Low Regularity Numerical Schemes for SPDE

Recontre ANR, Brest, 2024

Jacob Armstrong Goodall
Joint work with Yvain Bruned

May 23, 2024

Overview

- Setting: Schrödinger's equation
- Picard Iteration for Duhamel's formula
- Discretising iterated integrals
- Limitations at Higher order
- Resonance Based Structure Preserving Schemes
- Geometric Structure
- Kernel Approximations
- Discretisation Maps
- Resonance Runge-Kutta
- Theorem for Structure Preserving Scheme

Setting

$$i\partial_t u(t,x) + \mathscr{L}(\partial_x) u(t,x) = |\partial_x|^\alpha p(u(t,x),\overline{u}(t,x)) + |\partial_x|^\beta f(u(t,x),\overline{u}(t,x))W(t,x), \quad u(0,x) = v(x), \tag{1}$$

Two important examples are

$$\text{SNLSE: } \mathscr{L} = \partial_x^2 \quad p = |u|^2 u \quad f = uW(x,t)$$

$$\text{Manakov System: } \mathscr{L} = \partial_x^2 \quad p = |u|^2 u \quad f = \sum_{i=1}^{3} \sigma_i u \circ W(t)$$

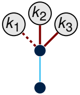
Goal 1: Find temporal discretisation of the above equations in the low regularity setting.
Goal 2: Extend these discretisation to those that preserve structure.

Duhamel Iterations

The Duhamel form of the NLSE is

$$\begin{aligned} u(t) = e^{it\Delta}v - ie^{it\Delta}\int_0^t e^{-is\Delta}u(s)\,|u(s)|^2\,ds \\ - ie^{it\Delta}\int_0^t e^{-is\Delta}u(s)\Phi dW(s). \end{aligned} \tag{2}$$

- This formula can be iterated once by substituting $u(s) = e^{is\Delta}v$.
- Again by substituting each occurring integral into every other.
- This produces a tree structure.

$T_1 = \Pi$ 

$= -ie^{-itk^2}\int_0^t e^{isk^2}e^{isk_1^2}e^{-isk_2^2}e^{-isk_3^2}ds.$

Duhamel Iterations

The first iteration is

$$u(t) = e^{it\Delta}v - ie^{it\Delta}\int_0^t e^{-is\Delta}\left(e^{is\Delta}v\right)^2 e^{-is\Delta}\bar{v}ds$$
$$- ie^{it\Delta}\int_0^t e^{-is\Delta}\left(e^{is\Delta}v\right)\Phi dW(s) + \mathcal{O}(t^{\frac{3}{2}})$$

The second order iteration will include all terms that scale linearly in time. For instance if we iterate the stochastic convolution we obtain

$$e^{it\Delta}\int_0^t e^{-is\Delta}\left(e^{is\Delta}\int_0^s e^{-is_1\Delta}\left(e^{is_1\Delta}v\right)\Phi dW(s_1)\right)\Phi dW(s) \sim t$$

which is of order $\mathcal{O}(t)$ because $dW(t)$ scales as $\sqrt{t}$.

Discretisation of Iterated Integrals

The primary challenge is to discretise the iterated integrals appearing in the expansion of Duhamel's Formula.

$$\int_0^t e^{-is\Delta}\left(e^{-is\Delta}\bar{v}\right)\left(e^{is\Delta}v\right)\left(e^{is\Delta}v\right)ds = \sum_{k=-k_1+k_2+k_3} e^{ikx}\bar{v}_{k_1}v_{k_2}v_{k_3} \int_0^t e^{isP(k_1,k_2,k_3)}ds,$$

The resonance approach relies on our ability to solve

$$\int_0^t e^{2ik_1^2 s}ds = \frac{e^{2ik_1^2 t}-1}{2ik_1^2}. \tag{3}$$

The other part of the operator, e^{isP}, can be discretised by Taylor expansion of the operator $e^{is\mathscr{L}_{\mathrm{low}}} = e^{is\left(P-2k_1^2\right)}$

The reason this is an improvement in terms of regularity is that the polynomial $P(k) - 2k_1^2 = 2k_1k_2 + 2k_2k_3 + 2k_1k_3$ is 'first order'. The terms map back to physical space as follows:

$$k_1^2 \bar{v}_{k_1} v_{k_2} v_{k_3} \mapsto (\Delta \bar{v}) v^2$$

while for the cross terms we have

$$k_1 k_2 \bar{v}_{k_1} v_{k_2} v_{k_3} \mapsto (\nabla \bar{v})(\nabla v) v.$$

So by eliminating the higher order terms by exact integration we have successfully lowered th regularity we ask on the initial conditions.

Discretisation of Iterated Integrals

Considering the first stochastic integral in Duhamel's Formula and apply the Fourier transform to the initial data and the white noise then we have

$$\int_0^t e^{-is\Delta}\left(e^{is\Delta}v\right)\Phi dW(s) = \sum_{k=k_1+k_2} e^{ikx}\Phi_{k_2}v_{k_1}\int_0^t e^{is(k_2^2+2k_1k_2)}dW_{k_2}(s). \tag{4}$$

Proceeding as in the deterministic case, we would like to solve the integral:

$$\int_0^t e^{isk_2^2}dW_{k_2}(s). \tag{5}$$

But this has no pathwise solution. As such we must Taylor expand the entire operator, which gives,

$$\int_0^t e^{is(k_2^2+2k_1k_2)}dW_{k_2}(s) = W_{k_2}(t) - W_{k_2}(0) + \mathcal{O}(t^{3/2}k_1k_2^2).$$

Low Regularity Scheme

Theorem

A low regularity scheme for stochastic NLS with multiplicative noise (2) of order $\mathcal{O}(t^{3/2})$ is given in Fourier space by:

$$
\begin{aligned}
U_k^{n,r}(v,t) &= e^{-itk^2} v_k - \sum_{k=-k_1+k_2+k_3} e^{-itk^2} \frac{e^{2ik_1^2 t} - 1}{2k_1^2} \bar{v}_{k_1} v_{k_2} v_{k_3} \\
&\quad - \sum_{k=k_1+k_2} i e^{-itk^2} \Phi_{k_2} (W_{k_2}(t) - W_{k_2}(0)) v_{k_1} \\
&\quad - \sum_{k=k_1+k_2+k_3} e^{-itk^2} \int_0^t \Phi_{k_2} (W_{k_2}(s) - W_{k_2}(0)) \Phi_{k_3} dW_{k_3}(s) v_{k_1}
\end{aligned}
$$

where one has to assume v to be in H^1 and that $\mathrm{Tr}\left((\Delta\Phi)^2\right) < +\infty$.

Limitations at Higher Order

Continuing Duhamel iterations to order $\mathcal{O}(t^2)$ by plugging the stochastic term into the nonlinearity gives

$$I = \sum_{k=k_1+k_2-k_3+k_4} e^{ikx} v_{k_1} \bar{v}_{k_3} v_{k_4} \Phi_{k_2} \int_0^t e^{isP_1} \int_0^s e^{is_1 P_2} dW_{k_2}(s_1) ds,$$

where $P_1 = 2k_3^2 - 2k_3(k_1 + k_2 + k_4) + 2k_1(k_2 + k_4) + 2k_2 k_4$ and $P_2 = k_2^2 + 2k_1 k_2$. We Taylor expand within the stochastic integral to obtain

$$\int_0^t e^{isP_1(k)} \int_0^s e^{is_1 P_2} dW_{k_2}(s_1) ds = \int_0^t e^{isP_1} \Big(W_{k_2}(s) - W_{k_2}(0) + \mathcal{O}(s^{3/2} k_1 k_2^2) \Big) ds.$$

Limitations at Higher Order

To proceed as in the deterministic setting we would observe that the only part of P_1 corresponding to a second order differential operator is $2k_3^2$ which would lead us to consider the integral

$$\int_0^t e^{2isk_3^2} \left(W_{k_2}(s) - W_{k_2}(0)\right) ds.$$

But this has no path-wise solution and we are thus forced to Taylor expand the operator $e^{isP_1} = 1 + \mathcal{O}(sP_1)$, preventing us from obtaining a low regularity approximation.

Structure Preserving Schemes

Next, we want to develop the idea of resonance schemes to obtain preservation of structural properties of the equation. For symplectic schemes we must consider the Stratanovich form of the SNLSE

$$\partial_t u + \partial_x^2 u + \lambda |u|^{2p} u = \kappa \Phi \sigma(u) \circ \xi(x,t),$$

- The discretisation of the Ito form corresponds to explicit methods
- The discretisation Stratanovich form corresponds to midpoint rule.

This comes from the definition of the integrals themselves i.e.

$$\int_0^t H(s) dW(s) = \lim_{n\to\infty} \sum_{s_i, s_{i-1} \in \pi} H(s_{i-1}) \left(W_{s_i} - W_{s_{i-1}} \right)$$

$$\int_0^t H(s) \circ dW(s) = \lim_{n\to\infty} \sum_{s_i, s_{i-1} \in \pi} \left(\frac{H_{s_i} - H_{s_{i-1}}}{2} \right) \left(W_{s_i} - W_{s_{i-1}} \right)$$

Geometric Structure: Deterministic

Consider Then The Hamiltonain equations of motion are

$$\dot{\mu}^k = \frac{\partial H}{\partial \nu_k}, \quad \dot{\nu}_k = \frac{\partial H}{\partial \mu^k}. \tag{6}$$

- The Hamiltonian is a function $H : M \to \mathbb{R}$ and a solution to the Hamiltonian system is a curve $\left(\mu^k(t), \nu_k(t)\right)$ in M
- The phase space M is $2n-$dimensional with coordinates μ^k and momenta ν_k for $k = 1, \ldots, n$.

For the NLSE, the following structures are conserved:

$$H(u) = \int \frac{1}{4} |\partial_x u|^2 - \frac{\lambda}{2p+2} |u|^{p+1}, \quad \int |u|^2 \, dx. \tag{7}$$

Geometric Structure: Stochastic

For the SNLSE, the generalised Hamiltonian equations of motion with noise are derived as follows,

$$\dot{\mu} = -\frac{\delta H_0}{\delta \nu} - \frac{\delta H_1}{\delta \nu} \circ \xi(t) \tag{8}$$

$$\dot{\nu} = \frac{\delta H_0}{\delta \mu} + \frac{\delta H_1}{\delta \mu} \circ \xi(t) \tag{9}$$

where $\delta F[\rho, \phi] = \frac{d}{d\varepsilon} F[\rho + \varepsilon \phi]_{\varepsilon=0}$, the functional derivative, and,

$$H_0(u) = -\frac{1}{2} \int |\nabla u|^2 \, dx + \frac{\lambda}{2p+2} \int |u|^{p+1} \, dx$$

and

$$H_1(u) = \frac{\kappa}{2} \int |u| \, dx. \tag{10}$$

Again, both the Hamiltonian and the mass are preserved.

Kernel Approximations

- Taylor expansion breaks symplectic structure
- An approximation based on polynomial interpolation can be used instead

$$
\begin{aligned}
e^{-2iskk_1+2isk_2k_3} &= e^{-2iskk_1} + e^{2isk_2k_3} - 1 + \left(e^{-2iskk_1} - 1\right)\left(e^{2isk_2k_3} - 1\right) \\
&\approx e^{-2iskk_1} + e^{2isk_2k_3} - 1 := \mathcal{K}(s; k, k_1, k_2, k_3).
\end{aligned}
$$

The kernel approximation above has the important symmetry property,

$$
\mathcal{K}(s; k, k_1, k_2, k_3) = \overline{\mathcal{K}(s; k_2, k_3, k, k_1)}. \tag{11}
$$

It's integral can be mapped to physical space

$$
\int_0^s \left[e^{-2skk_1} + e^{2isk_2k_3} - 1\right] ds \tag{12}
$$

Discretising Stochastic Integral

For a stochastic scheme we also need to discretise two stochastic integrals

$$I_1 = \sum_{k\in\mathbb{Z}} e^{ikx} \sum_{k_1,k_2} \Phi_{k_2} u_{k_1} e^{it(k_1+k_2)} \int_0^t e^{kk_2+k_1k_2} dW_{k_2}(s)$$

$$I_2 = \sum_{k\in\mathbb{Z}} e^{ikx} \sum_{k_1,k_2} \Phi_{k_3} \Phi_{k_2} u_{k_1} e^{it(k_1+k_2)} \int_0^t e^{isP(k_1,k_2,k_3)} dW_{k_2}(s) dW_{k_3}(s)$$

In both cases we can only perform the approximations

$$e^{itP(k_1,k_2)} \approx 1 + \mathcal{O}(k_1 k_2^2 t)$$

$$e^{itP(k_1,k_2,k_3)} \approx 1 + \mathcal{O}(k_1 k_2^2 k_3^2 t)$$

Discretisation Map

In order to construct our Scheme we must define the following maps based on these discretisations

$$v \mapsto \mathcal{F}(v)$$
$$:= -i\mu \sum_{k\in\mathbb{Z}} e^{ixk} \sum_{k+k_1=k_2+k_3} \int_0^t \mathcal{K}(s;k_1,k_2,k_3) ds \overline{\hat{v}_{k_1}} \hat{v}_{k_2} \hat{v}_{k_3}$$
$$v \mapsto \mathcal{P}_1(v) := \frac{1}{2} \sum_{m\in\mathbb{Z}} e^{ixm} \sum_{a+b=m} v_{k_1} \Phi_{k_2} W_{k_2}(t)$$
$$v \mapsto \mathcal{P}_2(v) := \frac{1}{4} \sum_{m\in\mathbb{Z}} e^{ixm} \sum_{a+b=m} v_{k_1} \Phi_{k_2} \Phi_{k_3} (W_{k_2}(t) W_{k_3}(t) - t)$$

For the maps $\mathcal{P}_1, \mathcal{P}_2$ to have the correct symmetry properties we require $\Phi^* = \Phi$ and $\Phi_k = \Phi_{-k}$.

Resonance Based Runge-Kutta

Using the discretisation $\mathcal{F}$ we can introduce the following scheme

$$u_{n+1} = e^{it\partial_x^2} u_n + t \sum_{\alpha \in S} b^{\alpha} e^{it\partial_x^2} K_{\alpha},$$

$$K_{\alpha} = \mathcal{F}\left(t; c_q; u_n + t \sum_{\tilde{\alpha} \in S} a_{\alpha}^{\tilde{\alpha}} K_{\tilde{\alpha}}\right).$$

which with

$$b^{\tilde{\alpha}} b^{\alpha} = b^{\alpha} a_{\alpha}^{\tilde{\alpha}} + b^{\tilde{\alpha}} a_{\tilde{\alpha}}^{\alpha},$$

Conserves both the mass and the Hamiltonian.

Resonance Based Runge-Kutta

When we introduce the maps for the stochastic terms we get the following:

$$u_{n+1} = e^{it\partial_x^2} u_n + t \sum_{\alpha_i \in S} b_\alpha^{(0)} e^{it\partial_x^2} K_\alpha + t \sum_{\alpha_i \in S} b_\alpha^{(1)} e^{it\partial_x^2} Q_\alpha + \sqrt{t} \sum_{\alpha_i \in S} b_\alpha^{(2)} e^{it\partial_x^2} L_\alpha$$

$$K_\alpha = \mathscr{F}(U_n), L_\alpha = \mathscr{P}_1(U_n), Q_\alpha = \mathscr{P}_2(U_n)$$

Where

$$U_n = u_n + t \sum_{\tilde{\alpha}_i \in S} a_{\alpha,\tilde{\alpha}}^{(0)} e^{it\partial_x^2} K_{\tilde{\alpha}} + \sqrt{t} \sum_{\tilde{\alpha}_i \in S} a_{\alpha,\tilde{\alpha}}^{(1)} e^{it\partial_x^2} L_{\tilde{\alpha}} + t \sum_{\tilde{\alpha}_i \in S} a_{\alpha,\tilde{\alpha}}^{(2)} e^{it\partial_x^2} Q_{\tilde{\alpha}}$$

Structure Preservation

Theorem

For coefficients such that

$$b_{\alpha}^{(i)} b_{\tilde{\alpha}}^{(j)} - b_{\alpha}^{(i)} a_{\alpha,\tilde{\alpha}}^{(j)} - b_{\tilde{\alpha}}^{(j)} a_{\tilde{\alpha},\alpha}^{(i)} = 0, \quad i,j = 0,1,2$$

and discretisation map such that

$$\int_{\mathbb{T}} \overline{u_n} \mathscr{F}(u_n) dx = 0$$

and symmetric Hilbert-Schmidt operator Φ *such that*

$$\Phi_k = \Phi_{-k}$$

the stochastic resonance Runge-Kutta scheme is symplectic.

Thank You!