Symplectic integration methods for multidimensional disordered nonlinear lattices

Haris Skokos
Aristotle University of Thessaloniki, Greece

E-mail: hskokos@auth.gr
URL: http://users.auth.gr/hskokos/
Outline

• Symplectic Integrators: Application to disordered nonlinear lattices
  ✓ Models
    • The quartic Klein-Gordon (KG) disordered lattice
    • The disordered discrete nonlinear Schrödinger equation (DNLS)
  ✓ Symplectic integration of KG and DNLS models
  ✓ Numerical results: different dynamical behaviors

• Symplectic integration of variational equations: The Tangent Map (TM) method
  ✓ Chaos indicators
    • Lyapunov exponents
    • Generalized Alignment Index (GALI)
  ✓ Chaotic behavior of the KG model

• High order three part split symplectic integrators for the DNLS model

• Outlook
Autonomous Hamiltonian systems

Consider an $N$ degree of freedom autonomous Hamiltonian system having a Hamiltonian function of the form:

$$H(q_1, q_2, \ldots, q_N, p_1, p_2, \ldots, p_N)$$

The time evolution of an orbit (trajectory) with initial condition

$$P(0) = (q_1(0), q_2(0), \ldots, q_N(0), p_1(0), p_2(0), \ldots, p_N(0))$$

is governed by the Hamilton’s equations of motion

$$\frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i}, \quad \frac{dq_i}{dt} = \frac{\partial H}{\partial p_i}$$
Symplectic Integration schemes

Formally the solution of the Hamilton equations of motion can be written as:

\[
\frac{d\vec{X}}{dt} = \{H, \vec{X}\} = L_H \vec{X} \Rightarrow \vec{X}(t) = \sum_{n=0}^{t^n} \frac{n!}{n!} L^n_H \vec{X} = e^{tL_H} \vec{X}
\]

where \(\vec{X}\) is the full coordinate vector and \(L_H\) the Poisson operator:

\[
L_H f = \sum_{j=1}^{N} \left\{ \frac{\partial H}{\partial p_j} \frac{\partial f}{\partial q_j} - \frac{\partial H}{\partial q_j} \frac{\partial f}{\partial p_j} \right\}
\]

If the Hamiltonian \(H\) can be split into two integrable parts as \(H = A + B\), a symplectic scheme for integrating the equations of motion from time \(t\) to time \(t+\tau\) consists of approximating the operator \(e^{\tau L_H}\) by

\[
e^{\tau L_H} = e^{\tau (L_A + L_B)} = \prod_{i=1}^{j} e^{c_i \tau L_A} e^{d_i \tau L_B} + O(\tau^{n+1})
\]

for appropriate values of constants \(c_i, d_i\). This is an integrator of order \(n\).

So the dynamics over an integration time step \(\tau\) is described by a series of successive acts of Hamiltonians \(A\) and \(B\).
Symplectic Integrator $SABA_2^2C$

The operator $e^{\tau L_H}$ can be approximated by the symplectic integrator [Laskar & Robutel, Cel. Mech. Dyn. Astr. (2001)]:

$$SABA_2 = e^{c_1 \tau L_A} e^{d_1 \tau L_B} e^{c_2 \tau L_A} e^{d_1 \tau L_B} e^{c_1 \tau L_A}$$

with $c_1 = \frac{1}{2} - \frac{\sqrt{3}}{6}$, $c_2 = \frac{\sqrt{3}}{3}$, $d_1 = \frac{1}{2}$.

The integrator has only small positive steps and its error is of order $2$.

In the case where $A$ is quadratic in the momenta and $B$ depends only on the positions the method can be improved by introducing a corrector $C$, having a small negative step:

$$C = e^{-\tau^3 \frac{c}{2} L_{\{\{A,B\},B\}}}$$

with $c = \frac{2 - \sqrt{3}}{24}$.

Thus the full integrator scheme becomes: $SABAC_2 = C (SABA_2) C$ and its error is of order $4$. 
Interplay of disorder and nonlinearity

Waves in disordered media – Anderson localization
[Billy et al., Nature (2008)]

Waves in nonlinear disordered media – localization or delocalization?


Experiments: propagation of light in disordered 1d waveguide lattices [Lahini et al., PRL, (2008)]
The Klein – Gordon (KG) model

\[ H_K = \sum_{l=1}^{N} \frac{P_l^2}{2} + \frac{\tilde{\varepsilon}_l}{2} u_l^2 + \frac{1}{4} u_l^4 + \frac{1}{2W} (u_{l+1} - u_l)^2 \]

with fixed boundary conditions \( u_0 = p_0 = u_{N+1} = p_{N+1} = 0 \). Typically \( N = 1000 \).

Parameters: \( W \) and the total energy \( E \). \( \tilde{\varepsilon}_l \) chosen uniformly from \( \left[ \frac{1}{2}, \frac{3}{2} \right] \).

The discrete nonlinear Schrödinger (DNLS) equation

We also consider the system:

\[ H_D = \sum_{l=1}^{N} \varepsilon_l |\psi_l|^2 + \frac{\beta}{2} |\psi_l|^4 - (\psi_{l+1}\psi_l^* + \psi_{l+1}^* \psi_l) \]

where \( \varepsilon_l \) chosen uniformly from \( \left[ -\frac{W}{2}, \frac{W}{2} \right] \) and \( \beta \) is the nonlinear parameter.

Conserved quantities: The energy and the norm of the wave packet.
Distribution characterization

We consider normalized energy distributions in normal mode (NM) space:

\[ z_\nu \equiv \frac{E_\nu}{\sum_m E_m} \quad \text{with} \quad E_\nu = \frac{1}{2} \left( \dot{A}_\nu^2 + \omega_\nu^2 A_\nu^2 \right) \],

where \( A_\nu \) is the amplitude of the \( \nu \)th NM.

Second moment:

\[ m_2 = \sum_{\nu=1}^{N} (\nu - \bar{\nu})^2 z_\nu \quad \text{with} \quad \bar{\nu} = \sum_{\nu=1}^{N} \nu z_\nu \]

Participation number:

\[ P = \frac{1}{\sum_{\nu=1}^{N} z_\nu^2} \]

measures the number of stronger excited modes in \( z_\nu \). Single mode \( P=1 \), Equipartition of energy \( P=N \).
The KG model

We apply the SABAC$_2$ integrator scheme to the KG Hamiltonian by using the splitting:

$$H_K = \sum_{l=1}^{N} \left( \frac{p_l^2}{2} + \frac{\varepsilon_l}{2} u_l^2 + \frac{1}{4} u_l^4 + \frac{1}{2W} (u_{l+1} - u_l)^2 \right)$$

with a corrector term which corresponds to the Hamiltonian function:

$$C = \left\{ \left\{ A, B \right\}, B \right\} = \sum_{l=1}^{N} \left[ u_l (\varepsilon_l + u_l^2) - \frac{1}{W} (u_{l-1} + u_{l+1} - 2u_l) \right]^2.$$
The DNLS model

A 2nd order SABA Symplectic Integrator with 5 steps, combined with approximate solution for the B part (Fourier Transform): SIFT$_2$

\[ H_D = \sum_l \varepsilon_l |\psi_l|^2 + \frac{\beta}{2} |\psi_l|^4 - \left( \psi_{l+1}\psi_l^* + \psi_{l+1}^*\psi_l \right), \quad \psi_l = \frac{1}{\sqrt{2}}(q_l + ip_l) \]

\[ H_D = \sum_l \left( \frac{\varepsilon_l}{2}(q_l^2 + p_l^2) + \frac{\beta}{8}(q_l^2 + p_l^2)^2 \right) - q_n q_{n+1} - p_n p_{n+1} \]

\[ e^{\tau L_A}: \left\{ \begin{array}{l} q_l' = q_l \cos(\alpha_l \tau) + p_l \sin(\alpha_l \tau), \\ p_l' = p_l \cos(\alpha_l \tau) - q_l \sin(\alpha_l \tau), \end{array} \right. \]
\[ \alpha_l = \varepsilon_l + \beta(q_l^2 + p_l^2)/2 \]

\[ e^{\tau L_B}: \left\{ \begin{array}{l} \varphi_q = \sum_{m=1}^N \psi_m e^{2\pi iq(m-1)/N} \\ \varphi_q' = \varphi_q e^{2i \cos(2\pi(q-1)/N)\tau} \\ \psi_l' = \frac{1}{N} \sum_{q=1}^N \varphi_q' e^{-2\pi il(q-1)/N} \end{array} \right. \]
The DNLS model

Symplectic Integrators produced by Successive Splits (SS)

\[ H_D = \sum_l \left( \frac{\varepsilon_l}{2} \left( q_l^2 + p_l^2 \right) + \frac{\beta}{8} \left( q_l^2 + p_l^2 \right)^2 \right) - q_n q_{n+1} - p_n p_{n+1} \]

\[
\begin{cases}
q_l' = q_l \cos(\alpha_l \tau) + p_l \sin(\alpha_l \tau), \\
p_l' = p_l \cos(\alpha_l \tau) - q_l \sin(\alpha_l \tau),
\end{cases}
\]

Using the SABA_2 integrator we get a 2nd order integrator with 13 steps, SS(SABA_2)_2:

\[ \text{SS}(\text{SABA}_2)_2 = e^{\frac{(3-\sqrt{3})}{6} \tau} L_A \tau L_B e^{\frac{\sqrt{3} \tau}{3} L_A} \tau L_B e^{\frac{(3-\sqrt{3})}{6} \tau} L_A \]

\[ \tau' = \tau / 2 \]
Different Dynamical Regimes


Δ: width of the frequency spectrum, d: average spacing of interacting modes, δ: nonlinear frequency shift.

Weak Chaos Regime: \( \delta < d, \quad m_2 \sim t^{1/3} \)
Frequency shift is less than the average spacing of interacting modes. NMs are weakly interacting with each other. [Molina, PRB (1998) – Pikovsky, & Shepelyansky, PRL (2008)].

Intermediate Strong Chaos Regime: \( d < \delta < \Delta, \quad m_2 \sim t^{1/2} \rightarrow m_2 \sim t^{1/3} \)
Almost all NMs in the packet are resonantly interacting. Wave packets initially spread faster and eventually enter the weak chaos regime.

Selftrapping Regime: \( \delta > \Delta \)
Frequency shift exceeds the spectrum width. Frequencies of excited NMs are tuned out of resonances with the nonexcited ones, leading to selftrapping, while a small part of the wave packet subdiffuses [Kopidakis et al., PRL (2008)].
Different spreading regimes

For $t=10$

- $\log_{10}(n_2)$ vs $\log_{10}t$: slope 1/3
- $\log_{10}P$ vs $\log_{10}t$: slope 1/6

For $t=10$

- $\log_{10}\epsilon$ vs $N$: $\epsilon$ is constant at $N=1000$
Different spreading regimes
Crossover from strong to weak chaos

\[ \alpha(\log t) = \frac{d \langle \log m_2 \rangle}{d \log t} \]

\( W = 4 \)

Average over 1000 realizations!

DNLS \( \beta = 0.04, 0.72, 3.6 \)

KG E = 0.01, 0.2, 0.75

\( \alpha = 1/2 \)

\( \alpha = 1/3 \)
Symplectic integration of variational equations
Autonomous Hamiltonian systems

We study $N$ degree of freedom autonomous Hamiltonian systems of the form:

$$H(\vec{q}, \vec{p}) = \frac{1}{2} \sum_{i=1}^{N} p_i^2 + V(\vec{q})$$

As an example, we consider the Hénon-Heiles system:

$$H_2 = \frac{1}{2}(p_x^2 + p_y^2) + \frac{1}{2}(x^2 + y^2) + x^2y - \frac{1}{3}y^3$$

Hamilton equations of motion:

$$\begin{align*}
\dot{x} &= p_x \\
\dot{y} &= p_y \\
\dot{p}_x &= -x - 2xy \\
\dot{p}_y &= y^2 - x^2 - y
\end{align*}$$

Variational equations:

$$\begin{align*}
\delta \dot{x} &= \delta p_x \\
\delta \dot{y} &= \delta p_y \\
\delta \dot{p}_x &= -(1 + 2y)\delta x - 2x\delta y \\
\delta \dot{p}_y &= -2x\delta x + (-1 + 2y)\delta y
\end{align*}$$
Chaos detection methods

The maximum Lyapunov exponent of a given orbit characterizes the mean exponential rate of divergence of trajectories surrounding this orbit.

\[ mLCE = \lambda_1 = \lim_{t \to \infty} \frac{1}{t} \ln \frac{\| \hat{w}(t) \|}{\| \hat{w}(0) \|} \]

\[ \lambda_1 = 0 \rightarrow \text{Regular motion (} \propto t^{-1} \text{)} \]

\[ \lambda_1 \neq 0 \rightarrow \text{Chaotic motion} \]

Following the evolution of \( k \) deviation vectors with \( 2 \leq k \leq 2N \), we define (Ch.S. et al., 2007) the Generalized Alignment Index (GALI) of order \( k \) :

\[ \text{GALI}_k (t) = \| \hat{w}_1 (t) \wedge \hat{w}_2 (t) \wedge ... \wedge \hat{w}_k (t) \| \]

Chaotic motion:

\[ \text{GALI}_k (t) \propto e^{[\lambda_1 - \lambda_2] + (\lambda_1 - \lambda_3) + ... + (\lambda_1 - \lambda_k)]t} \]

Regular motion on an \( s \)-dimensional torus with \( s \leq N \):

\[ \text{GALI}_k (t) \propto \begin{cases} \text{constant} & \text{if} \quad 2 \leq k \leq s \\ \frac{1}{t^{k-s}} & \text{if} \quad s < k \leq 2N - s \\ \frac{1}{t^{2(k-N)}} & \text{if} \quad 2N - s < k \leq 2N \end{cases} \]
Tangent Map (TM) Method


We apply the $\text{SABAC}_2$ integrator scheme to the Hénon-Heiles system by using the splitting:

$$
A = \frac{1}{2}(p_x^2 + p_y^2), \quad B = \frac{1}{2}(x^2 + y^2) + x^2y - \frac{1}{3}y^3,
$$

with a corrector term which corresponds to the Hamiltonian function:

$$
C = \{\{A, B\}, B\} = (x + 2xy)^2 + (x^2 - y^2 + y)^2
$$

We approximate the dynamics by the act of Hamiltonians $A$, $B$ and $C$, which correspond to the symplectic maps:

$$
e^{\tau_LA} : \begin{cases}
x' = x + p_x \tau \\
y' = y + p_y \tau \\
p'_{x} = p_{x} \\
p'_{y} = p_{y}
\end{cases}
$$

$$
e^{\tau_LB} : \begin{cases}
x' = x \\
y' = y \\
p'_{x} = p_{x} - x(1 + 2y)\tau \\
p'_{y} = p_{y} + (y^2 - x^2 - y)\tau
\end{cases}
$$

$$
e^{\tau_LC} : \begin{cases}
x' = x \\
y' = y \\
p'_{x} = p_{x} - 2x(1 + 2x^2 + 6y + 2y^2)\tau \\
p'_{y} = p_{y} - 2(y - 3y^2 + 2y^3 + 3x^2 + 2x^2y)\tau
\end{cases}
$$
Tangent Map (TM) Method

Any symplectic integration scheme used for solving the Hamilton equations of motion, which involves the act of Hamiltonians A, B and C, can be extended in order to integrate simultaneously the variational equations.

\[
\begin{align*}
\tau A: & \quad \left\{ 
\begin{array}{l}
x' = x + p_x \tau \\
y' = y + p_y \tau \\
p'_{x} = p_x \\
p'_{y} = p_y \\
\end{array}
\right. \\
\tau AV: & \quad \left\{ 
\begin{array}{l}
x' = x + p_x \tau \\
y' = y + p_y \tau \\
p'_{x} = p_x \\
p'_{y} = p_y \\
\end{array}
\right. \\
\tau BV: & \quad \left\{ 
\begin{array}{l}
x' = x \\
y' = y \\
p'_{x} = p_x - x(1 + 2y) \tau \\
p'_{y} = p_y + (y^2 - x^2 - y) \tau \\
\end{array}
\right. \\
\tau CV: & \quad \left\{ 
\begin{array}{l}
x' = x \\
y' = y \\
p'_{x} = p_x - 2x(1 + 2x^2 + 6y + 2y^2) \tau \\
p'_{y} = p_y - 2(y - 3y^2 + 2y^3 + 3x^2 + 2x^2y) \tau \\
\end{array}
\right.
\end{align*}
\]
Chaotic behavior of the KG model

Ch.S., I. Gkolas & S. Flach, 2012 (in preparation)
KG: Weak Chaos (E=0.4)
KG: Weak Chaos (E=0.4)

$t = 1000000000.00$

**Second Moment**

- Slope 1/3

**Participation Number**

- Slope 1/6

**Energy Distribution**

Slope -1
Single site excitations: Different spreading regimes

KG $W = 4$, $E = 0.4, 1.5$

Average over 20 realizations
Block excitations: Different spreading regimes

$W = 4$, $E/L = 0.01$, $0.2$, $0.75$

Average over 20 realizations
High order three part split symplectic integrators for the DNLS model

Three part split symplectic integrators for the DNLS model

Three part split symplectic integrator of order 2, with 5 steps: $ABC_2$

$$H_D = \sum_l \left( \frac{\varepsilon_l}{2} \left( q_i^2 + p_i^2 \right) + \frac{\beta}{8} \left( q_i^2 + p_i^2 \right)^2 \right)$$

$ABC_2 = e^{2L_A} e^{2L_B} e^{\tau L_C} e^{2L_B} e^{2L_A}$

This low order integrator has already been used by e.g. Chambers, MNRAS (1999) – Goździewski et al., MNRAS (2008).
2\textsuperscript{nd} order integrators: Numerical results
4th order symplectic integrators

Starting from any 2nd order symplectic integrator $S_{2nd}$, we can construct a 4th order integrator $S_{4th}$ using a composition method [Yoshida, Phys. Let. A (1990)]:

$$S_{4th}(\tau) = S_{2nd}(x_1 \tau) \times S_{2nd}(x_0 \tau) \times S_{2nd}(x_1 \tau)$$

$$x_0 = -\frac{2^{1/3}}{2 - 2^{1/3}} , \quad x_1 = \frac{1}{2 - 2^{1/3}}$$

Starting with the 2nd order integrators $SS(SABA_2)_2$ and $ABC_2$ we construct the 4th order integrators:

• $SS(SABA_2)_4$ with 37 steps
  • $ABC_4$ with 13 steps
4th order integrators: Numerical results
Outlook

• Disordered nonlinear lattices:
  ✓ Quantify the chaotic behavior of energy spreading: Find theoretical or empirical laws for the evolution of Lyapunov exponents.
  ✓ Use covariant Lyapunov vectors and frequency map analysis in order to study the chaotic nature of energy spreading: Do ‘chaotic hot spots’ exist?
  ✓ Determine the limiting states of wave packets.
  ✓ Identification of the selftrapped and spreading parts of wave packets.
  ✓ Extension to higher spatial dimensions, and interactions beyond nearest neighbors.

• Three part split symplectic integrators
  ✓ Computation of chaos indicators for the DNLS model.
  ✓ Different techniques for constructing high order integrators.
  ✓ Investigate the possible use of corrector terms.
  ✓ Applications to other dynamical systems (e.g. models studied at UCT).

• Chaos detection techniques
  ✓ Behavior of GALI\(_k\) indices for time dependent Hamiltonians, dissipative systems, and time series.
  ✓ Computation of the spectrum of LCEs using the compound matrix theory.
  ✓ Review paper: Comparative study of the various existing methods.
Main references

• Disordered systems
  ✓ S. Flach, D.O. Krimer, Ch.S. (2009) PRL, 102, 024101
  ✓ Ch.S., S. Flach (2010) PRE, 82, 016208
  ✓ J.D. Bodyfelt, T.V. Laptyeva, Ch.S., D.O. Krimer, S. Flach (2011) PRE, 84, 016205

• TM method

• Chaos indicators: Lyapunov exponents, GALI

• Three part split symplectic integrators
Summary

• Multidimensional disordered nonlinear lattices:
  ✓ The use of symplectic schemes allow us to follow their evolution for very long time intervals.
  ✓ We predicted theoretically and verified numerically the existence of different dynamical behaviors: a) Weak Chaos Regime: \( \delta<d, \ m_2 \sim t^{1/3} \), b) Intermediate Strong Chaos Regime: \( d<\delta<\Delta, \ m_2 \sim t^{1/2}, \rightarrow m_2 \sim t^{1/3} \), c) Self-trapping Regime: \( \delta>\Delta \)
  ✓ Generality of results: a) Two different models: KG and DNLS, b) Predictions made for DNLS are verified for both models.

• Numerical schemes based on symplectic integrators can be used for the efficient integration of the variational equations of multidimensional Hamiltonian systems.
  ✓ Our results suggest that Anderson localization is eventually destroyed by the slightest amount of nonlinearity, since spreading does not show any sign of slowing down.
  ✓ Energy spreading is a chaotic phenomenon, as Lyapunov exponent estimators decrease following an evolution different than in the case of regular motion.

• Three part split symplectic integrators
  ✓ Proved to be efficient integration methods suitable for the integration of the DNLS model.
  ✓ The 4th order integrator allows integration of the DNLS model for very long times.
  ✓ A systematic way of constructing high order three part split symplectic integrators was introduced.