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Explicit Symplectic Splitting Methods Applied to PDE's

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ABSTRACT. The symplectic integration of Hamiltonian partial differential equations with constant symplectic structure is discussed, with a consistent, Hamiltonian approach. The stability, accuracy, and dispersion of different explicit splitting methods are analyzed, and we give the circumstances under which the best results can be obtained. Many different treatments and examples are compared.

1. Introduction

A standard method of developing integrators for PDE's is to derive an *ad hoc* discretization in space and time, and then study the properties (convergence, stability) of that method. However, because symplectic integrators have shown an ability to capture the long-time dynamics of Hamiltonian ODE's, one would like to apply them to Hamiltonian PDE's as well. A natural approach is to discretize both the Hamiltonian function (an integral) and the Hamiltonian (Poisson) structure, then form the resulting ODE's. In principle this deals with all Hamiltonian PDE's at once, and provides a simple framework for incorporating symmetries of the phase space (Casimir functions), spatial symmetries (in the Hamiltonian function), and temporal symmetries (such as reversibility, a property of some symplectic integrators). Unfortunately some symmetries, such as those giving rise to integrals of more than second degree, cannot be preserved in the discrete system, and furthermore, symplectic integrators can be difficult to construct for exotic Poisson structures.

The main difference from the low-dimensional ODE case is that the equations are stiff—they contain widely different time-scales. Hence any numerical dissipation will have a severe effect; but standard conservative schemes (Crank-Nicolson, leapfrog on $u_t = u_x$) have undesirable attributes such as implicitness,

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parasitic waves, and low order. Hamiltonian methods have no parasitic waves, extend easily to any order, and are often explicit. However, note that if one wants to compute $u(T)$ accurately for fixed T then conventional methods will always do better—this only depends on the truncation error of the method used. This is not an appropriate test for symplectic integrators: one should concentrate instead on phase space structures (e.g. the shape of a traveling wave) and not on temporal errors (its speed). Whether or not accumulating phase errors (e.g. of angles on Liouville tori) corrupt the dynamics depends on the particular system studied, and on the measured property being structurally stable in the space of Hamiltonian systems.

We outline Hamiltonian systems in §2, and symplectic splitting methods in §3. These may be applied when $H = T(p)+V(q)$, ("P-Q splitting") but the best methods are possible when the nonlinear terms in H may be integrated exactly, as often happens ("L-N splitting"). Proposition 1 proves sufficient conditions for the much more accurate Runge-Kutta-Nyström methods to apply in this case. Sections 4 and 5 analyze the stability and dispersion of the two different splittings with different integrators—L-N splitting turns out to be more accurate and more stable, and if the equation is linear in its highest derivatives, dispersion errors are almost eliminated. Examples appear throughout.

2. Hamiltonian partial differential equations

Olver [**12**] is a good introduction to the structure of Hamiltonian ODE's and PDE's. Here we give a brief overview. A Hamiltonian dynamical system consists of a triple $(M, \{\cdot,\cdot\}, H)$ where M is a smooth manifold (the *phase space*), $H : M \to R$ is the Hamiltonian function, and $\{\cdot,\cdot\}$ is a Poisson bracket, a bilinear, skew-adjoint operator satisfying the Jacobi identity and the Leibniz rule. The bracket can be written in coordinates x_i as

$$\{F, G\} = (\nabla F)^T J(x)(\nabla G)$$

where $F,\ G : M \to R$ and J is called the Poisson tensor. A change of variables $x \to X = \phi(x)$ induces a bracket in the new variables by

$$\{F \circ \phi, G \circ \phi\}_X = \{F, G\}_x \circ \phi$$

or, in coordinates,

$$(D_x\phi)J(x)(D_x\phi)^T = \widetilde{J}(X).$$

If $J = \widetilde{J}$, ϕ is called a Poisson map; the time-map of the Hamiltonian dynamical system

$$\dot{x} = \{x, H\} = J(x)\nabla H(x)$$

is a Poisson map. A symplectic (or Poisson) integrator is one for which a time step is a Poisson map. Casimirs are functionals C such that $\{C, F\} = 0\ \forall F$, hence integrals of the motion for any H. When the phase space is infinite dimensional, we write the triple as $(\mathcal{M}, \{\cdot,\cdot\}, \mathcal{H})$, and the Poisson operator as $\mathcal{J}$. Typically $\mathcal{M}$ consists of sets of smooth functions on a finite dimensional space Z i.e. an

element in $\mathcal{M}$ is $u(x)$, $x \in Z$. The Hamiltonian $\mathcal{H} : \mathcal{M} \to R$ is a functional on this space, and the bracket can be written as

$$\{\mathcal{F}, G\}[u] = \int_Z \frac{\delta \mathcal{F}}{\delta u} \mathcal{J}(u) \frac{\delta \mathcal{G}}{\delta u}\, dx$$

where $\delta\mathcal{F}/\delta u$ is the variational derivative. When $\mathcal{J}$ is constant over $\mathcal{M}$, the Jacobi identity is trivially satisfied, and one need only check skew-adjointness. The most common cases are the canonical $\mathcal{J} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$ and the Gardner–Zakharov–Faddeev operator $\mathcal{J} = \partial_x$, which appears for example in the Korteweg–de Vries equation.

To reduce a Hamiltonian PDE to a set of Hamiltonian ODE's which can be symplectically integrated, our approach is to discretize $\mathcal{J}$ and $\mathcal{H}$ separately and then form the resulting dynamical system. $\mathcal{H}$ is an integral which can be discretized in any (suitably accurate) way, being careful to maintain the symmetry of any derivatives in $\mathcal{H}$. If $\mathcal{J}$ is constant, it may be discretized by replacing the differential operators by any (matrix) difference operator D, for example, central or pseudo-spectral differences. In what follows D will be any appropriate matrix difference operator. Some points to remember are that $\partial_x \partial_x = \partial_{xx}$ usually breaks down when discretized, $\mathcal{H}$ may be integrated by parts as necessary to get compact differences, and that for equations involving odd derivatives we may get 1-point-more-compact differences using staggered grids.

Consider periodic boundary conditions. Finite differences introduce excessive dispersion and will usually be inadequate, but full-spectral, pseudo-spectral and anti-aliased schemes are all possible, by treating the nonlinear terms in $\mathcal{H}$ (not $\dot{u}$) appropriately. The time-continuous dynamics are the same whether one works in Fourier or physical variables; usually the choice is made to minimize the number of Fourier transforms required per time-step.

EXAMPLE 1. $\mathcal{H} = -\int (u_x)^2\, dx = \int u u_{xx}\, dx$ may be discretized as $H = \sum_{i,j} u_i D_{ij} u_j$ where D is a matrix difference operator approximating ∂_{xx}. Then $(dH)_i = \sum_j (D_{ij} + D_{ji}) u_j$. This approximates $2u_{xx}$ only if $D_{ij} = D_{ji}$, i.e. the matrix D must be symmetric. So Chebyshev-spectral or finite differences skewed at boundaries are not suitable.

3. Symplectic integration

Suppose the Hamiltonian may be split into two parts—the "P-Q" splitting:

$$H = T(p) + V(q).$$

This was first considered by Feng [4]. Later we will also consider "L-N" splitting

$$H = L(u) + N(u)$$

where L has linear dynamics and N is nonlinear. Let $X_T = JdT$, etc., be the associated vector fields, and e^{kX} be the time-k flow of the vector field X. If

$J = \begin{bmatrix} 0 & K \\ -K^T & 0 \end{bmatrix}$ then the following map is an explicit, first-order approximation of the true flow e^{kX_H} [**13**]:

$$e^{kX_T} e^{kX_V} = e^{kX} \tag{3.1}$$

which is computed as

$$p^{n+1} = p^n - k\left(K^T V'(q^n)\right), \qquad q^{n+1} = q^n + k\left(KT'(p^{n+1})\right).$$

In (3.1),

$$X = X_T + X_V + k[X_T, X_V] + \mathcal{O}(k^2) = Jd\widehat{H} \tag{3.2}$$

where

$$\widehat{H} = H + H_0 + \mathcal{O}(k^2), \qquad H_0 = -k\{T, V\} \tag{3.3}$$

where the error (due to the noncommutativity of T and V) is expanded using the Campbell-Baker-Hausdorff (BCH) formula, and (3.3) follows because Hamiltonian vector fields form a Poisson algebra. The series in (3.2) is only an asymptotic series in k—it does not generally converge, although it will for linear systems for small enough k. Despite this problem, one might call H_0 the "autonomous Hamiltonian truncation error" (Yoshida [**17**]).

The leapfrog ("LF2") method extends the method (3.1) to second-order:

$$\varphi(k) = e^{\frac{1}{2}kX_T} e^{kX_V} e^{\frac{1}{2}kX_T} = e^{kX_{\widehat{H}}},$$

$$\widehat{H} = H + \frac{k^2}{24}\left(2\{V, \{T, V\}\} - \{T, \{T, V\}\}\right) + \mathcal{O}(k^4) \tag{3.4}$$

It is *symmetric*, that is, $\varphi(k)\varphi(-k) = 1$. Suzuki [**15**] and Yoshida [**16**] use this property to construct schemes of arbitrary order by concatenating $(2s+1)$ leapfrog stages and preserving the symmetry:

$$\varphi(w_s k) \ldots \varphi(w_1 k)\varphi(w_0 k)\varphi(w_1 k) \ldots \varphi(w_s k). \tag{3.5}$$

where $w_0 = 1 - 2(w_1 + \ldots + w_s)$. Particular schemes are given in Table 1. Other compositions, analagous to (3.4), can be made which preserve specified reversibilities of the continuous system [**14**]. A fourth-order scheme which has been rediscovered many times ([**2**], [**7**], [**15**], [**16**]) is LF4a, which has $s = 1$ (see Table 1). However, this method takes a large backwards step of $1.70k$, leading to poor accuracy and stability. A better fourth order method LF4b [**15**] whose largest step is $-0.66k$, has $s = 2$, and one can show that this is close to the most accurate fourth-order method of this type. The best sixth-order method, LF6a, is Yoshida's Method A which has $s = 3$.

If $T(p)$ is quadratic (i.e. one may write $\ddot{q} = f(q)$), one can do significantly better by simply concatenating several stages of (3.1): $\varphi = \prod_{i=s}^{1} e^{a_i kX_T} e^{b_i kX_V}$. These are known as Runge-Kutta-Nyström (RKN) methods. The most accurate

Table 1. Symplectic Integrators

I. General methods

$$\varphi(w_s k)\dots\varphi(w_1 k)\varphi(w_0 k)\varphi(w_1 k)\dots\varphi(w_s k), \qquad w_0 = 1 - 2(w_1 + \dots + w_s)$$

where $\varphi(k)$ is any symmetric method, such as leapfrog

(LF2:) $$e^{\frac{1}{2}kX_A}e^{kX_B}e^{\frac{1}{2}kX_A}, \qquad H = A + B$$

LF4a: $s = 1$, $w_1 = (2 - 2^{1/3})^{-1}$

LF4b: $s = 2$, $w_1 = w_2 = (4 - 4^{1/3})^{-1}$

LF6a: $s = 3$, $w_1 = -1.17767998417887$, $w_2 = 0.235573213359357$, $w_3 = 0.78451361047756$

II. Runge-Kutta-Nyström methods, $\varphi = \prod_{i=s}^{1} e^{a_i kX_T}e^{b_i kX_V}$.

LF4c: $s = 4$,

$a_1 = 0.5153528374311229364$	$b_1 = 0.1344961992774310892$
$a_2 = -0.085782019412973646$	$b_2 = -0.2248198030794208058$
$a_3 = 0.4415830236164665242$	$b_3 = 0.7563200005156682911$
$a_4 = 0.1288461583653841854$	$b_4 = 0.3340036032863214255$

LF6b: $s = 8$,

	$b_1 = 0$
$a_1 = -1.0130879789881764712$	$b_2 = 0.00016600692650939825$
$a_2 = 1.1874295738027426347 8$	$b_3 = -0.379624214274416219$
$a_3 = -0.018335852095646462$	$b_4 = 0.6891374118628092527 4$
$a_4 = 0.3439942572810802984 5$	$b_5 = 0.3806415909701951358 6$
$a_i = a_{9-i},\ i = 5,6,7,8$	$b_i = b_{10-i},\ i = 6,7,8$

4th- and 5th-order methods (in the sense of minimizing the Hamiltonian truncation error) are due to McLachlan and Atela [**10**]; the 4th-order one, LF4c, has $s = 4$ stages. Okunbor and Skeel [**11**] give sixteen 8-stage, 6th-order methods. Their method 13 (LF6b) has the smallest truncation error, about 0.02 times that of LF6a.

If both X_L and the nonlinear vector field X_N can be integrated exactly, then one may use the same composition methods with L-N splitting ($\varphi = e^{kX_L}e^{kX_N}$, etc.) This will usually be superior in that more (or all) or the derivatives in H will be treated exactly, and for weak nonlinearities, the truncation error will be asymptotically smaller. Furthermore, the more accurate RKN methods may still sometimes be used:

PROPOSITION 1. *Let* $J = \begin{bmatrix} 0 & K \\ -K^T & 0 \end{bmatrix}$ *and* $H = L(q,p) + N(q)$ *where* L *is a quadratic polynomial in* p *and* q. *Then any canonical Runge-Kutta-Nyström method of order five or less, or any symmetric (i.e.* $\varphi(k)\varphi(-k) = 1$*) method of order six or less, maintains its order of accuracy when applied to this splitting.*

PROOF. The special requirement of RKN for the splitting $H = T(p) + V(q)$ is that certain terms in the expansion of $e^{a_i k X_T} e^{b_i k X_V} \ldots$ contain a factor T''' and hence vanish identically. We compare these terms to those appearing in the expansion via the BCH formula, namely higher-order commutators of

$$\{T, V\} = -W_j T_j, \qquad T_j = \frac{\partial T}{\partial p_j}, \quad W_j = \sum_i \frac{\partial V}{\partial q_i} K_{ij}.$$

The first vanishing term is at $\mathcal{O}(k^4)$, which corresponds to a 4th-order method. It is $\{V, \{V, \{T, V\}\}\} = T_{ijk} W_i W_j W_k$. For the L-N splitting this term is $L_{ijk} W_i W_j W_k$ which is also identically zero (although $\partial L / \partial q$ does enter in the other terms). At fifth order, the two zero terms (in P-Q) are the two commutators of this one, hence also zero in L-N. At sixth order this simplicity breaks down: the twelve terms in the BCH expansion reduce to eight for both the P-Q and the L-N splitting. These eight contain five distinct terms in the P-Q case but eleven in the L-N case (the extra terms containing $\partial L / \partial q$, etc); hence the order conditions in the two cases are different. But if the method is symmetric, the sixth-order terms are identically zero, so the RKN methods do then carry over to the L-N splitting.

EXAMPLE 2. De Frutos, Ortega and Sanz-Serna have given two treatments of the Boussinesq equation $\mathcal{J} = \begin{bmatrix} 0 & \partial_x \\ \partial_x & 0 \end{bmatrix}$, $\mathcal{H} = \int \frac{1}{2}(p^2 + (q_x)^2 + q^2) + \frac{1}{3} q^3 \, dx$. The first method [**5**] is unconditionally stable; this is achieved by time-averaging the stiffest $(D^4 q)$ term:

$$(q^{n+1} - 2q^n + q^{n-1})/k^2 = -\frac{1}{4} D^4 (q^{n+1} + 2q^n + q^{n-1}) + Dq^n + D((q^n)^2) \tag{3.6}$$

where superscripts denote time-levels and D is the pseudo-spectral difference operator, but could just as well be the (diagonal) spectral difference operator or even ∂_x. Rearranging terms, this can be written as a map φ:

$$\begin{aligned} p^{n+\frac{1}{2}} &= p^{n-\frac{1}{2}} + k(I + \frac{k^2}{4} D^4)^{-1}(-D^3 q^n + Dq^n + D(q^n)^2) \\ &\equiv p^{n-\frac{1}{2}} + k \quad E \quad N(q^n) \\ q^{n+1} &= q^n + k D p^{n+\frac{1}{2}} \end{aligned} \tag{3.7}$$

showing that stability is achieved by braking the high modes severely; in fact $k = O(h^2)$ is required for consistency. Secondly, a direct calculation of $\varphi' J \varphi'^T$ shows that φ is a Poisson map iff $EN' = N'E$, which is not true here. It is true if $N(q)$ is linear; in this case the method is equivalent to leapfrog with the high modes braked in the Hamiltonian. (A similar method of gaining unconditional stability is used in Dai [**3**] for the variable-coefficient Schrödinger equation.)

Their second method (de Frutos et al. [**6**]) is equivalent to (3.7) with $E = I$. In our framework this is P-Q splitting with time-stepping $e^{kX_T} e^{kX_V}$, which is

second-order if the unknowns are staggered in time (q^n, $p^{n+\frac{1}{2}}$). They prove convergence and nonlinear stability for this method. Consider instead the equivalent LF2; the Hamiltonian truncation errors (3.4) for the P-Q and L-N splittings are

$$\text{P-Q:} \qquad -\frac{k^2}{24}\int -pp_{xx} + p^2 + 2qp^2 + 2(-q_{xx} + q + q^2)^2\,dx$$

$$\text{L-N:} \qquad -\frac{k^2}{24}\int \qquad\qquad 2qp^2 \qquad\qquad + 2q^4\,dx$$

or their corresponding discretizations. For strong nonlinearities, both are $\mathcal{O}(q^4)$; for $q \sim p \sim 1$, L-N has two terms against nine, and no derivatives (which can be larger); and for weak nonlinearities ($q \sim p \ll 1$), L-N is $\mathcal{O}(q^3)$ whereas P-Q is $\mathcal{O}(q^2)$. In addition, one may use the optimal RKN integrators; and the L-N splitting gains a factor $\frac{\pi}{2}$ in the stability criterion.

Integrals of the system are conserved if they are integrals of each part of the Hamiltonian separately. This is clearly the case for linear integrals (conserved by any consistent scheme anyway) and for bilinear integrals under both the P-Q and L-N splittings. When J is constant, Casimirs are linear functions and hence conserved.

4. Behavior of P-Q splitting

With finite differences, P-Q splitting must be used, because computing e^{kX_L} requires a Fourier transform. Even if L-N splitting is feasible, there is still the question of how the splitting acts on any derivatives remaining in N. For a simple analysis, we consider the linear wave equation $\dot{q} = p$, $\dot{p} = q_{xx}$ with P-Q splitting, and investigate the above methods with regard to stability and dispersion. The time-stepping is identical if one works in real or in Fourier space; choose the latter, so that the modes uncouple, and a change of scale reduces each to a linear oscillator:

$$\dot{q} = p, \qquad \dot{p} = -q.$$

Write one time step of the method as an explicit linear map

$$\begin{pmatrix} q^1 \\ p^1 \end{pmatrix} = A(k) \begin{pmatrix} q^0 \\ p^0 \end{pmatrix} = \begin{pmatrix} A_{11}(k) & A_{12}(k) \\ A_{21}(k) & A_{22}(k) \end{pmatrix} \begin{pmatrix} q^0 \\ p^0 \end{pmatrix}$$

where the polynomials $A_{ij}(k)$ can be found explicitly. One has by induction in the number of stages that A_{11} and A_{22} are even functions and A_{12} and A_{21} are odd. For symmetric methods, writing out the symmetry condition shows that $A_{11} = A_{22}$. Because the methods are symplectic, $\det A = 1$, and thus by standard stability analysis, the method is stable iff $|\mathrm{tr} A(k)| < 2$. The exact solution for the linear oscillator is $A_0 = \begin{pmatrix} \cos k & \sin k \\ -\sin k & \cos k \end{pmatrix}$, so $A(k)$ for a method of order p will agree with this up to terms of order k^p; thus the first wrong term in $\mathrm{tr} A$ is of order k^{p+2} for even-order methods.

PROPOSITION 2. *Consider $q_{tt} = q_{xx}$ discretized with time-step k and spatial mesh size h and a symplectic integrator with matrix $A(k)$ defined above. Let k^* be the least positive root of $|\mathrm{tr}A(k)| = 2$. Then the stability criterion, depending on the spatial discretization, is*

$$\begin{aligned} &\textit{(a) Pseudo-spectral differences:} && \frac{k}{h} \leq \frac{1}{\pi} k^* \\ &\textit{(b) Second-order finite differences:} && \frac{k}{h} \leq \frac{1}{2} k^* \\ &\textit{(c) Fourth-order finite differences:} && \frac{k}{h} \leq \frac{\sqrt{3}}{4} k^* \end{aligned}$$

PROOF. For the spectral discretization with Fourier modes $-\frac{M}{2}+1 \leq m \leq \frac{M}{2}$, we require stability for each oscillator ($\ddot{q}_m = -m^2 q_m$) separately; rescaling leads to $mk \leq k^*$ for $0 \leq m \leq \frac{M}{2}$. Then $M = 2\pi/h$ gives (a). (b) and (c) follow from standard von Neumann stability analysis.

EXAMPLE 3. For leapfrog, $\mathrm{tr}A/2 = 1 - k^2/2$ so $k^* = 2$. We therefore have stability in the spectral approximation for $k/h \leq \frac{2}{\pi} \sim 0.6366$. LF4a is worse: we find $2k^{*2} = 12 - 6(w + w^2) + 3\sqrt{-8 + 2w + 4w^2}$, where $w = \sqrt[3]{2}$; $k^* \sim 1.5734$ and we need $k/h \leq 0.5008$.

For the other methods the roots of the polynomials must be found numerically, and the corresponding stability criteria are given in Table 2. Notice that they are quite good—for non-symplectic methods (e.g. three-time-level leapfrog), one typically needs Courant numbers k/h near 1 with finite differences, and near $1/\pi$ with spectral differences. The results apply to any linear PDE with P-Q splitting: if the time-continuous problem has eigenvalues $i\sigma_m$, then the stability criterion is $k\sigma_m < k^*$.

Table 2. Stability criteria, P-Q splitting

k/h is the stability criterion for spectral differencing of the linear wave equation; a is the first ($\mathcal{O}(k^p)$) term in the expansion of the phase speed error.

Method	k^*	k/h	Phase error a
LF2	2	0.6366	-4.2×10^{-2}
LF4a	1.5734	0.5008	6.6×10^{-2}
LF4b	2.7210	0.8661	9.3×10^{-4}
LF4c	3.0389	0.9673	1.1×10^{-4}
LF6a	2.2691	0.7223	-3.8×10^{-3}
LF6b	3.0674	0.9764	-1.3×10^{-6}

No general time-integrator can be free of dispersion in general. Historically this has led to schemes which introduce artificial dissipation of the high modes

to prevent "wiggles." Indeed Crank-Nicolson (symplectic for a linear PDE) is often frowned on for just this reason. Now we have expressly disallowed numerical dissipation. Does dispersion mean that we cannot expect good long-time behavior from symplectic integrators? Certainly it does in the case of the linear wave equation, for which any initial condition will eventually disperse into its constituent modes as all phase accuracy is lost. However, for nonlinear and particularly for near-integrable equations, we can hope that phase locking inherent in the system will prevent this. (Consider the ODE case of coupled oscillators, for example.) In addition, it turns out that some integrators (e.g. LF4c) and L-N splitting have negligible dispersion errors.

We take $k \leq k^*$ and calculate the eigenvectors of A; separating real and imaginary parts show that the phase space is foliated by similar invariant ellipses, of which one is

$$B\begin{pmatrix}\cos\alpha\\ \sin\alpha\end{pmatrix} = \begin{pmatrix} A_{12} & 0\\ \cos\theta - A_{11} & \sin\theta\end{pmatrix}\begin{pmatrix}\cos\alpha\\ \sin\alpha\end{pmatrix}.$$

Applying the map to this ellipse and using $\det A = 1$ gives

$$AB\begin{pmatrix}\cos\alpha\\ \sin\alpha\end{pmatrix} = B\begin{pmatrix}\cos(\alpha-\theta)\\ \sin(\alpha-\theta)\end{pmatrix}$$

where $\cos\theta = \mathrm{tr}A/2$. Thus the map moves a point an angle θ around the ellipse each time-step, giving a dispersion relation θ. The exact map has $\theta = k$, and we are only considering a single wave, so the most natural error measure is the relative phase speed of that wave, $c = \theta/k$. Because $\cos\theta = \cos k + ak^{p+2} + o(k^{p+2})$ for even-order methods, we have $c \sim 1 - ak^p$ for small k (see Table 2.) At $k = k^*$, $c = \pi/k^*$. The figure shows c for different methods and also illustrates their stability limits.

5. Stability of L-N splitting

There are two approaches to the linear stability of splitting methods. Firstly, one can make general statements based on the generic bifurcations of symplectic vector fields and maps, giving sufficient conditions for linear stability. Secondly, the eigenvalues of the time-map can be computed explicitly for particular examples; the generic sufficient conditions turn out to be often necessary as well.

Here we are thinking of integrating $H = L + N$ with one of the composition methods in Table 1 with the resulting map $\widehat{\varphi}$ linearized about some steady state. Now $\widehat{\varphi} = e^{kX_{\widehat{H}}} = C$ is linear and hence is the time-k map of some autonomous linear Hamiltonian $\widehat{H}$ which can be found directly: $\widehat{H} = u^T B u$ where $C^T B C = B$. In this case the asymptotic series

$$\widehat{H} = H + k^p H_0 + \ldots \tag{5.1}$$

(cf. (3.4)) will converge to $\widehat{H}$ for k small enough. However, one cannot use the series to examine stability because near the onset of instability, typically all its terms are the same order in k. Examining the first term in (5.1) can determine

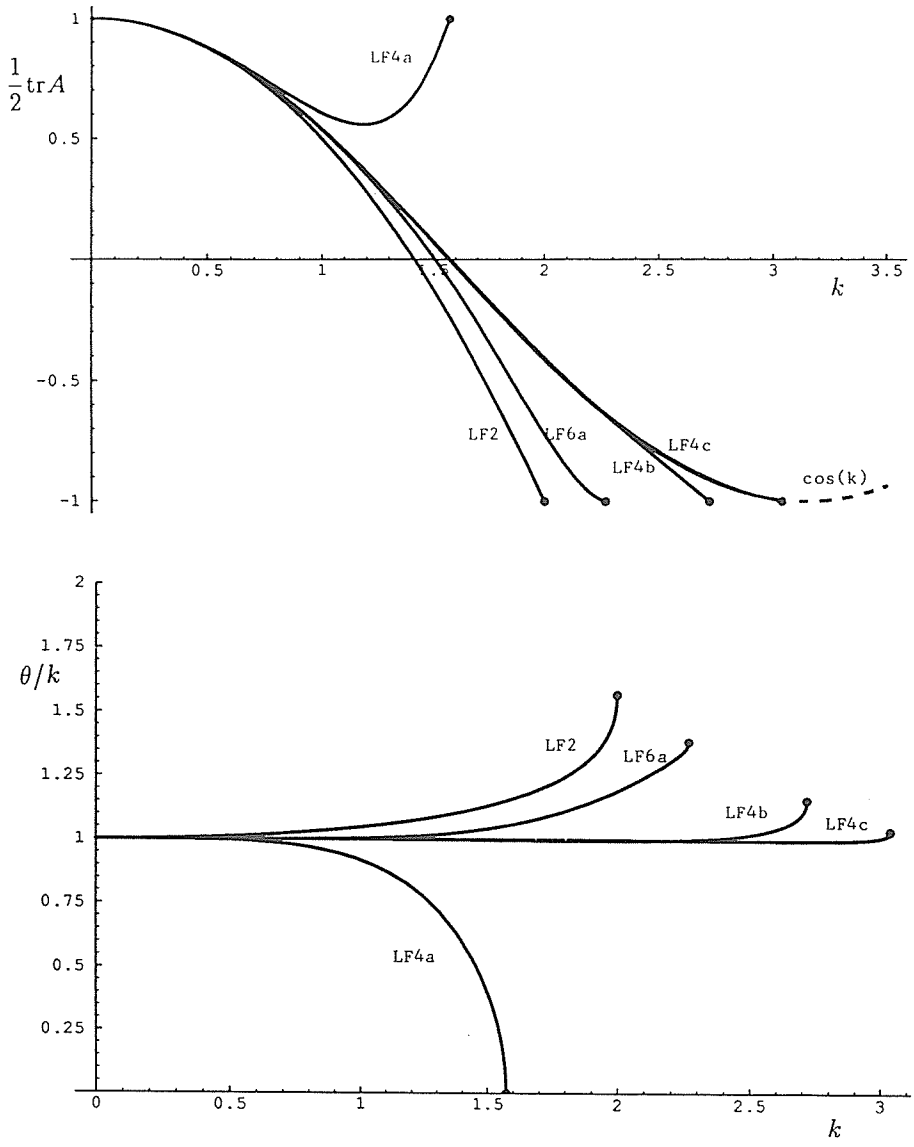

FIGURE. Stability & accuracy for explicit P-Q splitting. Top: $\frac{1}{2}\mathrm{tr}A$ for five explicit methods applied to the linear oscillator; the true solution is $\cos k$. The • shows the stability limit for each method. LF4c and LF6b are indistinguishable here. Bottom: Relative phase speed c for each method.

when the conditions of the following proposition are *not* satisfied, and can help in choosing a good splitting of H. Then (roughly, if dispersion errors are $o(1)$ as $k \to 0$) two time-steps per period of the fastest wave are sufficient for stability:

PROPOSITION 3. *Suppose X_H has pure imaginary eigenvalues $\{\pm i\sigma_m\}_{m=1}^M$, $\sigma_1 \le \ldots \le \sigma_M$, any multiple eigenvalues have positive signature, and any zero eigenvalues are associated with zeros of both X_L and X_N. Let $k \to 0$ with $k\sigma_M = k^*$ held fixed, and assume that in this limit $\widehat{\varphi}$ is a small perturbation of $\varphi = e^{kX_H}$. (One may need to rescale the independent variables to get $\varphi \sim 1$ first.) Then, for M sufficiently large, the method $\widehat{\varphi}$ is generically linearly stable for $k^* < \pi$.*

PROOF. We are investigating the stability of the fixed point at the origin to small symplectic perturbations. The nonunit eigenvalues of φ are $e^{ik\sigma_m}$ which are are bounded away from -1 if $k^* < \pi$. Because the eigenvalues of the vector field have positive signature, so do those of its time-k flow. These are just the requirements for generic stability of the origin when φ is perturbed to $\widehat{\varphi}$ (Arnol'd [**1**], MacKay [**8**], [**9**]). Finally, if zero eigenvalues of X_H come from zeros in X_L and X_N, then there is a corresponding zero in $X_{\widehat{H}}$, so the $+1$ eigenvalues of φ are fixed and do not split.

Notes:

1. If $H = T(p) + V(q)$, eigenvalues are guaranteed to have positive signature [**9**].
2. At $\pm k\sigma_m = \pi$, φ has a double eigenvalue at -1. In the perturbed map $\widehat{\varphi}$ this generically splits into a real pair, signaling loss of stability in this mode. It may be a bubble of instability or a permanent loss.
3. The proposition applies if $H = L(q,p) + N(q)$ and N has fewer derivatives of q than L—as in the nonlinear wave equation $q_{tt} = q_{xx} + V'(q)$ and the Boussinesq equation (example 2).

EXAMPLE 4: A NONLINEAR WAVE EQUATION. Sine-Gordon $q_{tt} - q_{xx} + \sin(q) = 0$ linearized about $q = 0$ is Klein-Gordon. Consider LF2 with L-N splitting on this equation: each mode decouples into a linear map

$$A = e^{\frac{1}{2}kX_L} e^{kX_N} e^{\frac{1}{2}kX_L}$$

$$= \begin{pmatrix} \cos(mk) - \frac{k}{2m}\sin(mk) & \frac{k}{2m^2}(\cos(mk) - 1) + \sin(mk)/m \\ -\frac{k}{2}(\cos(mk) + 1) - m\,\sin(mk) & \cos(mk) - \frac{k}{2m}\sin(mk) \end{pmatrix}$$

$$\cos\theta = \frac{1}{2}\mathrm{tr}A = \cos(mk) - \frac{k}{2m}\sin(mk) \tag{5.2}$$

The stability limit for large m is indeed $mk < \pi$, but beyond this there are bubbles of instability. Consider k small with $mk = x$ held fixed, so $\frac{1}{2}\mathrm{tr}A = \cos x - \frac{1}{2}k^2\sin(x)/x$. Solving by series for x near $l\pi$ shows that this is larger than 1 in absolute value for $x \in (l\pi - k^2/l\pi, l\pi)$. However, these instabilities

are unlikely to be triggered as they are only $k/l\pi$ times as wide as the spacing between modes, hence one can easily choose k so as to avoid them. The maximum growth rate in the bubbles is only $k^2/2\pi$.

Numerical experiments show that the formal stability limit can indeed be exceeded by a factor of three or four without the nonlinear terms triggering any instability, even for strong nonlinearities.

Expanding (5.2) for small k and any m gives the numerical dispersion relation:

$$\theta/k = \sqrt{1+m^2} + \frac{k^2}{24\sqrt{1+m^2}} + \mathcal{O}(k^4)$$

which is $\mathcal{O}(k^2)$ away from the true relation, uniformly in m. This, and the smaller truncation errors, are the great advantages of the L-N splitting.

6. A numerical example

For a numerical test of the above analyses consider the nonlinear wave equation

$$\dot{q} = p, \quad \dot{p} = -q_{xx} + q^3$$

on $[0, 2\pi]$ with periodic boundary conditions; the Hamiltonian discretized by pseudo-spectral differences and the (spectral) trapezoidal rule for the integral; and the time-integrator LP4c. (The advantage of this equation is that it is not integrable but it is known that C^∞ initial data stays C^∞ for all time.) The initial conditions considered are $p = 0$, $q = a\cos x$ for various amplitudes a. Standard properties of symplectic integrators were confirmed: (a) the energy error did not increase secularly with time; (b) the bilinear momentum integral $\int pq_x\,dx$ ($\sum mp_m q_{-m}$ for the ODE's) was conserved within round-off error; and (c) the above accuracy and stability analyses were confirmed (nonlinear terms could destabilize the calculation only when the solution was extremely poorly resolved spatially).

When $|q|$ is small the relative truncation error of P-Q splitting is $\mathcal{O}(1)$, against $\mathcal{O}(q^2)$ for L-N, so the latter is clearly superior then. Its maximum energy error was 2.4 times smaller at $a = 0.5$, and 3.2 times smaller at $a = 2$.

For all amplitudes a, P-Q splitting was stable for Courant numbers $c = k/h <\sim 0.94$ (cf. $k/h < 0.9673$ in Table 2). L-N was stable for $c <\sim 14$ when $a = 0.5$ (but only useful for $c < 5$) and for $c < 3$ when $a = 2$—L-N has no *linear* stability limit here. Clearly linear–nonlinear splitting is preferred when feasible.

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