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# A note on the numerical integration of the KdV equation via isospectral deformations

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**Abstract**

The main purpose of this paper is to test the performance of Lie group integrators as applied to a semi-discrete version of the KdV equation.

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## 1. Introduction

We consider the numerical approximation of the KdV equation

$$u_t + u_{xxx} - 3uu_x = 0. \tag{1.1}$$

In this manuscript we will focus our attention on the Lax formulation of the equation. Consider the Schrödinger operator

$$L = -D^2 + u \tag{1.2}$$

where $D = \frac{\mathrm{d}}{\mathrm{d}x}$ represents differentiation with respect to the $x$ variable. It is well known that if $u$ evolves according to the KdV equation then the operator $L$ is unitarily equivalent, i.e. $L$ is such that

$$U^*(t)L(t)U(t) = L(0) \tag{1.3}$$

and $U(t)$ is a one-parameter family of unitary operators in $L_2(-\infty, \infty)$. The flow $L(t)$ is isospectral. This can otherwise be expressed by the following equation:

$$L_t = [B, L] \tag{1.4}$$

where $B$ is the infinitesimal generator of the family $U(t)$. For $B = D$ (skew-adjoint) (1.4) reduces to $u_t = u_x$, the infinitesimal generator of translations leaving $L$ invariant. If we consider

$$B = -4D^3 + 2(uD + Du) \tag{1.5}$$

equation (1.4) reduces to the KdV equation. There is a hierarchy of operators $B$ defining nonlinear evolutionary equations though (1.4), which leave the Schrödinger operator $L$ invariant. The operators $L$ and $B$ are self- and skew-adjoint respectively with respect to the inner product of $L_2(-\infty, \infty)$. In [1] Adler described the orbit symplectic structure of Konstant–Kirillov for the KdV equation. In his analysis, using the theory of pseudo-differential operators, the author identifies the formal Lie group $G$, the formal Lie algebra $\mathfrak{g}$ and the Lie coadjoint group action of $G$ over $\mathfrak{g}^*$ necessary to define the Konstant–Kirillov symplectic form. In this context we will be mostly concerned with the analogous adjoint action.

Several authors have been recently considering the use of Lie group actions in the numerical integration of ordinary differential equations (ODEs) on manifolds (see [14] for an overview on the subject). The main idea of these methods is based on the assumption that the vector field of the given differential equation can be expressed in terms of a Lie group action on the manifold. Advancing in time the solution of a transformed problem in the Lie algebra using a Runge–Kutta (RK) method and then transforming back the result to the manifold, it is possible to obtain approximations of the flow that preserve the orbits. More specifically in the case of isospectral flows the methods preserve the spectrum of the operators. In the case of the KdV equation (and other completely integrable systems) the Lax formulation of the equation involves infinite-dimensional operators and in practice the above-mentioned numerical methods can be applied only after a suitable space discretization of the operators $L$ and $B$ that allows us to work with finite-dimensional operators.

Semi-discretizations preserving symmetries or the Hamiltonian structure of PDEs have been considered recently in [2, 3, 17–20].

In the KdV case one can consider semi-discretizations that describe an isospectral flow in a finite-dimensional space. A famous example of such discretization was given by Kac and Van Moerbeke in [15, 16]. We refer to [24] for a study of the convergence of the solutions of the Kac–Van Moerbeke (KVM) discretization to the solutions of (1.1). In this paper we are interested in producing discretizations in space and time of the KdV equation by applying a numerical method to the KVM system of ODEs.

Integrable discretizations of both space and time for the KdV equation have been studied by Hirota [13], whereas numerical methods for the time integration of isospectral flows have been considered by Calvo and collaborators [4].

The spectrum of the discrete Schrödinger operator is in any case just a discretization of the spectrum of $L$ and what we are guaranteed to preserve with our time-stepping procedure is just the discrete and obviously not the true spectrum of $L$.

In a more general way we are interested in finding discretizations of the operators $L$ and $B$ that are respectively self- and skew-adjoint with respect to an opportune discretization of the inner product of $L_2$. With straightforward computation it is possible to verify that, given $\phi \in L_2$, $[B, L]\phi = BL\phi - LB\phi = u_{xxx}\phi + 6uu_x\phi$ and the operator $[B, L]$ does not contain $D$ or powers of $D$. This fact is a consequence of the rules of composition of the operator $D$. This feature plays an important role also in the discrete version of the problem and in the KVM discretization it is represented by the fact that $[\tilde{B}, \tilde{L}]$ is a matrix with the same sparsity pattern as $\tilde{L}$.

We conjecture that considering restrictions of $L$ and $B$ to finite-dimensional subspaces of functions in $L_2$, and imposing certain constraints of regularity on these functions, it is possible to define other suitable discretizations $\tilde{L}$ and $\tilde{B}$ ensuring the desired properties for $\tilde{D}$.

The main purpose of this paper is to test the performance of Lie group integrators as applied to a semi-discrete version of the KdV equation, and to discuss which features of the infinite-dimensional problem should be maintained in the semi-discrete system in order to apply these time integration strategies.

In the next section we will give a brief introduction to the methods of integration on manifolds based on the use of Lie group actions with particular consideration to the case of isospectral flows and sparse matrices.

In the third and last section we will consider the application of these methods to the discretization of the KdV equation.

## 2. Methods based on Lie group actions

Consider the differential equation

$$y' = F(t, y) \qquad y \in \mathcal{M}$$

with $F(t, \cdot) \in X(\mathcal{M})$ a vector field on the manifold $\mathcal{M}$; assume that

$$F(t, y) = \lambda_*(f(t, y))(y). \tag{2.6}$$

Here $f : \mathbb{R} \times \mathcal{M} \to \mathfrak{g}$ ($\mathfrak{g}$ a Lie algebra) and $\lambda_* : \mathfrak{g} \to X(\mathcal{M})$ and it is obtained as follows: assume

$$\Lambda : \mathrm{G} \times \mathcal{M} \to \mathcal{M}$$

is a Lie group action, choose

$$\phi : \mathfrak{g} \to \mathrm{G}$$

a coordinate map form $\mathfrak{g}$ to G, define

$$\lambda : \mathfrak{g} \times \mathcal{M} \to \mathcal{M}$$

a Lie algebra action by $\lambda(v, p) = \Lambda(\phi(v), p)$,

$$\lambda_*(v)(p) = \left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} \lambda(tv, p)$$

and $f : \mathbb{R} \times \mathcal{M} \to \mathfrak{g}$. We will consider cases in which $\mathfrak{g} \subset \mathfrak{gl}(n)$.

Consider $\mathrm{d}\phi_w : \mathfrak{g} \to \mathfrak{g}$,

$$\mathrm{d}\phi_w(v) = \left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} (\phi(v + tw)).$$

Then, given $p \in \mathcal{M}$, the vector field $\varphi(t, u) = \mathrm{d}\phi_u^{-1}(f(t, \lambda_p(u)))$, with $\lambda_p : \mathfrak{g} \to \mathcal{M}$ and $\lambda_p(u) = \lambda(u, p)$ is such that

$$\lambda'_p \circ \varphi = F \circ \lambda_p.$$

As an immediate consequence if

$$u(t)' = \varphi(u(t)) \tag{2.7}$$

then

$$(\lambda_p \circ u)' = \lambda'_p \circ u' = \lambda'_p \circ \varphi \circ u = F \circ (\lambda_p \circ u).$$

It is possible to use an RK method for the integration for ODEs on the Lie algebra equation (2.7) and transform the obtained approximation back to the manifold $\mathcal{M}$ at every time step. This leads to the following algorithm originally due to Munthe–Kaas (MK):

*Generalized RK–MK algorithm*

$p := y_n$
for $i = 1$ to $s$ do
  $u_i := h \sum a_{ij} \tilde{k}_j$
  $k_i = f(t_n + c_i h, \lambda(u_i, p))$,
  $\tilde{k}_i := \mathrm{d}\phi_{u_i}^{-1}(k_i)$
end do
$v := h \sum b_i \tilde{k}_i$
$y_{n+1} = \lambda(v, p)$

where $\{a_{i,j}\}$, $i = 1, \ldots, s$, $j \leqslant i-1$ and $b_i$, $i = 1, \ldots, s$ are the coefficients of a classical, explicit RK method with $s$ stages [12]. In the previous algorithm the numerical solution is advanced in the Lie algebra by computing $v$ as a linear combination of the stages $\tilde{k}_i$ and then transformed to the manifold by applying the Lie algebra action. For a more extensive description of the RK–MK methods we refer to the original article of MK [21] and for its generalizations to [9] and [23]. Similar strategies have been explored by Zanna in [26] and by Diele and collaborators in [8] with particular focus on the application to isospectral flows.

Suppose now we want to apply the previous algorithm to an isospectral flow of the type

$$L_t = [B(L), L] \tag{2.8}$$

$L(0) = L_0$ with $L$ an $n \times n$ symmetric matrix, $L \in \mathrm{Sym}(n)$ and $B : \mathrm{Sym}(n) \to \mathfrak{so}(n)$; we then need to identify the Lie group action, the map $f$ of equation (2.6), to choose a coordinate map and to obtain the Lie algebra action. The Lie group action we consider is the adjoint action, $B$ plays the role of $f$ and given a coordinate map, local diffeomorphism $\phi : \mathfrak{so}(n) \to SO(n)$, the Lie algebra action is

$$\lambda(P, S) := \phi(P)^* S \phi(P);$$

by differentiation one obtains that

$$\lambda_*(P)(S) = [P, S].$$

We recognize in (2.8) the framework required in (2.6).

Several possible choices are available for the coordinate map $\phi : SO(n) \to \mathfrak{so}(n)$. Perhaps the most natural one consists in taking $\phi = \exp$ the matrix exponential, that leads to the following expression for $\mathrm{d}\phi_u^{-1}$:

$$\mathrm{d}\exp_u^{-1}(v) = \left.\frac{z}{\mathrm{e}^z - 1}\right|_{\mathrm{ad}_u}(v). \tag{2.9}$$

For computing (2.9) usually one considers truncations of the corresponding Taylor expansion of the same order in the step size $h$ of the considered RK method. When $n \geqslant 4$, some techniques for the exact computation of the exponential of skew-symmetric matrices are available [25]; however, the computational costs can be high and this is one of the main motivations for considering the use of alternative coordinate maps.

Among other choices for the coordinate map $\phi$ rational maps can be considered [6], and in particular all the diagonal Padé approximants of the exponential map are suitable. For example if we consider $\phi(u) = (I - u/2)^{-1}(I + u/2)$, the Cayley map, we have $\mathrm{d}\phi_u^{-1}(v) = (I - u/2)v(I + u/2)$ in an explicit closed form.

A third and last option that we want to mention here is based on the composition of elementary exponentials: one can take for example $\phi(u) = \mathrm{e}^{u_1 e_1} \cdots \mathrm{e}^{u_d e_d}$, where $e_1, \ldots, e_d$ are a basis of the Lie algebra $\mathfrak{g}$ that in our case is $\mathfrak{so}(n, \mathbb{R})$.

The straightforward computation of $\mathrm{d}\phi_u^{-1}(v)$ implies high computational costs, but in the case of semi-simple Lie algebras over $\mathbb{C}$ it is possible to derive explicit expressions for $\mathrm{d}\phi_u^{-1}$ that can be computed at a competitive cost [23]; these results do not apply in the $\mathfrak{so}(n, \mathbb{R})$ case.

In this last case one can instead opt for finding cheap approximations of the correct order for $\mathrm{d}\phi_u^{-1}(v)$ when $u, v \in \mathfrak{so}(n, \mathbb{R})$. In [5] and [6] the authors propose a strategy based on the use of compositions of elementary exponentials for constructing approximations of the exponential map of order $p$ in the step size that are coordinate maps in their own right. The use of such maps combined with the same-order approximation of $\mathrm{d}\exp_u^{-1}$ gives a method of order $p$.

For $u \in \mathfrak{g}$, and $\mathfrak{g}$ of dimension $d$, let $e_1, \ldots, e_d$ be a basis for $\mathfrak{g}$, and $u = \sum_{l=1}^{d} u_l e_l$ consider

$$\phi(u) = \exp(\alpha_1(u)e_1) \cdots \exp(\alpha_d(u)e_d)$$

with $\alpha_j : \mathfrak{g} \to \mathbb{R}$ if the Jacobian of $[\alpha_1, \ldots, \alpha_d]$ is invertible for $u$ sufficiently close to the origin in $\mathfrak{g}$, $\phi(u)$ is a coordinate map. More generally consider

$$\phi(u) = \exp(U_1) \cdots \exp(U_k)$$

where the $\{U_i\}_{i=1}^k$ are defined as follows: let $\{S_i\}_{i=1}^k$ define a partition of the set of indices $\mathcal{I} = \{1, \ldots, d\}$, i.e.

$$\cup_{i=1}^k S_i = \mathcal{I} \qquad S_i \cap S_j = O \quad i \neq j$$

we define now

$$U_i := \sum_{j \in S_i} \lambda_j(u) e_j$$

with $\lambda_j : \mathfrak{g} \to \mathbb{R}$. Using the Baker–Campbell–Hausdorff (BCH) formula for $U_1, \ldots, U_k$ we find $Y(u) = \sum_{l=1}^d y_l(u) e_l$ such that $\phi(u) = \exp(Y(u))$ and also in this case if for $u$ close enough to the origin the Jacobian of $[y_1, \ldots, y_d]$ is invertible, then $\phi$ is a coordinate map.

We illustrate this strategy in the appendix with a special instance of these techniques that is particularly interesting in the $\mathfrak{so}(n, \mathbb{R})$ case.

Parametrizing the element $u \in \mathfrak{g}$ with the step size $h$ it is easy to realize that if $\phi(hu) = \exp(hu) + \mathcal{O}(h^{p+1})$ it is possible to take the series of $\mathrm{d}\exp_{hu}^{-1}$ truncated at order $p$ as an order $p$ approximation of $\mathrm{d}\phi_{hu}^{-1}$.

In the case of sparse matrices, the main drawback in the application of these methods is due to the fact that the application of $w = \mathrm{d}\phi_u^{-1}(v)$ with $u$ and $v$ sparse gives a result $w$ of reduced sparsity. This implies that at each time step, in the computation of the Lie algebra action in the method, the coordinate map is applied to matrices of decreasing sparsity. To avoid this problem it is possible to use methods that are simply based on the composition of elementary flows, for which however the number of exponentials to be computed is much higher than in this case [7].

## 3. Discrete KdV and Lie group integrators

In this section we consider the use of the methods described in the previous section in the numerical integration of the following system of differential equations known as the KVM equation [15]:

$$\frac{\mathrm{d}R_n}{\mathrm{d}t} = \mathrm{e}^{-R_{n-1}(t)} - \mathrm{e}^{-R_{n+1}(t)} \tag{3.10}$$

for $n = 2, \ldots, N-1$ with $\frac{\mathrm{d}R_1}{\mathrm{d}t} = -\mathrm{e}^{-R_2(t)}$ and for our purposes we assume $N$ finite and consider $\frac{\mathrm{d}R_N}{\mathrm{d}t} = \mathrm{e}^{-R_{N-1}(t)}$, and setting $a_i = \frac{1}{2}\mathrm{e}^{-\frac{1}{2}R_i(t)}$ for $i = 1, \ldots, N$ and $b_i = a_i a_{i+1}$ for $i = 1, \ldots, N-1$ we define the following $(N+1) \times (N+1)$ matrices:

$$L = \begin{bmatrix} 0 & a_1 & 0 & \cdots & 0 \\ a_1 & \ddots & \ddots & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & a_N \\ 0 & \cdots & 0 & a_N & 0 \end{bmatrix} \qquad B = \begin{bmatrix} 0 & 0 & b_1 & \cdots & 0 \\ 0 & \ddots & \ddots & \ddots & \vdots \\ -b_1 & \ddots & \ddots & \ddots & b_{N-1} \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & -b_{N-1} & 0 & 0 \end{bmatrix}.$$

We will apply algorithm (2) to the isospectral flow

$$L_t = [B, L]$$

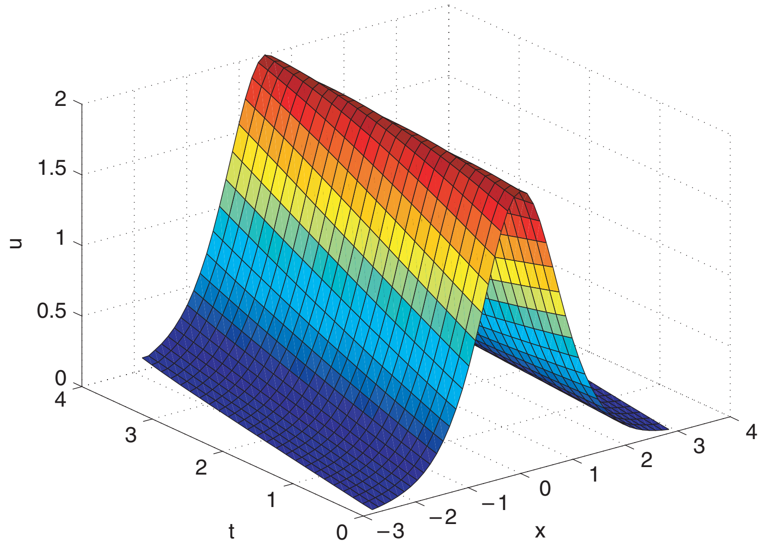


**Figure 1.** Evolution of the one-soliton solution.
(This figure is in colour only in the electronic version, see www.iop.org)

in order to obtain a numerical approximation of $R_i(t)$ $i = 1, \ldots, N$ that preserves the spectrum of the operator $L$. We will then use the obtained approximations to derive a numerical solution of the KdV equation.

Consider the solutions of the scaled version of (3.10) obtained by replacing $R_n(t)$ with $r_n(t) = h_x^{-2} R_n(t/h_x^3)$ and with infinite $n$. Consider then an interpolating function $r_{h_x}(x, t)$ whose values in the nodes $x_n = nh_x$ coincide with $r_n(t)$ and define $U_{h_x}(x + h_x^{-2}2t, t) := r_{h_x}(x, t)$; in [24] the author gives the details of the convergence of $U_{h_x}$ to the general solution of the KdV equation.

As mentioned in the previous section different coordinate choices give rise to different Lie group methods; in the numerical experiments we will compare the use of exp the classical exponential map computed using the built-in function of `Matlab expm` and a map obtained by symmetric composition of elementary exponentials as described in the appendix by (A.1) and (A.2).

The coefficients of the RK method in (2) are chosen to be the coefficients of the classical RK4 (explicit RK of order four) [12].

The map $\mathrm{d}\phi_u^{-1}$ for both choices of coordinate map is substituted by the order four approximation obtained by truncation of the series:

$$\mathrm{d}\phi_u^{-1}(v) = v - 1/2\mathrm{ad}_u(v) + 1/12\mathrm{ad}_u^2(v) - 1/720\mathrm{ad}_u^4(v) + \mathcal{O}(h^6)$$

the method is implemented using the free Lie algebra strategy that reduces the number of commutators [22]. The Lie algebra action used for advancing the solution from $L_n$ to $L_{n+1}$ is given by $\lambda(v, L_n) = \phi(hv)L_n\phi(-hv)$ with $\phi(hv)$ either the exponential of $hv$ or a composition of elementary exponentials given by (A.1) and (A.2).

We notice that in the case of matrices of the sparsity of $B$ the coordinate map described by (A.1) and (A.2) will be computed in a number of $\mathcal{O}(n^2)$ operations; this appears to be competitive compared with the algorithms that efficiently compute exponentials of skew-symmetric sparse matrices and that in any case require $\mathcal{O}(n^3)$ operations.

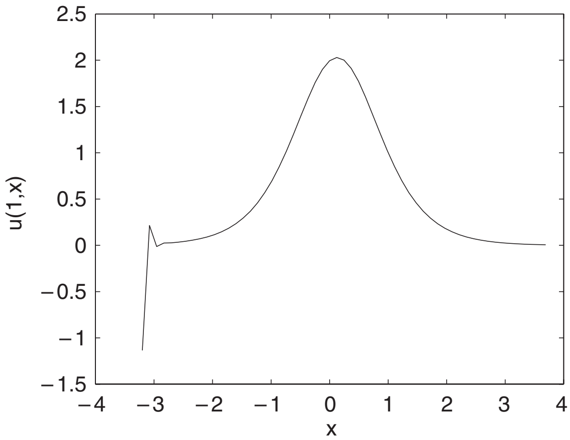


**Figure 2.** RK4 numerical solution at $t = 1$.

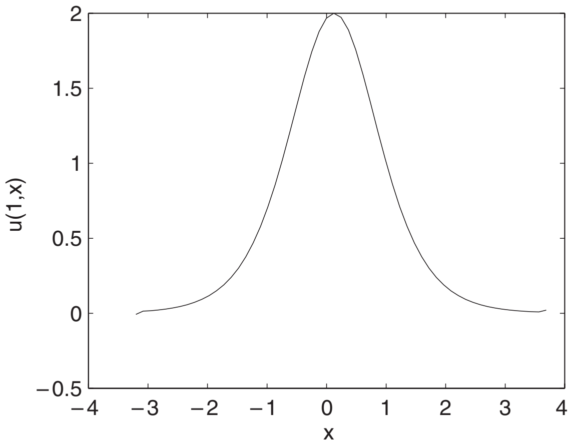


**Figure 3.** RK–MK with exponential, numerical solution at $t = 1$.

In figure 1 we report the evolution of one soliton computed using the RK–MK algorithm of the previous section combined with exp as coordinate map.

In our example we took $N = 65$ and $h_x = 8/65$, taking in other words the interval $[-4, 4]$ as our approximation of the real line. The values of the numerical solution are plotted in an interval of amplitude 5.6616 corresponding to 47 of the 65 nodes of the space grid; the initial space interval is $[-2.83, 2.83]$ and it moves with the soliton; at $t = 4$ it is $[-1.8503, 3.8113]$; we integrated for $t \in [0, 4]$ with 240 steps and initial value $2\,\mathrm{sech}^2(x)$.

In figures 2–4 we compare the results obtained integrating the previous problem on the time interval $[0, 1]$ with three different strategies: in figure 2 the built-in function of `Matlab ode45` applied to the system (3.10) with relative tolerance $1 \times 10^{-9}$ and absolute tolerance $1 \times 10^{-12}$; in figure 3 the classical RK–MK method with the exponential as coordinate map and in figure 4 the RK–MK combined with the coordinate map defined by (A.1) and (A.2). In the plots the space interval is larger compared to the previous experiment and it corresponds to 57 of the 65 nodes on the space grid.

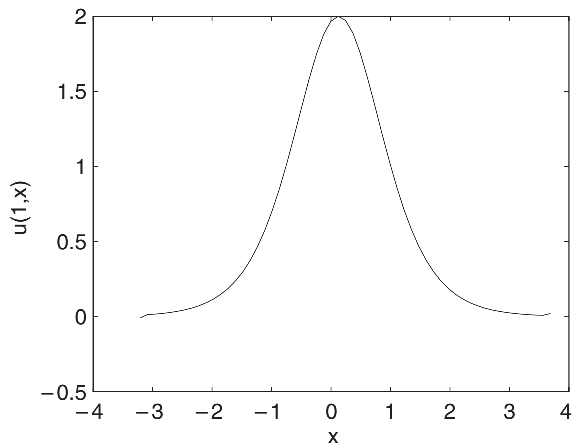


**Figure 4.** RK–MK with composition of exponentials, numerical solution at $t = 1$.

As we can see the two Lie group methods perform identically and both better then the `Matlab` routine that implements a classical RK method. Given that the approximation of the soliton for the KdV equation is obtained just by scaling and interpolating the numerical solution obtained for the KVM, the figures presented are also indicative of the performance of the methods on the KVM system.

The simulation of two interacting solitons has not been properly tested yet and in any case it appears more difficult, numerical instability occurs for big enough $t$.

In [11] Goodman and Lax observed that the semi-discrete scheme of [15] coincides with the use of a special finite-difference discretization for the conservation law

$$u_t + (\tfrac{1}{2}u^2)_x = 0 \tag{3.11}$$

namely

$$\frac{\mathrm{d}}{\mathrm{d}t}u_n + u_n\frac{u_{n+1} - u_{n-1}}{2\Delta} = 0. \tag{3.12}$$

Using the explicit classical RK of order 4 (RK4) for integrating the system (3.11) Goodman and Lax observed an oscillatory behaviour in the numerical solution for times $t$ greater than a certain critical time.

This unstable behaviour appears as a disadvantage also in our context and sets limits to the possibility of using the KVM discretization for numerical purposes.

Our interest in investigating the KVM equation as a discretization of the KdV equation is motivated by the fact that the KVM is a completely integrable system and can be written in the Lax formalism, which is natural for the application of Lie group methods.

Our attempts to find alternative more stable semi-discretizations for the Lax formulation of the KdV that maintain the geometrical properties of the infinite-dimensional problem have for the moment not been successful.

Given the good features of pseudo-spectral methods in handling soliton equations [10], we will try in the future to combine these semi-discretization strategies with the ideas of this paper.

## Appendix

We here illustrate an example of a coordinate map based on the symmetric composition of elementary exponentials.

Suppose $u \in \mathfrak{so}(n, \mathbb{R})$ is a skew-symmetric matrix; we consider a symmetric composition of exponentials

$$\phi(u) = \exp(U_1) \cdots \exp(U_{n-1}) \cdots \exp(U_1) \tag{A.1}$$

where the $U_i$ are explicit functions of the entries of $u$. More precisely we express

$$U_i := U_i^0 + U_i^1$$

and we now define $U_i^0 := \boldsymbol{u}_i \boldsymbol{e}_i^{\mathrm{T}} - \boldsymbol{e}_i \boldsymbol{u}_i^{\mathrm{T}}$ with $\boldsymbol{u}_i = -[0, \ldots, 0, u_{i,i+1}, \ldots, u_{i,n}]^{\mathrm{T}}$ and $\boldsymbol{e}_i$ the $i$th vector of the canonical basis of $\mathbb{R}^n$. Analogously $U_i^1 := \boldsymbol{q}_i \boldsymbol{e}_i^{\mathrm{T}} - \boldsymbol{e}_i \boldsymbol{q}_i^{\mathrm{T}}$ with $\boldsymbol{q}_i = -[0, \ldots, 0, q_{i,i+1}, \ldots, q_{i,n}]^{\mathrm{T}}$ and $q_{i,j}$ are the entries of the skew-symmetric matrix $Q$ defined by

$$Q = \frac{1}{12} \sum_{l=2}^{n-1} 2(\bar{\boldsymbol{u}}_l \hat{\boldsymbol{u}}_l^{\mathrm{T}} - \hat{\boldsymbol{u}}_l \bar{\boldsymbol{u}}_l^{\mathrm{T}}) + \frac{1}{2}(\bar{\boldsymbol{u}}_l \boldsymbol{u}_l^{\mathrm{T}} - \boldsymbol{u}_l \bar{\boldsymbol{u}}_l^{\mathrm{T}}) \tag{A.2}$$

$$+ \frac{1}{12} \sum_{l=2}^{n-1} \boldsymbol{u}_l \left( \sum_{k=1}^{l-1} u_{k,l} \boldsymbol{u}_k - \check{\boldsymbol{u}}_l \right)^{\mathrm{T}} - \left( \sum_{k=1}^{l-1} u_{k,l} \boldsymbol{u}_k - \check{\boldsymbol{u}}_l \right) \boldsymbol{u}_l^{\mathrm{T}} \tag{A.3}$$

$$+ \frac{1}{12} \sum_{l=2}^{n-1} \frac{1}{2} \boldsymbol{u}_l^{\mathrm{T}} \boldsymbol{u}_l (\hat{\boldsymbol{u}}_l \boldsymbol{e}_l^{\mathrm{T}} - \boldsymbol{e}_l \hat{\boldsymbol{u}}_l^{\mathrm{T}}) + \check{\boldsymbol{u}}_l \boldsymbol{e}_l^{\mathrm{T}} - \boldsymbol{e}_l \check{\boldsymbol{u}}_l^{\mathrm{T}} \tag{A.4}$$

with

$$\boldsymbol{e}_k^{\mathrm{T}} \bar{\boldsymbol{u}}_l = \begin{cases} -\boldsymbol{u}_k^{\mathrm{T}} \boldsymbol{u}_l & k = 1, \ldots, l-1 \\ 0 & \text{otherwise} \end{cases}$$

$$\boldsymbol{e}_k^{\mathrm{T}} \hat{\boldsymbol{u}}_l = \begin{cases} u_{k,l} & k = 1, \ldots, l-1 \\ 0 & \text{otherwise} \end{cases}$$

and

$$\boldsymbol{e}_k^{\mathrm{T}} \check{\boldsymbol{u}}_l = \begin{cases} \boldsymbol{u}_k^{\mathrm{T}} \hat{\boldsymbol{u}}_l & k = 1, \ldots, l-1 \\ 0 & \text{otherwise.} \end{cases}$$

The cost of computing $Q$ is in this case $\approx 5n^3$ flops, but if the rows of the matrix $u$ are such that just one element per row is nonzero then the complexity reduces to $\approx 5n^2$. This is in fact the case of our application.

If we assume that the entries of $u$ are of order one in a parameter $h$ it is possible to show that (A.1) is an approximation of order four in $h$ of $\exp(u)$. Moreover the given explicit formula for $Q$ is the second term in the symmetric BCH formula for

$$\exp(U_1^0) \cdots \exp(U_{n-1}^0) \cdots \exp(U_1^0)$$

and $U_i^0 = \boldsymbol{u}_i \boldsymbol{e}_i^{\mathrm{T}} - \boldsymbol{e}_i \boldsymbol{u}_i^{\mathrm{T}}$, namely

$$Q = \frac{1}{12} \sum_{l=2}^{k-1} [U_1^0 + \cdots + U_{l-1}^0 + \tfrac{1}{2} U_l^0, [U_1^0 + \cdots + U_{l-1}^0, U_l^0]].$$

## References


[1] Adler M 1979 On a trace functional for formal pseudo-differential operators and the symplectic structure of the Korteweg–de Vries type equations *Inv. Math.* **50** 219–48

[2] Bakirova M I, Dorodnitsyn V A and Kozlov R V 1997 Symmetry preserving difference schemes for some heat transfer equations *J. Phys. A: Math. Gen.* **30** 8139–55

[3] Budd C J, Collins G J, Huang W Z and Russell R D 1999 Self-similar numerical solutions of the porous-medium equation using moving mesh methods *Phil. Trans. R. Soc.* A **357** 1047–78

[4] Calvo M P, Iserles A and Zanna A 1997 Numerical solution of isospectral flows *Math. Comput.* **66** 1461–86

[5] Celledoni E and Iserles A 1999 Methods for the approximation of the matrix exponential in a Lie-algebraic setting *Technical Report* 1999-015 MSRI
Celledoni E and Iserles A 1999 *IMA J. Numer. Anal.* at press

[6] Celledoni E and Iserles A 2000 Approximating the matrix exponential from a Lie algebra to a Lie group *Math. Comput.* **69** 1457–80

[7] Crouch P E and Grossman R 1993 Numerical integration of ordinary differential equations on manifolds *J. Nonlinear Sci.* **3** 1–33

[8] Diele F, Lopez L and Politi T 1998 One step semi-explicit methods based on the Cayley transform for solving isospectral flows *J. Comput. Appl. Math.* **89** 219–23

[9] Engø K 1999 On the construction of geometric integrators in the RK–MK class *Bus. Inf. Technol.* **40** 41–61

[10] Fornberg B 1996 *A Practical Guide to Pseudospectral Methods (Cambridge Monographs on Applied and Computational Mathematics)* (Cambridge: Cambridge University Press)

[11] Goodman J and Lax P 1988 On dispersive difference schemes *Commun. Pure Appl. Math.* **41** 591–613

[12] Hairer E, Nørsett S P and Wanner G 1993 *Solving Ordinary Differential Equations I. Nonstiff Problems* 2nd revised edn (Berlin: Springer)

[13] Hirota R 1977 Nonlinear partial difference equations I. A difference analogue of the Korteweg–de Vries equation *J. Phys. Soc. Japan* **43** 1429–33

[14] Iserles A, Munthe-Kaas H Z, Nørsett S P and Zanna A 2000 Lie-group methods *Acta Numer.* **9** 215–365

[15] Kac M and Van Moerbeke P 1975 On an explicitly soluble system of nonlinear differential equations related to certain Toda lattices *Adv. Math.* **16** 160–9

[16] Kac M and Van Moerbeke P 1975 Some probabilistic aspects of scattering theory *Functional Integration and its Applications: Proc. Int. Conf. (London, 1974)* (Oxford: Clarendon) pp 87–96

[17] Kozlov R 2000 Conservation laws of semidiscrete Hamiltonian equations *NTNU Department of Mathematical Sciences Technical Report*
Kozlov R 2000 *J. Math. Phys.* at press

[18] McLachlan R and Robidoux N Integral-preserving and skew-adjoint discretizations of partial differential equations *Massey University Technical Report*

[19] McLachlan R I 1994 Symplectic integration of Hamiltonian wave equations *Numer. Math.* **66** 465–92

[20] McLachlan R I and Roubidoux N 1999 Antisymmetry, pseudospectral methods, weighted residual discretizations, and energy conserving partial differential equations *Massey University Technical Report*

[21] Munthe-Kaas H 1999 High order Runge–Kutta methods on manifolds *Appl. Numer. Math.* **29** 115–27

[22] Munthe-Kaas H and Owren B 1999 Computations in a free Lie algebra *Phil. Trans. R. Soc.* A **357** 957–81

[23] Owren B and Marthinsen A 2000 Integration methods based on canonical coordinates of the second kind *Numer. Math.* at press

[24] Schwarz M 1982 Korteweg–de Vries and nonlinear equations related to the Toda lattice *Adv. Math.* **44** 132–54

[25] Trefethen L N and Bau D 1997 *Numerical Linear Algebra* (Philadelphia, PA: SIAM)

[26] Zanna A 1999 Collocation and relaxed collocation for the Fer and the Magnus expansions *SIAM J. Numer. Anal.* **36** 1145–82