Multi-revolution composition methods for highly oscillatory problems

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joint work with
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Plan of the talk

1. The class of multi-revolution composition methods (MRCM)
2. Order conditions and convergence analysis
3. Numerical experiments
4. Extension to stochastic highly oscillatory systems

References

- P. Chartier, J. Makazaga, A. Murua, and G. Vilmart, Multi-revolution composition methods for highly oscillatory differential equations. *Preprint.*
- P. Chartier, F. Mehats, M. Thalammer, Multi-revolution composition methods for time-dependent Schrödinger equations. *in preparation.*
- G. Vilmart, Weak second order multi-revolution composition methods for highly oscillatory stochastic differential equations with additive or multiplicative noise. *Preprint.*

Highly oscillatory problems

We consider highly oscillatory problems (HOP) of the form

$$\frac{d}{dt}y_\varepsilon(t) = \varepsilon^{-1}A_\varepsilon y_\varepsilon(t) + g(y_\varepsilon(t)), \qquad 0 \le t \le T,$$

with solution $y_\varepsilon(t) \in \mathbb{R}^d$ and

- A_ε is a $d \times d$ skew-symmetric matrix with eigenvalues in $2i\pi\mathbb{Z}$ (making $t \mapsto e^{t\varepsilon^{-1}A}$ an ε-periodic map)
- $\varepsilon \ll 1$ (scales as the inverse of the frequency)
- g is a smooth nonlinearity.

Remarks.

- It includes several Hamiltonian partial differential equations (spatially discr.), in particular the nonlinear Schrödinger eq.
- Standard integrators usually have a stepsize restriction $h \le C\varepsilon$ for stability/accuracy. Trigonometric methods require filters to reduce resonances (see Gautchi type methods).

Multi-revolution methods

see Calvo, Jay, Montijano, Rández (2003, 2004, 2007)
(multi-revolution Runge-Kutta methods in the context of Astronomy).
Idea The flow-map over one period ε is a near-identity map:

$$\varphi_\varepsilon : \mathbb{R}^d \to \mathbb{R}^d, \qquad \varphi_\varepsilon(y) = y + \mathcal{O}(\varepsilon).$$

Iterating N times the map φ_ε accounts for integrating the differential system over a time interval of length $H = N\varepsilon$.

Considering a smooth near-identity map

$$(\varepsilon, y) \mapsto \varphi_\varepsilon(y) = y + \varepsilon\Theta_\varepsilon(y),$$

the idea is to approximate $N = \mathcal{O}(1/\varepsilon)$ compositions of φ_ε,

$$\varphi_\varepsilon^N = \underbrace{\varphi_\varepsilon \circ \cdots \circ \varphi_\varepsilon}_{N \text{ times}}$$

with a method with cost and accuracy independent of ε.

Definition of multi-revolution composition methods

Definition: Semi discrete MRCM

Given $s \geq 1$, define for all $N \geq N_0$, $H = N\varepsilon \leq H_0$,

$$\Psi_{N,H}(y) := \varphi_{\alpha_1(N)H} \circ \varphi^*_{\beta_1(N)H} \circ \cdots \circ \varphi_{\alpha_s(N)H} \circ \varphi^*_{\beta_s(N)H}(y) \simeq \varphi^N_\varepsilon(y)$$

where $\alpha_j(N)$ and $\beta_j(N)$ are scalars depending on N and satisfying $\sum_{j=1}^s (\alpha_j(N) + \beta_j(N)) = 1$, and where $\varphi^*_\varepsilon := \varphi^{-1}_{-\varepsilon}$ is the adjoint of φ_ε.

Remark: comput. advantageous compared to φ^N_ε for $2s \ll N$.

Example: Method of order 2

With $s = 1$, given by $\alpha_1 = \frac{1}{2} + \frac{1}{2N}$ and $\beta_1 = \frac{1}{2} - \frac{1}{2N}$:

$$\varphi_{\alpha_1 H} \circ \varphi^{-1}_{-\beta_1 H}(y) = \varphi^N_\varepsilon(y) + \mathcal{O}(H^3).$$

Definition of multi-revolution composition methods

If φ_ε is not known exactly, we consider instead an approximation

$$\Phi_{\varepsilon,h}(y) \approx \varphi_\varepsilon(y).$$

We assume the following accuracy estimate with order $q \geq 1$,

$$\Phi_{\varepsilon,h}(y) - \varphi_\varepsilon(y) = \mathcal{O}(\varepsilon h^q),$$

obtained using e.g. a standard Strang splitting with stepsize h between the periodic linear part and the nonlinear part.

Definition: Fully-discrete composition methods

Given $s \geq 1$, define for all $N \geq 1$, $H \leq H_0$, $h \leq h_0$,

$$\Psi_{N,H,h}(y) = \Phi_{\alpha_1(N)H,h} \circ \Phi^*_{\beta_1(N)H,h} \circ \cdots \circ \Phi_{\alpha_s(N)H,h} \circ \Phi^*_{\beta_s(N)H,h}(y)$$

where H is called the macro step and h the micro step, and where $\Phi^*_{\varepsilon,h} := \Phi^{-1}_{-\varepsilon,h}$ is the adjoint of $\Phi_{\varepsilon,h}$.

Ingredient 1: Formalism of trees to derive the order conditions

B_∞-series associated to a map $a : T_\infty \cup \{\emptyset\} \to \mathbb{R}$

Assume $\varphi_\varepsilon = y + \varepsilon d_1(y) + \varepsilon^2 d_2(y) + \varepsilon^3 d_3(y) + \dots$

Consider formal series indexed by labelled rooted trees: $\textcircled{1}, \textcircled{2}, \begin{smallmatrix}\textcircled{1}\\ | \\ \textcircled{2}\end{smallmatrix}, \dots$

$$
\begin{aligned}
B_\infty(a, \varepsilon, y) &= a(\emptyset)y + \sum_{\tau \in T_\infty} \frac{\varepsilon^{\|\tau\|}}{\sigma(\tau)} a(\tau) F(\tau)(y) \\
&= a(\emptyset)y + \varepsilon a(\textcircled{1}) d_1(y) + \varepsilon^2 a(\textcircled{2}) d_2(y) \\
&\quad + \varepsilon^2 a\left(\begin{smallmatrix}\textcircled{1}\\ | \\ \textcircled{1}\end{smallmatrix}\right) d_1'(y) d_1(y) + \varepsilon^3 a(\textcircled{3}) d_3(y) + \varepsilon^3 a\left(\begin{smallmatrix}\textcircled{1}\\ | \\ \textcircled{2}\end{smallmatrix}\right) d_2'(y) d_1(y) \\
&\quad + \dots
\end{aligned}
$$

where

$$
\begin{aligned}
F(\textcircled{j})(y) &= d_j(y), \\
F([\tau_1, \dots, \tau_m]_j)(y) &= d_j^{(m)}(y)(F(\tau_1)(y), \dots, F(\tau_m)(y)).
\end{aligned}
$$

Ingredient 2: rigorous estimates on the remainders in Taylor series

To derive the order conditions, we compare equal powers of H in the B_∞-series $B(e_N, H, y)$ and $B(a, H, y)$.
The remainder of the Taylor series is estimated rigorously using the following lemma.

Lemma

Assume that $(y, \varepsilon) \mapsto \Theta_\varepsilon(y)$ is of class C^{p+1} with respect to (y, ε) on $B_{2R}(y_0) \times [-\varepsilon_0, \varepsilon_0]$ for a given $R > 0$ and a given $\varepsilon_0 > 0$. Then, there exists a constant H_0 such that for all ε and $N \geq 1$ with $H = N\varepsilon \leq H_0$,

$$\left\|\partial_\varepsilon^{p+1} \varphi_\varepsilon^N\right\| \leq CN^{p+1}, \qquad \left\|\partial_H^{p+1} \varphi_{H/N}^N\right\| \leq C,$$

in $B_R(y_0)$, where C is independent of N and ε.

Main ingredient of the proof of the lemma: the Faà-di-Bruno formula.

Ingredient 3: Eliminating redundant order conditions

For instance, for order 4, there are 7 conditions + 14 superfluous conditions.

Definition: Hall set

Given an order relation $<$ (compatible with $|\cdot|$), define $\mathcal{H} \subset T_\infty$ by

$$(i) \quad \forall i \geq 1, \; \textcircled{\scriptsize i} \in \mathcal{H}$$
$$(ii) \quad \tau \in H \text{ iff } \exists u, v \in H, u > v, \text{ such that } \tau = u \circ v.$$

Theorem (Murua & Sanz-Serna)

Consider $B(a, \varepsilon, y)$ and $B(b, \varepsilon, y)$ two B_∞-series obtained as compositions and let $p \geq 1$. The following statements are equivalent:

$$(i) \quad \forall \tau \in T_\infty, \; \|\tau\| \leq p, \; a(\tau) = b(\tau),$$
$$(ii) \quad \forall \tau \in \mathcal{H}, \; \|\tau\| \leq p, \; a(\tau) = b(\tau).$$

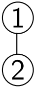
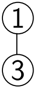
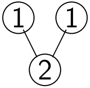
Order 1, 2:	①, ②	$\sum_{k=1}^{s}(\alpha_k+\beta_k)=1,\ \sum_{k=1}^{s}(\alpha_k^2-\beta_k^2)=N^{-1}$
Order 3:	③	$\sum_{k=1}^{s}(\alpha_k^3+\beta_k^3)=N^{-2}$
		$\sum_{k=1}^{s}(\alpha_k^2-\beta_k^2)\sum_{\ell=1}^{k}{}'(\alpha_\ell+\beta_\ell)=\frac{N^{-1}-N^{-2}}{2}$
Order 4:	④	$\sum_{k=1}^{s}(\alpha_k^4-\beta_k^4)=N^{-3}$
		$\sum_{k=1}^{s}(\alpha_k^3+\beta_k^3)\sum_{\ell=1}^{k}{}'(\alpha_\ell+\beta_\ell)=\frac{N^{-2}-N^{-3}}{2}$
		$\sum_{k=1}^{s}(\alpha_k^2-\beta_k^2)\Big(\sum_{\ell=1}^{k}{}'(\alpha_\ell+\beta_\ell)\Big)^2=\frac{N^{-1}(1-N^{-1})(2-N^{-1})}{6}$

Table: Fourth-order conditions for MRCMs.

Convergence of MRCM (semi-discrete)

Theorem

Consider a semi-discrete MRCM with coefficients $\alpha_i(N)$, $\beta_i(N)$, $i = 1, \ldots, s$ bounded with respect to N for all $N \geq N_0$ and satisfying the algebraic order conditions up to order p. Then, for all $H \leq H_0$, $N \geq N_0$,

$$\|\Psi_{N,H}(y) - \varphi_\varepsilon^N(y)\| \leq CH^{p+1}$$

where $H = N\varepsilon$ and the constant C is independent of N, ε.

Convergence of MRCM (fully-discrete)

Theorem

Consider a fully-discrete MRCM satisfying the order p conditions. Assume further the order q estimate $\|\Phi_h - \varphi_\varepsilon\|_R \leq C\varepsilon h^q$. Then

$$\|\Psi_{H,h}(y) - \varphi_\varepsilon^N(y)\| \leq C(H^{p+1} + Hh^q)$$

where $H = N\varepsilon$, $h \leq \varepsilon$ and C is independent of N, ε, H, h.

Remarks: This yields the global error estimate

$$\|\Psi_{H,h}^m(y_0) - y(Hm)\| \leq C(H^p + h^q),$$

for all $H = N\varepsilon \leq H_0$ and $Hm \leq T$.
Notice that $y(t)$ is approx. at times t that are integer multiples of the oscillatory period (similarly to the Stroboscopic Averaged Method (SAM) by Chartier, Murua & Sanz-Serna, 2011)

Fermi-Pasta-Ulam type problem

Hamiltonian: $$E_\varepsilon(p,q) = \frac{1}{2}\sum_{i=4}^{6} p_i^2 + \frac{1}{2\varepsilon^2}\sum_{i=4}^{6} q_i^2 + \frac{1}{2}\sum_{i=1}^{3} p_i^2 + V(q)$$

where $V(q)$ is a quartic potential.
HOP with an ε-dependent linear part with eigenvalues 0, i and $-i$.

- Micro method: Strang splitting $\Phi_{\varepsilon,h} := (\Xi_{h,\varepsilon})^n$ with $h = 2\pi/n$ (we take e.g. $n = 4$ or 8).
- Time interval length: $T = 2\pi\varepsilon^{-1}$ (i.e. $\mathcal{O}(\varepsilon^{-2})$ fast oscillations).
- Quantities of interest: the stiff spring energies

$$I_j = \frac{1}{2}p_{3+j}^2 + \frac{1}{2\varepsilon^2}q_{3+j}^2, \quad j = 1,2,3,$$

the adiabatic invariant $I = I_1 + I_2 + I_3$ and the energy $E_\varepsilon(p,q)$.

Global error at time $t = 2\pi$ (semi-discrete)

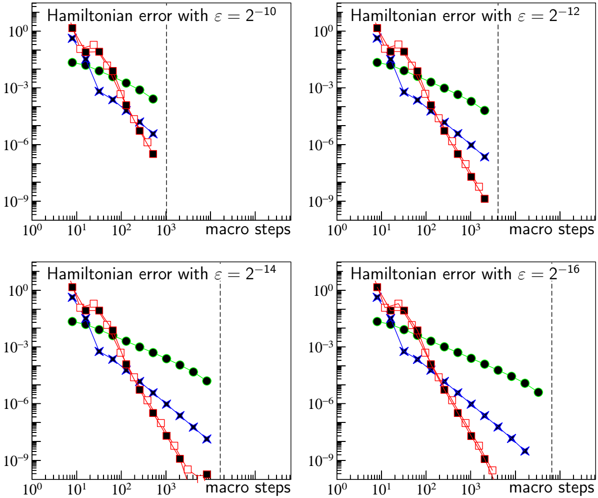


Figure: Hamiltonian error for MRCMs versus number of macro steps. Orders 1 (circles), 2 (squares), 4 ($s = 3$ white stars, $s = 4$ black stars).

Global error at time $t = 2\pi$ (fully-discrete)

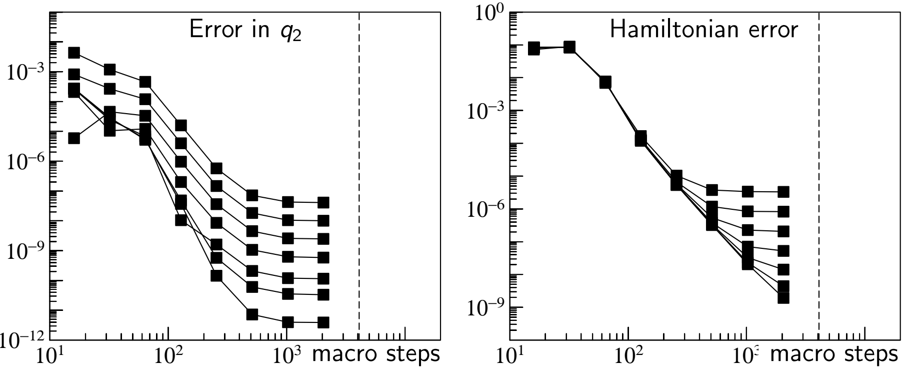


Figure: Fourth-order MRCM with $\varepsilon = 2^{-12}$.
Errors with versus number of macro steps.
The lines correspond respectively to $h = 2^{-j}\pi, j = 1, \dots, 7$.

Conclusion: H and h should be refined simultaneously (here $H^4 \sim h^2$).

Energy exchanges on the time interval $(0, 2\pi\varepsilon^{-1})$

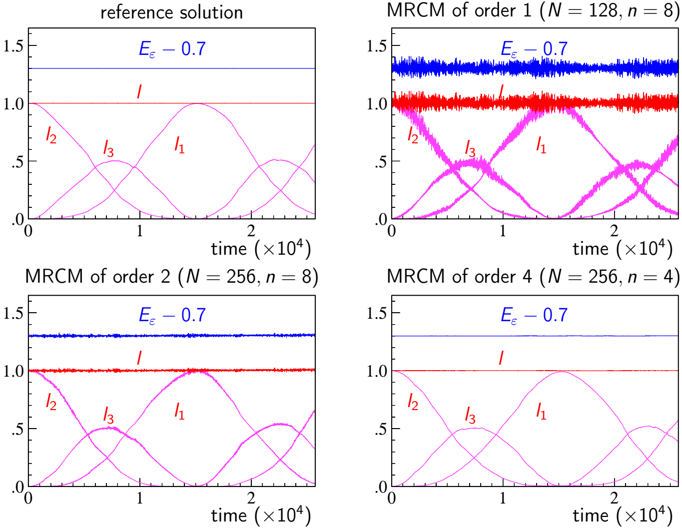


Figure: $\varepsilon = 2^{-12}$. MRCMs of orders 1, 2, 4. Reference solution computed with 10^8 constant steps by the standard Deuflhard method.

The nonlinear Schrödinger equation

The problem involves a cubic nonlinearity $|\psi^\varepsilon|^2\psi^\varepsilon$ with excitation factor $2\cos(2x)$.

$$\begin{aligned} i\partial_t\psi^\varepsilon &= -\Delta\psi^\varepsilon + 2\varepsilon\cos(2x)|\psi^\varepsilon|^2\psi^\varepsilon, \quad t \geq 0, \\ \psi(0,x) &= \cos x + \sin x. \end{aligned}$$

(unique global solution $\psi^\varepsilon(t,\cdot)$ in $H^s(\mathbb{T}_{2\pi})$ for all $s \geq 0$).

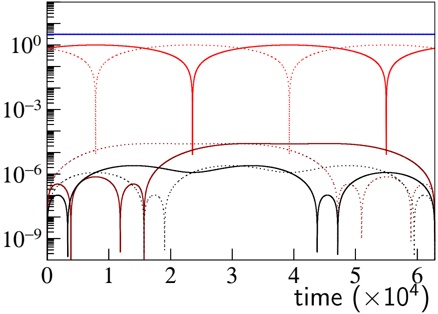
Theorem (Grébert & Villegas-Blas, 2011)

Consider the Fourier expansion of $\psi^\varepsilon(t,x) = \sum_{k\in\mathbb{Z}} \xi_k(t)e^{ikx}$. For ε small enough, one has for all $|t| \leq \varepsilon^{-9/8}$ the following estimates:

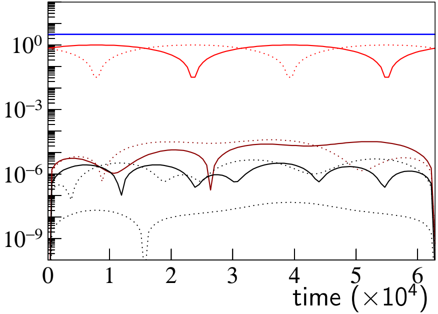
$$\begin{aligned} |\xi_1(t)|^2 &= \frac{1+\sin(2\varepsilon t)}{2} + \mathcal{O}(\varepsilon^{1/8}), \\ |\xi_{-1}(t)|^2 &= \frac{1-\sin(2\varepsilon t)}{2} + \mathcal{O}(\varepsilon^{1/8}). \end{aligned}$$

Beating effect for the NLS, time interval $2\pi\varepsilon^{-1}$

reference solution (Strang splitting)



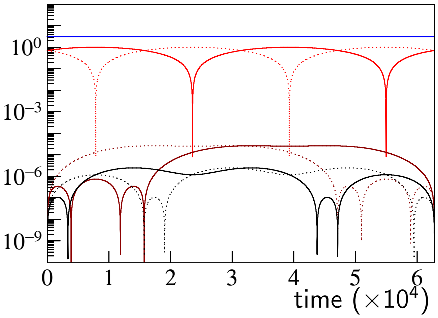
MRCM of order 2 ($N = 100$)



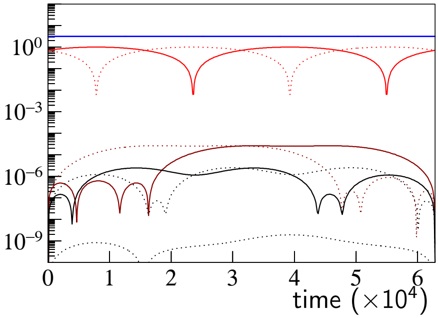
$\varepsilon = 10^{-4}$, Hamiltonian, and modes $|\xi_1|, |\xi_{-1}|$ $|\xi_3|, |\xi_{-3}|$, $|\xi_5|, |\xi_{-5}|$.

Beating effect for the NLS, time interval $2\pi\varepsilon^{-1}$

reference solution (Strang splitting)

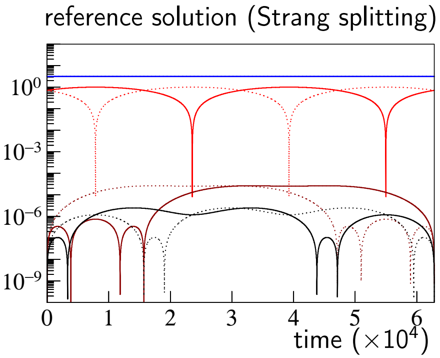


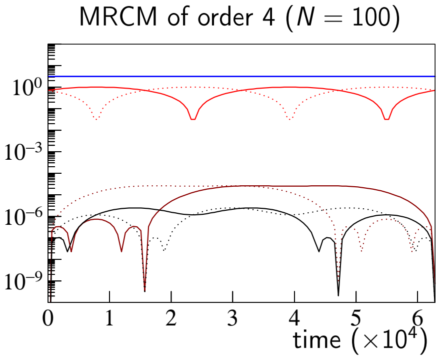
MRCM of order 2 ($N = 20$)



$\varepsilon = 10^{-4}$, Hamiltonian, and modes $|\xi_1|, |\xi_{-1}|$ $|\xi_3|, |\xi_{-3}|$, $|\xi_5|, |\xi_{-5}|$.

Beating effect for the NLS, time interval $2\pi\varepsilon^{-1}$





$\varepsilon = 10^{-4}$, Hamiltonian, and modes $|\xi_1|, |\xi_{-1}|$ $|\xi_3|, |\xi_{-3}|$, $|\xi_5|, |\xi_{-5}|$.

Extension to stochastic highly-oscillatory systems

For systems of (Itô) SDEs with general (noncommutative) noise,

$$dX(t) = (\varepsilon^{-1}AX(t)+f(X(t)))dt+\sum_{r=1}^{m} g^r(X(t))dW_r(t), \quad 0 \leq t \leq T,$$

we consider the stochastic MRCM based on the order 2 method

$$\varphi_{\alpha_1 H} \circ \varphi_{-\beta_1 H}^{-1}(y) = \varphi_\varepsilon^N(y) + \mathcal{O}(H^3).$$

We approximate φ_ε by a Strang splitting between oscillatory and non-oscillatory parts.

Theorem: weak order two global error estimate

Let $T > 0$. Assume $f, g^r \in C^6$ with bounded derivatives. Then, for all $\phi \in C_P^6(\mathbb{R}^d, \mathbb{R})$, and all $h = 1/n$ and $H = N\varepsilon$ small enough,

$$|\mathbb{E}(\phi(X_k) - \mathbb{E}(\phi(X(kH))| \leq C(H^2 + h^2), \qquad kH \leq T,$$

where C is independent of $\varepsilon, H, n, k, N, h$.

Back to the nonlinear Schrödinger equation

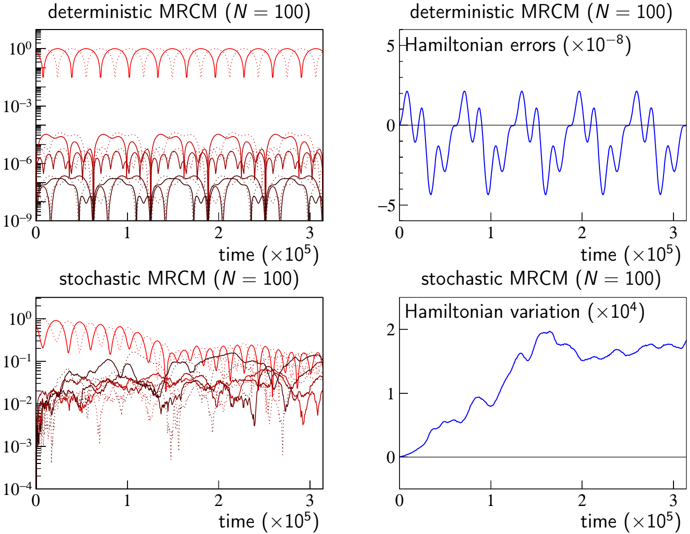


Figure: $\varepsilon = 10^{-4}$. MRCMs of orders 2. Top: deterministic case.
Bottom: Stratonovitch space-time multiplicative noise $g(u) = u \circ \dot{W}(x,t)$.

Weak convergence of order 2 (stochastic NLS)

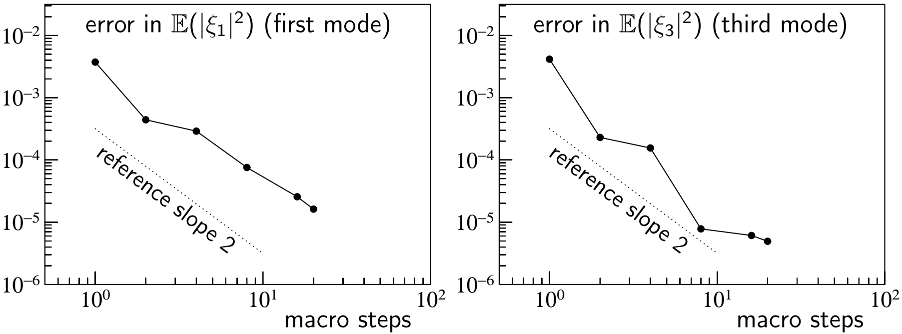


Figure: $\varepsilon = 10^{-4}$. Convergence curves for S-MRCM of orders 2: Weak error versus number of macro steps ($\ell = 128$ Fourier modes, $n = 100$ micro steps per macro steps, number of samples for Monte-Carlo$=10^5$).

Conclusions on multi-revolution composition meth.

We introduced a new class of integrators with large time steps for highly oscillatory problems.

- The schemes retain the advantages of composition methods: their are intrinsically geometric (the scheme inherits the symplecticity for Hamiltonian problems, conservation of quadratic first integrals, etc).
- It can be interpreted as an homogenization integrator, in the spirit of the Heterogeneous multiscale method (HMM, E, Engquist, 2003): it involves a macro step $H = N\varepsilon$ and a micro step h, and for $\varepsilon \to 0$ (i.e. $N \to \infty$) we recover the solution of the averaged system $\frac{dz(t)}{dt} = \Theta_0(z(t))$.
- The approach applies to stochastic highly oscillatory problems.