High order three part split symplectic integrators: Application to the disordered discrete nonlinear Schrödinger equation

Ch. Skokos,1 E. Gerlach,2 J.D. Bodyfelt,3 G. Papanikos,4 and S. Eggel5

1Physics Department, Aristotle University of Thessaloniki, GR-54124, Thessaloniki, Greece
2Lohrmann Observatory, Technical University Dresden, D-01062, Dresden, Germany
3The Ohio State University, ElectroScience Laboratory, 1320 Kinneer Road, Columbus, OH 43212, USA
4School of Mathematics, Statistics and Actuarial Science, University of Kent, Canterbury, CT2 7NF, UK
5IMCCE, Observatoire de Paris, 77 Avenue Denfert-Rochereau, F-75014, Paris, France

(Dated: June 5, 2013)

PACS numbers: 05.45.-a, 45.10.-b, 02.60.Jh, 05.60.Cd

While symplectic integration methods based on operator splitting are well established in many branches of science, high order methods for Hamiltonian systems that split in more than two parts have not yet been studied in detail. We demonstrate ways to construct high order symplectic integrators for Hamiltonian systems that can be split in exactly three integrable parts. Using these techniques for the integration of the disordered, discrete nonlinear Schrödinger equation, we show that three part split symplectic integrators are more efficient than other numerical methods for the long time integration of multidimensional systems, with respect to both accuracy and computational time.

Following the time evolution of a dynamical system is generally accomplished by solving its corresponding equations of motion. If, for instance, the system under consideration can be described by an autonomous Hamiltonian function $H(\vec{q}, \vec{p})$, with $\vec{q}, \vec{p}$ respectively being vectors of the generalized coordinates and momenta, the equations of motion can be readily derived via Hamilton’s equations. One then attempts to determine the solution $\vec{x}(t) = (\vec{q}(t), \vec{p}(t))$, $t > 0$, for any given initial condition $\vec{x}(0)$. Formally this solution can be described by the action of the operator $e^{iL_H}$, with $L_H = \sum_i H_{\partial q_i} \partial_{q_i} - H_{\partial p_i} \partial_{p_i}$, on the initial condition, i.e. $\vec{x}(t) = e^{iL_H} \vec{x}(0)$. The Hamiltonian is said to be integrable if the action of this operator is known explicitly and the solution of the Hamiltonian equations of motion can be written in a closed, analytic form.

Unfortunately, this task is rarely possible, but in most cases the true solution can be approximated numerically. General purpose numerical integration methods for ordinary differential equations are capable of providing such approximations.

In this respect, the so-called symplectic integration techniques are of particular interest, as they are explicitly designed for the integration of Hamiltonian systems (see, for example, Chap. VI of [1], [2] and references therein). Assume that $H(\vec{q}, \vec{p})$ can be written as $H(\vec{q}, \vec{p}) = A(\vec{q}, \vec{p}) + B(\vec{q}, \vec{p})$, so that the action of operators $e^{iL_A}$ and $e^{iL_B}$ is known, and the solution of their Hamiltonian equations of motion can be written analytically, while $e^{iL_H}$ does not permit a closed analytical solution of its equations of motion. Then, a symplectic scheme for integrating the equations of motion from time $t$ to time $t+\tau$ consists of approximating the operator $e^{iL_H} = e^{i(L_A + L_B)}$ by a product of $j$ operators $e^{i\tau L_A}$ and $e^{i\tau L_B}$, which represent exact integrations of Hamiltonians $A(\vec{q}, \vec{p})$ and $B(\vec{q}, \vec{p})$ over times $c_i\tau$ and $d_i\tau$ respectively, i.e. $e^{iL_H} = \prod_{i=1}^{j} e^{i\tau L_A} e^{i\tau L_B} + O(\tau^{n+1})$. The constants $c_i$ and $d_i$ are appropriately chosen to increase the order of the remainder of this approximation. In practice, using this symplectic integrator (SI) we approximate the dynamics of the real Hamiltonian $H = A + B$ by a new one, $K = A + B + O(\tau^n)$, introducing an error term of order $\tau^n$ in each integration step, and the SI is said to be of order $n$.

By their construction SIs preserve the symplectic nature of the Hamiltonian system and keep bounded the error of the computed value of $H$ (which is an integral of the system, commonly referred as the ‘energy’) irrespectively of the total integration time. Generally, this is not the case with non-symplectic integration algorithms. As a consequence, SIs permit the use of relatively large integration time steps $\tau$ for acceptable levels of energy accuracy, resulting in lower CPU time requirements.

Recently, it was shown that SIs are also highly efficient in the integration of the variational equations needed for the computation of chaos indicators like the maximum Lyapunov Characteristic Exponent (mLCE) and the Smaller (SALI) and Generalized Alignment Index (GALI) when using the so-called ‘Tangent Map’ method. Due to these benefits, SIs became a standard technique in Hamiltonian dynamics with particular importance in long time integrations of multidimensional systems. Several SIs of different orders based on operator splitting have been developed over the years by various researchers.

In many cases of practical interest the Hamiltonian can be written as a sum of the system’s kinetic energy $T(\vec{p})$, dependent only on the momenta $\vec{p}$, and the potential $V(\vec{q})$, dependent only on the positions $\vec{q}$. In such
cases, the obvious choice for the application of a SI is to consider $A = T(\hat{p})$ and $B = V(\hat{q})$. Yet in many physical problems the corresponding Hamiltonian cannot be split in two integrable parts. The question then naturally arises whether it is possible to exploit the advantages of SIs for such systems as well.

In this paper we present a systematic way to construct efficient, high order SIs for Hamiltonians that can be split in three integrable parts. Particular cases of second order three part split SIs, connected with astronomical problems, have been reported in literature $[11]$. In these works, the considered Hamiltonians were expressed as $H = A(\hat{q}, \hat{p}) + B(\hat{q}, \hat{p}) + C(\hat{q}, \hat{p})$, the action of operators $e^{\tau L_A}$, $e^{\tau L_B}$ and $e^{\tau L_C}$ was analytically obtained, the second order SI of 5 steps

$$ABC^2(\tau) = e^{\tau L_A} e^{\tau L_B} e^{\tau L_C} e^{\tau L_B} e^{\tau L_A} \tag{1}$$

was constructed, and its performance was studied. This integrator represents the simplest form of a symmetric SI that can be constructed for a Hamiltonian which splits in three distinct parts. Surprisingly enough, no systematic attempts for obtaining general high order three part split SIs have been performed to date, although integrator $[11]$ showed a good numerical performance. Nevertheless, the idea of three part split was implemented for constructing second and fourth order integration schemes for a particular complicated molecular model $[12]$, while recently an adaptation of high order three part split methods was attempted to treat a specific astronomical problem $[8]$.

Our study fills this void by presenting a systematic way to construct higher order three part split SIs, based on the composition technique proposed by Yoshida $[6]$. Starting from a SI $S^{2n}(\tau)$ of order $2n$, we can construct a SI $S^{2n+2}(\tau)$ of order $2n+2$, as

$$S^{2n+2}(\tau) = S^{2n}(z_1 \tau) S^{2n}(z_0 \tau) S^{2n}(z_1 \tau), \tag{2}$$

with $z_0 = -2^{1/(2n+1)}/[2 - 2^{1/(2n+1)}]$ and $z_1 = 1/[2 - 2^{1/(2n+1)}]$. Applying this procedure to the second order SI $[11]$ we obtain the fourth order SI of 13 steps

$$ABC^4(\tau) = ABC^2(x_1 \tau) ABC^2(x_0 \tau) ABC^2(x_1 \tau), \tag{3}$$

with $x_0 = -2^{1/3}/(2 - 2^{1/3})$ and $x_1 = 1/(2 - 2^{1/3})$.

Equation (3) can be used repeatedly to construct higher order three part split SIs. Although such a procedure for constructing arbitrary SIs of even order with exact coefficients is straightforward, it is not optimal with respect to the number of required steps. As was already pointed out in $[6]$, alternative methods can be applied to obtain more economical integrators of high order, although the new coefficients can no longer be given in analytical form. Several sixth order SIs of this kind were presented in $[6]$. Here, we consider one corresponding to ‘solution A’ in $[6]$

$$ABC^6(\tau) = ABC^2(w_3 \tau) ABC^2(w_2 \tau) ABC^2(w_1 \tau) \times ABC^2(w_0 \tau) ABC^2(w_1 \tau) ABC^2(w_2 \tau) ABC^2(w_3 \tau) \tag{4}$$

having 29 steps. The exact values of $w_i$, $i = 0, 1, 2, 3$ can be found in $[1]$, Chap. V, Eq. (3.11) and $[6]$.

In order to investigate the efficiency of the different SI schemes we choose a multidimensional Hamiltonian system describing a one–dimensional chain of coupled, nonlinear oscillators. In particular we consider the Hamiltonian of the disordered discrete nonlinear Schrödinger equation (DNLS)

$$\mathcal{H}_D = \sum_i \epsilon_i |\psi_i|^2 + \frac{\beta}{2} |\psi_i|^4 - (\psi_{i+1} \psi_i^* + \psi_{i-1} \psi_i^*), \tag{5}$$

with complex variables $\psi_i$, lattice site indices $l$ and nonlinearity strength $\beta \geq 0$. The random on–site energies $\epsilon_l$ are chosen uniformly from the interval $[-\frac{W}{2}, \frac{W}{2}]$, with $W$ denoting the disorder strength. This model has two integrals of motion, as it conserves both the energy (5) and the norm $S = \sum_i |\psi_i|^2$, and has been extensively investigated in order to determine the characteristics of energy spreading in disordered systems $[13, 14, 17]$. These studies showed that the second moment, $m_2$, of the norm distribution grows subdiffusively in time $t$, as $t^a$, and the asymptotic value $a = 1/3$ of the exponent was theoretically predicted and numerically verified. Currently open questions on the dynamics of disordered systems concern the possible halt of wave packet’s spreading for $t \rightarrow \infty$ $[18]$, as well as the characteristics of its chaotic behavior $[19]$. Thus, providing the means to perform accurate long time simulations for the DNLS model within reasonable amounts of computational time is essential.

Applying the canonical transformation $\psi_l = (q_l + ip_l)/\sqrt{2}$, $\psi_l^* = (q_l - ip_l)/\sqrt{2}$, one can split (5) into a sum of three integrable parts A, B and C as follows

$$H_D = \sum_l \left\{ \frac{\epsilon_l |q_l|^2 + |p_l|^2}{A} + \frac{\beta}{8} \frac{|q_l|^2 + |p_l|^2}{B} - p_{l+1} p_l - q_{l+1} q_l \right\} \tag{6}$$

where $q_l$ and $p_l$ are respectively generalized coordinates and momenta. For these three parts the propagation of initial conditions $(q_l, p_l)$ at time $t$, to their final values $(q'_l, p'_l)$ at time $t + \tau$ is given by the operators

$$e^{\tau L_A} : \left\{ \begin{array}{r} q'_l = q_l \cos(\alpha_l \tau) + p_l \sin(\alpha_l \tau) \\ p'_l = p_l \cos(\alpha_l \tau) - q_l \sin(\alpha_l \tau) \end{array} \right., \tag{7}$$

$$e^{\tau L_B} : \left\{ \begin{array}{r} p'_l = p_l \\ q'_l = q_l - (p_{l-1} + p_{l+1}) \tau \end{array} \right., \tag{8}$$

$$e^{\tau L_C} : \left\{ \begin{array}{r} q'_l = q_l \\ p'_l = p_l + (q_{l-1} + q_{l+1}) \tau \end{array} \right., \tag{9}$$

with $\alpha_l = \frac{\epsilon_l}{\sqrt{\beta}}$. For $t \rightarrow \infty$, it is essential to choose $\alpha_l$ such that $\cos(\alpha_l \tau)$ remains close to unity. As the choice of $\alpha_l$ is restricted by the requirement that $\cos(\alpha_l \tau)$ remains close to unity, a natural choice for $\alpha_l$ is $\alpha_l = \frac{\epsilon_l}{\sqrt{\beta}}$.
with \( \alpha = \epsilon_1 + \beta(q_l^2 + p_l^2)/2 \). Thus, the DNLS model represents an ideal test case for our aforementioned three part split SIs.

In order to evaluate the efficiency of the SIs of (1), (3) and (4) we compare their performance to that of other numerical techniques. In [14–17] numerical integration schemes based on traditional two part split SIs were applied for the integration of Hamiltonian (6). These approaches were based on the split of \( H = A + B \), and the application of second order SIs of the so-called SABA–family [10]. In our study we implement the second order SI SABA2 using the split \( H_D = A + B \). The integration of the \( A \) part is performed according to (7), while different approaches for approximating the action of \( e^{t L_S} = e^{t L_B+c} \) are followed. In [14, 15] a numerical scheme based on Fourier transforms was implemented (see appendix of [15] for more details) leading to a second order integrator with 5 steps, which we name SIFT2 in the following. Another approach is to split the \( B \) part in two integrable parts as \( B = B + C \), and use the SABA2 SI to approximate its solution. This means that we perform two successive two part splits in order to integrate \( H_D \). This approach leads to a second order SI with 13 steps which we name SS2 (this scheme corresponds to the PQ method used in [17]). In addition, based on two part split SIs we construct an integrator of order higher than two by applying the composition procedure [2] to the SS2 integrator [21]. In this way we construct a fourth order SI with 37 simple steps which, to the best of our knowledge, has never been used before for the integration of the DNLS system, and we call it SS4.

Of course one can also use any general purpose non–symplectic integrator for the integration of (6). One disadvantage of such techniques is that different epochs of the system’s evolution are computed with different accuracy since these integrators do not keep the energy error bounded, but increase it as time increases. In particular for the DNLS model considered here the later stages of its evolution, which are of most importance since we are mainly interested in the asymptotic behavior of the system, are computed less accurately. As a representative of non–symplectic integrators we consider here the variable step Runge–Kutta method called DOP853, whose performance is controlled by the so–called one–step accuracy \( \delta \) [21].

In order to compare the performance of the various integration schemes we consider a particular disorder realization of the DNLS model with \( N = 1024 \) lattice sites. We fix the total norm of the system to \( S = 1 \), and following [10] we initially excite homogeneously 21 central sites by attributing to each one of them the same constant norm, but with a random phase, while for all other sites we set \( q_l(0) = p_l(0) = 0 \). Due to the nonlinear nature of the model the norm distribution spreads, keeping of course the total norm \( S = \sum_l(q_l^2 + p_l^2)/2 \) constant (\( S = 1 \)). The performance of the integration schemes is evaluated by their ability to (a) reproduce correctly the dynamics, which is reflected in the subdiffusive increase of \( m_2(t) \), (b) keep the values of the two integrals \( H_D, S \) constant, as monitored by the evolution of the absolute relative errors of the energy \( E_r(t) = (H_D(t) - H_D(0))/H_D(0) \), and norm \( S_r(t) = (|S(t) - S(0)|)/S(0) \), and (c) reduce the required CPU time \( T_r(t) \) for the performed computations.

Results obtained by the second order SIs ABC2, SS2 and SIFT2 and the non–symplectic integrator DOP853 are presented in Fig. 1. These integration methods correctly describe the system’s dynamical evolution since for all of them the wave packet’s \( m_2 \) shows practically the same behavior (Fig. 1). The time steps \( \tau \) of the three SIs were chosen so that all of them keep the relative energy error practically constant at \( E_r \approx 10^{-5} \) (Fig. 1b). Since we are interested in the accurate long time integration of the DNLS model we use \( \delta = 10^{-16} \) for the implementation of the DOP853 integrator. For \( t \approx 10^8 \) (which can be considered as a typical final integration time for long time simulations), this choice results practically in the same energy error obtained by all other tested integrators. From Fig. 1 we see that the relative norm error \( S_r \) increases for all used methods, exhibiting larger values yet lower increase rates, for the ABC2 and SS2 SIs. Nevertheless, our results indicate that all methods can keep \( S_r \) to acceptable levels (e.g. \( S_r \lesssim 10^{-2} \)), even for long time integrations. From Fig. 1 we see that the SIFT2 integration scheme is the most efficient one with respect to the CPU time needed for obtaining the results of Fig. 1.

For this reason we use the SIFT2 SI as a reference method, and compare in Fig. 2 its results with the ones obtained by our higher order SIs: the SS4, ABC4 and ABC6 methods. These higher order SIs reproduce correctly the evolution of \( m_2 \) (Fig. 2a), keep \( E_r \approx 10^{-5} \) (Fig. 2b), and show a slow increase of \( S_r \) with values remaining acceptably small (Fig. 2c). The ABC4 and ABC6 SIs require less CPU times respective to the SIFT2 method (Fig. 2d), with ABC6 showing the best performance. From the results of Fig. 2 we see that using the ABC6 with \( \tau = 0.15 \) we need \( \sim 1.5 \) times less CPU time than the SIFT2 with \( \tau = 0.05 \). Although one might argue that this CPU time gain factor is not too big, we should keep in mind that long time simulations up to \( t = 10^7 \) of the DNLS model with \( N \sim 1000 \) sites could require (depending on the particular computer used) up to \( \sim 10 \) days of computations. Thus a gain factor close to 2 is practically significant as it can considerably reduce the computation time. Our results indicate that the construction of efficient triple split SIs can allow the integration of the DNLS for longer times, and numerically tackle questions about the asymptotic behavior of wave packets.

In summary, we presented ways to use SIs for Hamil-
FIG. 1. Results for the integration of $H_D$ by the second order SIs ABC for $\tau = 0.005$, SS for $\tau = 0.02$, SIFT for $\tau = 0.05$ (g green; (b) blue; (bl) black), and the non–symplectic integrator DOP853 for $\delta = 10^{-16}$ (r red): (a) the absolute relative error $E_r(t)$, (c) the absolute relative norm error $S_r(t)$, and (d) the required CPU time $T_c(t)$ in seconds.

FIG. 2. Results for the integration of $H_D$ by the second order SI SIFT for $\tau = 0.05$ (bl black), the fourth order SIs SS for $\tau = 0.1$, ABC for $\tau = 0.05$ (b blue; (g) green), and the sixth order SI ABC2 for $\tau = 0.15$ (r red). The panels are as in Fig. 1. Note that in panel (d) the black and blue curves practically overlap.

Part of this work was carried out. Ch.S. was supported by the Research Committee of the Aristotle University of Thessaloniki (Prog. No 89317), and by the European Union (European Social Fund - ESF) and Greek national funds through the Operational Program “Education and Lifelong Learning” of the National Strategic Reference Framework (NSRF) – Research Funding Program: “THALES. Investing in knowledge society through the European Social Fund”.

* hskokos@auth.gr

[1] E. Hairer, C. Lubich and G. Wanner Geometric Numerical Integration. Structure-Preserving Algorithms for Ordinary Differential Equations, Springer Series in Computational Mathematics Vol. 31 (Springer, New York, 2002).

[2] R. I. McLachan and G. R. W. Quispel, J. Phys. A 39 5251 (2006); É. Forest, J. Phys. A 39 5321 (2006).

[3] G. Benettin et al., Meccanica 15 9 (1980); ibid 15 21 (1980); Ch. Skokos, Lect. Notes Phys. 790 63 (2010).

[4] Ch. Skokos, J. Phys. A 34 10029 (2001); Ch. Skokos et al., Prog. Theor. Phys. Supp. 150 439 (2003); ibid, J. Phys. A 37 6269 (2004); Ch. Skokos, T. C. Bountis and Ch. Antonopoulos, Physica D 231 30 (2007); ibid, Eur. Phys. J. Sp. T. 165 5 (2008); T. Manos, Ch. Skokos and Ch. Antonopoulos, Int. J. Bifurcation Chaos 22 1250218 (2012).

[5] Ch. Skokos and E. Gerlach, Phys. Rev. E 82 036704 (2010); E. Gerlach and Ch. Skokos, in Dynamical Sys-

Hamiltonian systems that do not split in two integrable parts, as traditional symplectic methods require, but in three. For such systems we constructed high order three part split SIs applying a systematic way for their creation: the composition method of [6], and emphasized their practical importance. In particular, we showed that such three part split SIs are more efficient numerical schemes than other symplectic and non-symplectic methods in terms of both accuracy and CPU time requirements, especially for the long time integration of multidimensional systems like the DNLS model.

We hope that our results will draw the interest of the community in the construction of three part split SIs, and will initiate future research both for the theoretical development of new integrators of this type, as well as for their applications to different dynamical systems. Keeping in mind that such SIs can provide efficient numerical schemes for the long time integration of Hamiltonian systems with many degrees of freedom (like the DNLS model), it would be interesting to investigate if the possible addition of a corrector term can improve their accuracy, as done for traditional two part split methods (see e.g. [2] [3] [4]).

Ch.S. would like to thank S. Anastasiou, G. Benettin and J. Laskar for useful discussions, as well as the Max Planck Institute for the Physics of Complex Systems in Dresden for its hospitality during his visits in July–August 2012 and January–February 2013, when part of this work was carried out. Ch.S. was supported by the Research Committee of the Aristotle University of Thessaloniki (Prog. No 89317), and by the European Union (European Social Fund - ESF) and Greek national funds through the Operational Program “Education and Lifelong Learning” of the National Strategic Reference Framework (NSRF) - Research Funding Program: “THALES. Investing in knowledge society through the European Social Fund”.

* hskokos@auth.gr

[1] E. Hairer, C. Lubich and G. Wanner Geometric Numerical Integration. Structure-Preserving Algorithms for Ordinary Differential Equations, Springer Series in Computational Mathematics Vol. 31 (Springer, New York, 2002).

[2] R. I. McLachan and G. R. W. Quispel, J. Phys. A 39 5251 (2006); É. Forest, J. Phys. A 39 5321 (2006).

[3] G. Benettin et al., Meccanica 15 9 (1980); ibid 15 21 (1980); Ch. Skokos, Lect. Notes Phys. 790 63 (2010).

[4] Ch. Skokos, J. Phys. A 34 10029 (2001); Ch. Skokos et al., Prog. Theor. Phys. Supp. 150 439 (2003); ibid, J. Phys. A 37 6269 (2004); Ch. Skokos, T. C. Bountis and Ch. Antonopoulos, Physica D 231 30 (2007); ibid, Eur. Phys. J. Sp. T. 165 5 (2008); T. Manos, Ch. Skokos and Ch. Antonopoulos, Int. J. Bifurcation Chaos 22 1250218 (2012).

[5] Ch. Skokos and E. Gerlach, Phys. Rev. E 82 036704 (2010); E. Gerlach and Ch. Skokos, in Dynamical Sys-
tems, Differential Equations and Applications, edited by W. Feng et al., Discr. Cont. Dyn. Syst. Supp. (2011) p. 475; E. Gerlach, S. Eggl and Ch. Skokos, Int. J. Bifurcation Chaos 22 1250216 (2012).

[6] H. Yoshida, Phys. Let. A 150 262 (1990).

[7] P. J. Channell and C. Scovel, Nonlinearity 3 231 (1990); E. Forest and R. D. Ruth, Physica D 43 105 (1990); J. Candy and W. Rozmus, J. Comp. Phys. 92 230 (1991); R. I. McLachan and P. Atela, Nonlinearity 5 541 (1992); H. Yoshida, Cel. Mech. Dyn. Astron. 56 27 (1993); R. I. McLachan, BIT 35 258 (1995); S. A. Chin, Phys. Let. A. 226 344 (1997); I. P. Omelyan, I. M. Myrglod and R. Folk, Phys. Rev. E 65 056706 (2002).

[8] S. Blanes et al., e-print arXiv:1208.0689; A. Farrés et al., e-print arXiv:1208.0716)

[9] I. P. Omelyan, I. M. Myrglod and R. Folk, Phys. Rev. E 66 026701 (2002)

[10] J. Laskar and P. Robutel, Cel. Mech. Dyn. Astr. 80 39 (2001).

[11] J. E. Chambers, Mon. Not. R. Astron. Soc. 304, 793 (1999); K. Goździewski, S. Breiter and W. Borczyk, Mon. Not. R. Astron. Soc. 383, 989 (2008); T. Quinn et al., Astron. J. 139, 803 (2010); J. E. Chambers, in Planets in Binary Star Systems, edited by N. Haghighipour, Astrophysics and Space Science Library 366 (2010) p. 239.

[12] I. P. Omelyan, J. Chem. Phys. 127 044102 (2007)

[13] G. Kopidakis et al., Phys. Rev. Let. 100 084103 (2008); J. D. Bodyfelt et al., Int. J. Bifurcation Chaos 21 2007 (2011).

[14] S. Flach, D. O. Krimer and Ch. Skokos, Phys. Rev. Let. 102 024101 (2009).

[15] Ch. Skokos et al., Phys. Rev. E 79 056211 (2009).

[16] T. V. Laptyeva et al., Europhys. Lett. 91 30001 (2010).

[17] J. D. Bodyfelt et al., Phys. Rev. E, 84 016205 (2011).

[18] M. Johansson, G. Kopidakis, and S. Aubry, Europhys. Lett., 91 50001 (2010); S. Aubry, Int. J. Bifurcation Chaos 21 2125 (2011).

[19] Ch. Skokos, I. Gkolias and S. Flach, in preparation.

[20] The successive splits methodology in combination with Yoshida’s composition technique was also implemented in 

[21] Freely available from http://www.unige.ch/~hairer/software.html.