$

We get order $n$ resonance with $h$ such that $\theta = 2\pi/n$, $n \in \mathbb{N}$

Example

The midpoint rule: (for the pendulum)
Why don’t trig integrators display these order three and four resonances?
2nd order DEs

\[ \ddot{y}(t) = -Ay(t) + g(y(t)), \quad A = \Omega^2 \]

Solution:

\[
\begin{bmatrix}
    y(t) \\
    \dot{y}(t)
\end{bmatrix} = R(t\Omega) \begin{bmatrix}
    y_0 \\
    \dot{y}_0
\end{bmatrix} + \int_0^t \begin{pmatrix}
    \Omega^{-1} \sin(t - s)\Omega \\
    \cos(t - s)\Omega
\end{pmatrix} g(y(s)) ds
\]

\[
R(t\Omega) = \begin{bmatrix}
    \cos(t\Omega) & \Omega^{-1} \sin(t\Omega) \\
    -\Omega \sin(t\Omega) & \cos(t\Omega)
\end{bmatrix}.
\]

i.e. exact for linear part, approximation for \( \int g(y(s)) ds \).
Replace $\int g(y(s)) \, ds$ by

\[
\frac{h}{2} \left[ h\Psi g(\Phi y_n) \right. \\
\left. + \Psi_0 g(\Phi y_n) \right]
\]

\[
\Phi = \phi(h\Omega), \quad \Psi = \psi(h\Omega), \quad \psi(\xi) = \text{sinc}(\xi)\psi_1(\xi), \quad \psi_0(\xi) = \cos(\xi)\psi_1(\xi).
\]
# Introduction to Trig Integrators

Common filter functions:

<table>
<thead>
<tr>
<th></th>
<th>$\psi(\xi)$</th>
<th>$\phi(\xi)$</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>(A)</td>
<td>$\text{sinc}^2(\frac{1}{2}\xi)$</td>
<td>1</td>
<td>Gautschi (1961)</td>
</tr>
<tr>
<td>(B)</td>
<td>$\text{sinc}(\xi)$</td>
<td>1</td>
<td>Deuflhard (1979)</td>
</tr>
<tr>
<td>(C)</td>
<td>$\text{sinc}^2(\xi)$</td>
<td>$\text{sinc}(\xi)$</td>
<td>García-Archilla et al. (1999)</td>
</tr>
<tr>
<td>(D)</td>
<td>$\text{sinc}^2(\frac{1}{2}\xi)$</td>
<td>$\text{sinc}(\xi)(1 + \frac{1}{3}\sin^2(\frac{1}{2}\xi))$</td>
<td>Hochbruck &amp; Lubich (1999)</td>
</tr>
<tr>
<td>(E)</td>
<td>$\text{sinc}^2(\xi)$</td>
<td>1</td>
<td>Hairer &amp; Lubich (2000)</td>
</tr>
<tr>
<td>(G)</td>
<td>$\text{sinc}^3(\xi)$</td>
<td>$\text{sinc}(\xi)$</td>
<td>Grimm &amp; Hochbruck (2006)</td>
</tr>
</tbody>
</table>

- Symplectic $\iff \psi(\xi) = \text{sinc}(\xi)\phi(\xi)$
- Finite time energy conservation $\iff \psi(\xi) = \text{sinc}^2(\xi)\phi(\xi)$
- Can find a $h\Omega$ dependent change of coordinates such that the transformed method is symplectic.
Experiments

(A) 

(B) 

(C) 

(D) 

(E) 

(F) 

(G) 

(MPT) 

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**Question and Answer**

**Q:** Why don’t trig integrators show order three and four resonances?

**A:** They do — at least for planar problems.

**Q:** Why hasn’t this been observed before? Have we been looking at the wrong things? Does the number of d.o.f. have something to do with it?
**Introduction to the F.P.U. problem**

Popular test problem for methods of highly oscillatory DEs.

6 springs, 3 soft (nonlinear) & 3 stiff (harmonic)

\[ H(x, \dot{x}) = \frac{1}{2} \dot{x}^T \dot{x} + \frac{1}{2} x^T \Omega x + U(x) \]

Adiabatic invariant

\[ I = \sum_j I_j, \quad I_j = \frac{1}{2} (\dot{x}_{1,j}^2 + \omega^2 x_{1,j}^2) \]
Experiments with the F.P.U. problem

(A)  

(B)  

(C)  

(D)  

(E)  

(G)  

(MPT)
More questions:

Q: What happened to those order three and four resonances?
A: They’re still there, but we’re looking at the wrong thing.
More questions:

Q: What happened to those order three and four resonances?
A: They’re still there, but we’re looking at the wrong thing.
Further experiments with the F.P.U. problem

\( h \omega / \pi \)

(A)  

(B)  

(C)  

(D)  

(E)  

(G)  

(MPT)  

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Further experiments with the F.P.U. problem
Further experiments with the F.P.U. problem

What if we want smaller errors in $\Delta_{\text{max}}H$ for a fixed $h\omega$?
Further experiments with the F.P.U. problem
Further experiments with the F.P.U. problem

Another comparison:

- The stiff springs slowly exchange oscillatory energy.
- Methods need $\psi(\xi)\phi(\xi) = \text{sinc}(\xi)$ to reproduce this.
Further experiments with the F.P.U. problem

(A)  
(B)  
(C)  
(D)  
(E)  
(G)  
(MPT)  
(LF)
Further experiments with the F.P.U. problem

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Still more questions:

Q: What’s the effect of getting these properties wrong?

A: It depends which quantity we’re interested in. Perhaps we should be looking at long-time statistics — this is a chaotic system after all.

Take some long runs: \( t \in [0, 1 \times 10^6] \).
Further experiments with the F.P.U. problem

|       | $\sigma l$ | $\Delta_{\text{max}} H$ | $\sigma l - \sigma l^{\text{ref}}$ | $\frac{1}{3} \sum |\mathbf{l}_j - \mathbf{l}_j^{\text{ref}}|$ |
|-------|------------|-------------------------|------------------------------------|--------------------------------|
| (A)   | 1.47e-02  | 2.58e-03                | -2.18e-04                         | 2.37e-03                      |
| (B)   | 1.31e-02  | 1.56e-02                | -1.84e-03                         | 1.49e-02                      |
| (C)   | 1.14e-02  | 4.45e-02                | -3.60e-03                         | 3.82e-03                      |
| (D)   | 1.48e-02  | 3.23e-03                | -1.89e-04                         | 1.31e-03                      |
| (E)   | 1.12e-02  | 4.38e-02                | -3.74e-03                         | 8.74e-03                      |
| (G)   | 9.20e-03  | 6.56e-02                | -5.77e-03                         | 2.37e-02                      |
| mid-pt| 1.47e-02  | 7.58e-04                | -2.87e-04                         | 3.05e-03                      |
| leap-frog | 1.50e-02 | 2.51e-03                | –                                 | –                             |

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Further experiments with the F.P.U. problem
None of the trig methods manage to capture all properties and some perform worse than the mid-point rule.

Q: What other properties are useful for measuring the performance of a method? Lyapunov exponents...?

Q: Is there a method which manages to get all/several properties correct?