Derivative-free high-order uniformly accurate schemes for highly-oscillatory systems

Philippe Chartier, Mohammed Lemou, Florian Méhats, Xiaofei Zhao

DERIVATIVE-FREE HIGH-ORDER UNIFORMLY ACCURATE SCHEMES FOR HIGHLY-OSCILLATORY SYSTEMS

PHILIPPE CHARTIER, MOHAMMED LEMOU, FLORIAN MÉHATS, AND XIAOFEI ZHAO

Abstract. In this paper, we address the computational aspects of *uniformly accurate* numerical methods for solving highly-oscillatory evolution equations. In particular, we introduce an approximation strategy that allows for the construction of arbitrary high-order methods using solely the right-hand side of the differential equation. No derivative of the vector field is required, while uniform accuracy is retained. The strategy is then applied to two different formulations of the problem, namely the *two-scale* and the *micro-macro* formulations. Numerical experiments on the Hénon-Heiles system, as well as on the Klein-Gordon equation and a Vlasov type problem all confirm the validity of the new strategy.

Keywords: Highly-oscillatory problem, Chapman-Enskog expansion, Standard averaging, Uniformly accurate method, High-order convergence.

AMS Subject Classification: 65L05, 65L20, 65L70.

1. Introduction

This paper is concerned with the numerical solution of oscillatory problems where possibly different time scales are present. More precisely, the class of systems considered here is of the form

$$\dot{u}(t) = f_{t/\varepsilon}(u(t)), \quad u(0) = u_0 \in X, \quad t \in [0,1], \tag{1.1}$$

where X is a Banach space for the norm $\|\cdot\|$, f_θ a function 2π-periodic in θ and $\varepsilon \in]0,1]$. In order to analyze numerical methods for (1.1), we will assume throughout the paper, that there exist an open set $\mathcal{K} \subset X$ with bounded closure and an open set $\mathcal{U}^0 \subset \mathcal{K}$, such that for all initial condition u_0 in $\mathcal{U}^0$ and all $\varepsilon \in]0,1]$, the solution $u(t)$ of (1.1) exists and remains in $\mathcal{K}$ for all times $t \in [0,1]$.

Many realistic physical phenomena are indeed modeled by a system of the form (1.1), where ε denotes a dimensionless parameter whose physical interpretation depends on the specific context. Examples of such problems originate, e.g., from molecular dynamics [21, 22] or from charged-particle dynamics under a strong magnetic field [13, 27, 19, 20]. When f_θ contains a pseudo-differential operator, then (1.1) is to be understood as an abstract model of a partial differential equation for which $u(t)$ evolves in a functional space. For instance, the nonlinear Klein-Gordon equation in the nonrelativistic limit regime [1, 2] and the oscillatory nonlinear Schrödinger equation [5] fall into that category.

When ε is small, the solution $u(t)$ of (1.1) oscillates (very) rapidly in time. As a consequence, solving (1.1) with the help of a standard numerical methods requires tiny steps and becomes computationally costly. In order to circumvent this difficulty, ad-hoc methods have been introduced which perform vastly better then standard ones for small ε-values. For instance, some of the authors of this article have introduced several schemes [7, 8], inspired by the theory of *averaging*. At the other end of the spectrum, when ε is of the order of 1, problem (1.1) ceases to be stiff and a classical integrator gives accurate result in a reasonable time. The true difficulty emerges for intermediate values of ε, for which, due to truncation errors, averaging techniques are too crude and, due to computational

cost, standard methods are inefficient. This has motivated the introduction of a new paradigm, the so-called *uniform accuracy*: uniformly accurate (UA) methods are indeed able to solve (1.1) with a precision and a computational cost that are independent of the value of $0 < \varepsilon \leq 1$. So far in the literature, UA methods have been constructed by different techniques by several authors [1, 3, 4, 6, 9, 10, 11, 12, 13, 15, 16, 18]. It is out of the scope of this paper to describe all of them and for an extensive comparison, we refer the interested reader to [25]. However, all these methods have in common that they necessitate not only an analytic expression of f_θ in (1.1), but also higher-order derivatives $\partial_u^p f_\theta$ in explicit form: instead of solving directly (1.1) the system is first transformed into a nonstiff one which is more amenable to numerical integration. The derivation of this new system is usually lengthy and tedious for non-trivial functions, and it has to be carried out for each occurrence of f_θ. In practice, this prevents UA schemes to be used by a broader group.

The purpose of this work is to show that it is actually possible to reformulate (1.1) as a non-stiff system through a *derivative-free formula*. This formula allows to construct a change of unknowns, introduced in [10], that lies at the core of the reformulation of the system. In its original version, this iteration suffers from the aforementioned drawback, i.e. it involves derivatives of f_θ. The idea is thus to replace these derivatives by forward finite differences with appropriate increments. Owing to this technique, we are able to construct UA methods of arbitrary orders without any pre-computed formulas. The derivation is accomplished in a completely systematic way.

We shall envisage two different core UA-methods from the literature: on the one hand, the two-scale formulation (TSF) method from [6], and on the other hand, the micro-macro decomposition approach [10]. Note that constructing high-order UA schemes in the two-scale formulation was regarded as a challenge in [10] as both the preparation of the initial datum and the design of an integrator are not straightforward. As already implied, the two techniques rely on the very same change of variables, either to prepare the initial datum in the TSF or to write the micro-macro decomposition. Altogether, our results pave the way for a toolbox of UA methods for solving (1.1) by only providing f_θ and u_0.

The rest of the paper is organized as follows. In Section 2, we present our derivative-free iteration. In Section 3, we present the high order UA schemes under two-scale formulation by the help of derivative-free averaging and the application to micro-macro decomposition framework in presented in Section 4. Numerical results are reported and conclusions are drawn in Section 5.

2. Derivative-free averaging

It was noticed by the authors of this paper, that a single mathematical object, namely the change of variables $(\theta, u) \mapsto \Phi_\theta(u)$ introduced in [24] (see also [5] where the same notations are adopted), is the key ingredient of *micro-macro* and *pullback* methods [10], as well as, as we shall see in Section 3, of two-scale methods [6]. This change of variables allows to write *formally* the solution of (1.1) in the following form

$$u(t) = \Phi_{t/\varepsilon} \circ \Psi_t \circ \Phi_0^{-1}(u_0)$$

where $(t, u) \mapsto \Psi_t(u)$ is a *smooth* with respect to ε (see [5, 10] for further details). In a first step, we thus present how this change of variables can be approximated iteratively. In a second step, we discuss the main modification we introduce in this work to avoid the computation of derivatives.

2.1. Computing the change of variables required in averaging.

The change of variables $(\theta, u) \mapsto \Phi_\theta^{[n]}(u)$ is by definition 2π-periodic with respect to θ and can be computed

by the following iteration[1] for $k = 0, \dots, n-1$ with $n \in \mathbb{N}$

$$\Phi_\theta^{[0]} = \mathrm{id}, \quad \Phi_\theta^{[k+1]} = \mathrm{id} + \varepsilon \int_0^\theta \Big(f_\tau \circ \Phi_\tau^{[k]} - \partial_u \Phi_\tau^{[k]} F^{[k]} \Big) d\tau - \varepsilon \left\langle \int_0^\theta \Big(f_\tau \circ \Phi_\tau^{[k]} - \partial_u \Phi_\tau^{[k]} F^{[k]} \Big) d\tau \right\rangle$$
$$F^{[0]} = \langle f \rangle, \quad F^{[k+1]} = \langle f \circ \Phi^{[k+1]} \rangle. \tag{2.1}$$

where $F^{[n]}$ referred to as the *averaged vector-field*. For instance, the first three iterates of (2.1) read

$$\Phi_\theta^{[0]} = \mathrm{id}, \quad \Phi_\theta^{[1]} = \mathrm{id} + \varepsilon \int_0^\theta \Big(f_\tau - \langle f \rangle \Big) d\tau - \varepsilon \left\langle \int_0^\theta \Big(f_\tau - \langle f \rangle \Big) d\tau \right\rangle,$$
$$\Phi_\theta^{[2]} = \mathrm{id} + \varepsilon \int_0^\tau \Big(f_\tau \circ \Phi_\tau^{[1]} - \partial_u \Phi_\tau^{[1]} \langle f \circ \Phi^{[1]} \rangle \Big) d\tau - \varepsilon \left\langle \int_0^\theta \Big(f_\tau \circ \Phi_\tau^{[1]} - \partial_u \Phi_\tau^{[1]} \langle f \circ \Phi^{[1]} \rangle \Big) d\tau \right\rangle,$$

and accordingly

$$F^{[0]} = \langle f \rangle, \quad F^{[1]} = \langle f \circ \Phi^{[1]} \rangle, \quad F^{[2]} = \langle f \circ \Phi^{[2]} \rangle.$$

Now, one of the main contributions of [10] is the following result (see Theorem 3.3 in [10] for a detailed version).

Theorem 2.1. *Suppose that the function $(\theta, u) \mapsto f_\theta(u)$ is p-times ($p \geq 1$) continuously differentiable w.r.t. θ and that for all $\theta \in \mathbb{T}$, it and all its derivatives can be analytically extended to a complex strip (in a complex neighbourhood of $\mathcal{K}$) on which they are uniformly bounded. Then, there exist two positive constants ε_0 and $\mathcal{Q}_p$ such that for $n \in \mathbb{N}^*$ and all $0 < (n+1)\varepsilon \leq \varepsilon_0$, the defect*

$$\delta_\theta^{[n]} = \frac{1}{\varepsilon} \partial_\theta \Phi_\theta^{[n]} + \partial_u \Phi_\theta^{[n]} \, F^{[n]} - f_\theta \circ \Phi_\theta^{[n]}, \tag{2.2}$$

where $\Phi^{[n]}$ and $F^{[n]}$ are defined by iteration (2.1), is p-times differentiable and satisfies

$$\forall \nu \in \{0, \dots, p\}, \ \forall \theta \in \mathbb{T}, \ \forall u \in \mathcal{K}, \quad \|\partial_\theta^\nu \delta^{[n]}(u)\| \leq \Big(\mathcal{Q}_p \, (n+1) \frac{\varepsilon}{\varepsilon_0} \Big)^n. \tag{2.3}$$

2.2. **A derivative-free iteration.** Note that from the computational point of view, all operations in (2.1) involving θ can be performed by Fast Fourier Transforms (FFTs). In contrast, computing the explicit form of $\partial_u \Phi_\theta^{[k]}$ becomes very complicated for large k as it involves high-order derivatives of $f_\theta(u)$. For instance, the derivative of $\Phi_\theta^{[1]}$ requires $\partial_u f_\theta$, the derivative of $\Phi_\theta^{[2]}$ involves $\partial_u^2 f_\theta$, and so on and so forth. Despite the fact that exact formulas have been previously derived in the literature [10, 12, 14, 15, 16, 18], either by tedious calculations or by using computer algebra systems, their intricacy as well as the necessity to have at our disposal the derivatives of f_θ are a serious burden. This is the reason why we replace (2.1) by the following iteration[2] for $k = 0, \dots, n-1$

$$\tilde{\Phi}_\theta^{[0]} = \mathrm{id}, \quad \tilde{\Phi}_\theta^{[k+1]} = \mathrm{id} + \varepsilon \int_0^\theta \Big(f_\tau \circ \tilde{\Phi}_\tau^{[k]} - D_{\varepsilon^k} \tilde{\Phi}_\tau^{[k]} \, \tilde{F}^{[k]} \Big) d\tau - \varepsilon \left\langle \int_0^\theta \Big(f_\tau \circ \tilde{\Phi}_\tau^{[k]} - D_{\varepsilon^k} \tilde{\Phi}_\tau^{[k]} \tilde{F}^{[k]} \Big) d\tau \right\rangle$$
$$\tilde{F}^{[0]} = \langle f \rangle, \quad \tilde{F}^{[k+1]} = \langle f \circ \tilde{\Phi}^{[k+1]} \rangle. \tag{2.4}$$

where, for all smooth function g on $\mathcal{K}$ and all $(u, v) \in \mathcal{K}^2$,

$$D_\eta g(u) \, v = \frac{1}{\eta} \left(g \left(u + \eta v \right) - g(u) \right)$$

[1]Here and in the sequel, if g_θ is a 2π-periodic function, then $\langle g_\theta \rangle$ represents its average $\frac{1}{2\pi} \int_0^{2\pi} g_\theta d\theta$.
[2]Note that $\tilde{\Phi}_\theta^{[0]} = \Phi_\theta^{[0]}$ and $\tilde{\Phi}_\theta^{[1]} = \Phi_\theta^{[1]}$.

stands for an approximation of $\partial_u g(u)\, v$. For instance, the first three iterates of (2.4) read

$$\tilde\Phi_\theta^{[0]} = \mathrm{id}, \quad \tilde\Phi_\theta^{[1]} = \mathrm{id} + \varepsilon \int_0^\theta \Big(f_\tau - \langle f\rangle\Big) d\tau - \varepsilon \left\langle \int_0^\theta \Big(f_\tau - \langle f\rangle\Big) d\tau \right\rangle,$$
$$\tilde\Phi_\theta^{[2]} = \mathrm{id} + \varepsilon \int_0^\theta \Big(f_\tau \circ \tilde\Phi_\tau^{[1]} - D_{\varepsilon^k} \tilde\Phi_\tau^{[1]} \rangle\Big) d\tau - \varepsilon \left\langle \int_0^\theta \Big(f_\tau \circ \tilde\Phi_\tau^{[1]} - D_{\varepsilon^k} \tilde\Phi_\tau^{[1]} \rangle\Big) d\tau \right\rangle.$$

Theorem 2.2. *Under the assumptions of Theorem 2.1, for any $n \in \mathbb{N}^*$ there exist two positive constants $\tilde\varepsilon_0$ and $\widetilde{\mathcal{Q}}_{p,n}$ such that the defect*

$$\widetilde\delta_\theta^{[n]} = \frac{1}{\varepsilon} \partial_\theta \widetilde\Phi_\theta^{[n]} + \partial_u \widetilde\Phi_\theta^{[n]}\, \widetilde F^{[n]} - f_\theta \circ \widetilde\Phi_\theta^{[n]}, \tag{2.5}$$

where $\widetilde\Phi^{[n]}$ and $\widetilde F^{[n]}$ are defined by iteration (2.4), is p-times differentiable and satisfies

$$\forall \nu \in \{0, \dots, p\},\ \forall \theta \in \mathbb{T},\ \forall u \in \mathcal{K}, \quad \|\partial_\theta^\nu \widetilde\delta^{[n]}(u)\| \le \widetilde{\mathcal{Q}}_{n,p}\, \varepsilon^n. \tag{2.6}$$

Sketch of proof. In order to avoid repeating the technicalities of the original proof of Theorem 2.1, we shall content ourselves here with the main arguments. We first notice that iterations (2.4) are well-defined for $\varepsilon > 0$ and are such that $\widetilde\Phi_\theta^{[k]}$ is 2π-periodic and p-times continuously differentiable w.r.t. θ. Moreover, it and all its derivatives up to order p are analytic w.r.t. u on the same (complex) domain as $\Phi_\theta^{[k]}$. The following estimate

$$\max_{0\le\nu\le p} \sup_{\theta\in\mathbb{T}} \|\partial_\theta^\nu \Phi_\theta^{[k]} - \partial_\theta^\nu \widetilde\Phi_\theta^{[k]}\| \le C_{k,p}\, \varepsilon^{k+1} \tag{2.7}$$

can then be proved (for some constant $C_{k,p} > 0$ depending only on bounds of $\partial_\theta^\nu \Phi_\theta^{[k-1]}$ and $\partial_\theta^\nu f_\theta$ for $\nu \le p$) by induction from formulas obtained in the proof of Proposition 2. of [10] and similar ones for the $\widetilde\Phi_\theta^{[k]}$. Just note that this is obvious for the first two iterates. Estimate (2.6) then follows from relations (2.7) and (2.2). □

We conclude this section with an algorithm for computing $\widetilde\Phi_\theta^{[n]}$ numerically. To this aim, we write

$$\widetilde\Phi_\theta^{[k]} = \mathrm{id} + \varepsilon \widetilde B_\theta^{[k]}, \quad k \ge 0, \tag{2.8}$$

with $\widetilde B_\theta^{[0]} = 0$, $\widetilde f_\theta^{[0]} = f_\theta$, $\widetilde F^{[0]} = \langle f\rangle$ and for $k \ge 0$

$$\widetilde B_\theta^{[k+1]} = \int_0^\theta \Big(\widetilde f_\tau^{[k]} - \widetilde F^{[k]} - \varepsilon D_{\varepsilon^k} \widetilde B_\tau^{[k]}\, \widetilde F^{[k]}\Big) d\tau - \left\langle \int_0^\theta \Big(\widetilde f_\tau^{[k]} - \widetilde F^{[k]} - \varepsilon D_{\varepsilon^k} \widetilde B_\tau^{[k]}\, \widetilde F^{[k]}\Big) d\tau \right\rangle$$
$$\widetilde f_\theta^{[k+1]} = f_\theta \circ (\mathrm{id} + \varepsilon \widetilde B_\theta^{[k+1]}), \quad \widetilde F^{[k+1]} = \left\langle \widetilde f^{[k+1]} \right\rangle \tag{2.9}$$

3. Two-scale formulation method

In this section, we consider the two-scale framework and present how the derivative-free change of variables $\widetilde\Phi_\theta^{[n]}$ of Section 2 can be used to construct arbitrary high order uniformly accurate schemes. Prior to that, we state Theorem 3.1, which establishes a connection between the so-called *preparation* procedure of the two-scale formulation and the map $\Phi_\theta^{[n]}$. Let us emphasize that this link had not been previously made formally, which motivates the proof given in Appendix. We then construct UA schemes for solving (1.1) of arbitrary orders.

Pseudo-code for computing the n-th order iteration (2.9)

Function: $\widetilde{B}_\theta^{[k]}(u)$
If $k=0$, then
$\diamond$ Returns 0
Else
$\diamond$ $k=k-1$
$\diamond$ Computes $\widetilde{f}_\theta^{[k]}(u)=f_\theta\Big(u+\varepsilon\widetilde{B}_\theta^{[k]}(u)\Big)$
$\diamond$ Computes $\widetilde{F}^{[k]}(u)=\langle\widetilde{f}^{[k]}(u)\rangle$
$\diamond$ Computes $\widetilde{I}_\theta^{[k+1]}(u)=\int_0^\theta\Big(\widetilde{f}_\tau^{[k]}(u)-\widetilde{F}^{[k]}(u)-\varepsilon D_{\varepsilon^k}\widetilde{B}_\tau^{[k]}(u)\,\widetilde{F}^{[k]}(u)\Big)d\tau$
$\diamond$ Returns $\widetilde{I}_\theta^{[k+1]}(u)-\langle\widetilde{I}^{[k+1]}(u)\rangle$
Endif

TABLE 1

3.1. **The choice of the initial condition.** The two-scale formulation of (1.1) is obtained by separating the slow and fast variables, respectively t and $\theta=t/\varepsilon$ explicitly, in a new unknown $U(t,\theta)$, and imposing the *diagonal* condition $U(t,t/\varepsilon)=u(t)$. In doing so, we obtain the following partial differential equation for U

$$\begin{cases}\partial_t U(t,\theta)+\dfrac{1}{\varepsilon}\partial_\theta U(t,\theta)=f_\theta(U(t,\theta)),\quad t>0,\ \theta\in\mathbb{T},\\ U(0,0)=u_0,\end{cases}\tag{3.1}$$

where $U(t,\theta)$ is periodic in θ on the torus $\mathbb{T}$. It was shown in previous publications [6, 12, 13, 14, 16, 18], that it is possible to choose an initial condition $U(0,\theta)=U_0(\theta)$ for equation (3.1) in such a way that $U(t,\theta)$ has uniformly (with respect to ε) bounded derivatives up to a certain order $k\in\mathbb{N}$. Whereas Chapman-Enskog expansions can be used to construct $U_0(\theta)$, this means of derivation remains somehow pedestrian and definitely unsystematic. In contrast, we hereby show in next theorem that

$$U(0,\theta)=\Phi_\theta^{[n]}(\widetilde{u}_0),\quad \widetilde{u}_0=(\Phi_0^{[n]})^{-1}(u_0).\tag{3.2}$$

is a perfectly suitable choice which furthermore paves the way for a systematic construction.

Theorem 3.1. *Under the assumptions of Theorem 2.1, the unique solution of equation* (3.1) *with initial condition* (3.2) *is p-times continuously differentiable with respect to both* $t\in[0,1]$ *and* $\theta\in\mathbb{T}$. *Moreover, there exists a constant* $\mathcal{C}_{p,n}>0$ *such that*

$$\forall\nu\le p,\ \forall\mu\le\min(p,n+1),\ \forall\theta\in\mathbb{T},\quad \|\partial_\theta^\nu\partial_t^\mu U(t,\theta))\|\le\mathcal{C}_{p,n}.$$

The proof of Theorem 3.1 is given in the Appendix. Now, according to Theorem 2.2, the conclusions of previous theorem remain true when replacing $\Phi_\theta^{[n]}$ by $\widetilde{\Phi}_\theta^{[n]}$ in (3.2). In Table 2, we give a brief description of the algorithm for computing (3.2).

3.2. **Uniformly accurate (UA) scheme of arbitrary order.** We are now in position to derive UA schemes of arbitrary order for solving (1.1). We choose here to solve the two-scale equation (3.1) with the help of an *exponential multistep method* of the form described below.

We first discretize the θ-variable as

$$\theta_l=l\Delta\theta, l=0,1,\dots,N_\theta,$$

Pseudo-code for computing the n-th order preparation

1. Input $n \in \mathbb{N}$ and u_0
2. Computes $\widetilde{u}_0$
   - $\widetilde{u}_0 = u_0$
   - For $k = 1 : n+1$ do
     $\widetilde{u}_0 = u_0 - \varepsilon \widetilde{B}_0^{[k-1]}(\widetilde{u}_0)$
     End do
3. Returns $U(0,\theta) = \widetilde{u}_0 + \varepsilon \widetilde{B}_\theta^{[n]}(\widetilde{u}_0)$

TABLE 2

with $\Delta\theta = 2\pi/N_\theta$ and N_θ some positive even integer. Applying Fourier transform to (3.1) on $\mathbb{T}$, we get for $\ell = -N_\theta/2, \dots, N_\theta/2 - 1$,

$$\frac{d}{dt}\widehat{U}_\ell(t) + \frac{i\ell}{\varepsilon}\widehat{U}_\ell(t) = \widehat{f}_\ell(t), \quad t > 0, \tag{3.3}$$

where

$$U(t,\theta) = \sum_{\ell=-N_\theta/2}^{N_\theta/2-1} \widehat{U}_\ell(t) \mathrm{e}^{i\ell\theta} \quad \text{and} \quad f_\theta(U(t,\theta)) = \sum_{\ell=-N_\theta/2}^{N_\theta/2-1} \widehat{f}_\ell(t) \mathrm{e}^{i\ell\theta}.$$

Now, given a time-step Δt and the grid

$$t_j = j\Delta t$$

Duhamel's formula for (3.3) between t_j and t_{j+1} ($n \geq 0$) writes

$$\widehat{U}_\ell(t_{j+1}) = \mathrm{e}^{-\frac{i\ell\Delta t}{\varepsilon}} \widehat{U}_\ell(t_j) + \int_0^{\Delta t} \mathrm{e}^{-\frac{i\ell}{\varepsilon}(\Delta t - s)} \widehat{f}_\ell(t_j + s) ds. \tag{3.4}$$

In order to obtain a $(n+1)$-th order UA scheme we thus approximate the function $\widehat{f}_\ell(t_j + s)$ by the n-th order Lagrange interpolation polynomial

$$\widehat{f}_\ell(t_j + s) \approx \sum_{k=0}^{n} \left(\prod_{\substack{l=0 \\ l \neq k}}^{n} \frac{s + l\Delta t}{(l-k)\Delta t} \right) \widehat{f}_\ell(t_{j-k}), \quad j \geq 0. \tag{3.5}$$

and use exact formulas for

$$p_{\ell,k}^{[n]} := \int_0^{\Delta t} \mathrm{e}^{-\frac{i\ell}{\varepsilon}(\Delta t - s)} \prod_{\substack{l=0 \\ l \neq k}}^{n} \frac{s + l\Delta t}{(l-k)\Delta t} ds, \quad 0 \leq k \leq n, \ \ell = -\frac{N_\theta}{2}, \dots, \frac{N_\theta}{2} - 1. \tag{3.6}$$

Note that the $p_{\ell,k}^{[n]}$ are universal coefficients and can be pre-computed and stored. Once incorporated in (3.4), we obtain the following approximation

$$\widehat{U}_\ell(t_{j+1}) \approx \mathrm{e}^{-\frac{i\ell\Delta t}{\varepsilon}} \widehat{U}_\ell(t_j) + \sum_{k=0}^{j} p_{\ell,k}^{[n]} \widehat{f}_\ell(t_{n-k}), \quad j \geq n. \tag{3.7}$$

It can be verified that the local truncation error is of size $\mathcal{O}(\Delta t^{n+2})$ uniformly in ε so that the overall scheme has indeed the claimed uniform order $n+1$ if ones uses the n-th order prepared initial data (3.2).

As far as starting values $\widehat{U}_\ell(t_1), \dots, \widehat{U}_\ell(t_n)$ as concerned, they can be obtained from lower order schemes. For instance, the first order interpolation polynomial has been used in [12, 14, 18] to get a second order UA scheme.

The full method is explicit and the computational cost at each step is $\mathcal{O}(N_\theta \log N_\theta)$. For its resemblance with Adams-Bashforth method, we shall refer to this scheme as the $(n+1)$-th order Adams-Bashforth two-scale formulation **(AB-TSF)** integrator. Note that in practice, the two-scale strategy requires a fresh restart from time to time. For that, we adapt straightforwardly the strategy proposed in [18].

4. Micro-macro decomposition method

The micro-macro decomposition method was originally proposed in [10] with the aim of removing the extra variable θ occurring in the two-scale formulation. Its interpolation property which helps the recovery of the whole oscillation trajectory was later pointed out in [13]. This distinguishable feature compares favourably with the two-scale formulation method in some applications. We refer the reader to [13] for a detailed comparison of the two methods.

4.1. Generating the micro-macro decomposition at arbitrary order.

We now follow the presentation of [10]: the solution $u(t)$ of (1.1) can be decomposed into a *macro* part $v(t)$ and a *micro* part $w(t)$ as follows

$$u(t) = \Phi^{[n]}_{\frac{t}{\varepsilon}}(v(t)) + w(t), \tag{4.1}$$

where $(v(t), w(t))$ is the solution of the *micro-macro* system

$$\dot{v} = F^{[n]}(v), \tag{4.2}$$

$$\dot{w} = f_{\frac{t}{\varepsilon}}\Big(\Phi^{[n]}_{\frac{t}{\varepsilon}}(v) + w\Big) - \Big(\frac{1}{\varepsilon}\partial_\theta \Phi^{[n]}_{\frac{t}{\varepsilon}} + \partial_u \Phi^{[n]}_{\frac{t}{\varepsilon}}\, F^{[n]}\Big)(v) \tag{4.3}$$

with initial conditions

$$v(0) = (\Phi^{[n]}_0)^{-1}(u_0), \quad w(0) = 0. \tag{4.4}$$

Theorem 2.1 then lies at the core of the following convergence result, which allows to derive UA methods of arbitrary orders from existing non-stiff methods. As a matter of fact, it is not difficult to show from estimate (2.3) that the the right-hand side of (4.2, 4.3) has bounded derivatives up to order $\min(p, n) + 1$. This was done with some details in [10] and the complete result is exposed in the theorem below.

Theorem 4.1. *Consider an approximation $(v_j, w_j)_{0\le j\le J}$ of (4.2, 4.3) at times $t_0 = 0 < t_1 < \ldots < t_J = 1$ obtained by a numerical method convergent of order q when applied to* (1.1) *with $\varepsilon = 1$. Then, under the assumptions of Theorem 2.1, this approximation yields a uniformly accurate approximation of order $r = \min(p, q, n)$ of the solution of* (1.1)*, i.e.*

$$\max_{0\le j\le J} \|\Phi^{[n]}(v_j) + w_j - u^\varepsilon(t_j)\|_X \le C\Delta t^r,$$

where the constant C is independent of ε *and the time grid size $\Delta t = \max_j(t_{j+1} - t_j)$ is assumed to be small enough.*

Taking into account Theorem 2.2, it is clear that the very same result holds true if we replace $\Phi^{[n]}$ by $\widetilde{\Phi}^{[n]}$. However, in order to keep the whole procedure free of derivative, equation (4.3) can not solved as such and will have to be slightly transformed.

4.2. **UA scheme to arbitrary order.** Leaning on the derivative-free construction of $\widetilde{\Phi}_\theta^{[n]}$, for any specified $n \in \mathbb{N}^*$, we aim at designing a $(n+1)$-th order UA scheme for (1.1). Denoting

$$g_\theta^{[n]}(v,w) := f_\theta\left(\widetilde{\Phi}_\theta^{[n]}(v) + w\right), \tag{4.5}$$

the n-th order micro-macro equations can be rewritten as

$$\dot{v} = \widetilde{F}^{[n]}(v), \quad \dot{w} = g_{t/\varepsilon}^{[n]}(v,w) - \frac{d}{dt}\left(\widetilde{\Phi}_{t/\varepsilon}^{[n]}(v)\right),$$

so that, by integrating both sides of each equation between t_j and $t_{j+1} + \Delta t$

$$v(t_{j+1}) - v(t_j) = \int_{t_j}^{t_{j+1}} \widetilde{F}^{[n]}\left(v(t)\right) dt, \quad j \geq 0, \tag{4.6a}$$

$$w(t_{j+1}) - w(t_j) = \int_{t_j}^{t_{j+1}} g_{t/\varepsilon}^{[n]}(v(t),w(t))dt - \widetilde{\Phi}_{t_{j+1}/\varepsilon}^{[n]}\left(v(t_{j+1})\right) + \widetilde{\Phi}_{t_j/\varepsilon}^{[n]}(v(t_j)). \tag{4.6b}$$

Replacing the function under the integral in (4.6a) by a $(n+1)$-th order interpolation at times $t_{j-n}, \ldots, t_j$, we obtain, for $j \geq n$

$$\int_{t_j}^{t_{j+1}} \widetilde{F}^{[n]}\left(v(t)\right) dt \approx \int_0^{\Delta t} \sum_{k=0}^{n} \left(\prod_{\substack{l=0 \\ l\neq k}}^{n} \frac{s + l\Delta t}{(l-k)\Delta t} \right) \widetilde{F}^{[n]}\left(v(t_{j-k})\right) ds = \sum_{k=0}^{n} q_k^{[n]} \widetilde{F}^{[n]}\left(v(t_{j-k})\right),$$

with

$$q_k^{[n]} := \int_0^{\Delta t} \left(\prod_{\substack{l=0 \\ l\neq k}}^{n} \frac{s + l\Delta t}{(l-k)\Delta t} \right) ds, \quad k = 0, \ldots, n, \tag{4.7}$$

and accordingly, for $j \geq n$, the numerical scheme for (4.6a) has the form

$$v_{j+1} \approx v_j + \sum_{k=0}^{n} q_k^{[n]} \widetilde{F}^{[n]}\left(v_{j-k}\right).$$

As far as equation (4.6b) is concerned, a Fourier expansion leads to

$$\begin{aligned} \int_{t_j}^{t_{j+1}} g_{t/\varepsilon}^{[n]}(v(t),w(t))dt &= \sum_{\ell \in \mathbb{Z}} \int_0^{\Delta t} \mathrm{e}^{i\ell\frac{(t_j+s)}{\varepsilon}} \widehat{(g^{[n]})}_\ell\left(v(t_j+s), w(t_j+s)\right) ds \\ &\approx \mathrm{e}^{i\ell\frac{t_{j+1}}{\varepsilon}} \sum_{\ell=N_\theta/2}^{N_\theta/2-1} \sum_{k=0}^{n} p_{\ell,k}^{[n]} \widehat{(g^{[n]})}_\ell\left(v(t_{j-k}), w(t_{j-k})\right), \end{aligned}$$

where the $\widehat{(g^{[n]})}_\ell(v,w)$ are the Fourier coefficients of $g_\theta^{[n]}$, and the $p_{\ell,k}^{[n]}$ are defined as in (3.6). Hence, the numerical scheme corresponding to equation (4.6b) takes the form, for $j \geq n$

$$w_{j+1} = w_j + \mathrm{e}^{i\ell\frac{t_{j+1}}{\varepsilon}} \sum_{\ell=N_\theta/2}^{N_\theta/2-1} \sum_{k=0}^{n} p_{\ell,k}^{[n]} \widehat{(g^{[n]})}_\ell\left(v_{j-k}, w_{j-k}\right) - \widetilde{\Phi}_{\frac{t_{j+1}}{\varepsilon}}^{[n]}\left(v_{j+1}\right) + \widetilde{\Phi}_{\frac{t_j}{\varepsilon}}^{[n]}\left(v_j\right). \tag{4.8}$$

As for the starting values v_{j+1} and w_{j+1}, $j = 0, \ldots, n-1$, they can be obtained by a method of lower order. An approximation of $u(t_j)$ is then recovered from the micro-macro decomposition, that is to say , for $j \geq 0$

$$u_{j+1} = \widetilde{\Phi}_{t_{j+1}/\varepsilon}^{[n]}(v_{j+1}) + w_{j+1}.$$

Overall, the full scheme is explicit with computational cost per step $\mathcal{O}(N_\theta \log N_\theta)$ and its local error can be proved to be of size $\mathcal{O}(\Delta t^{n+1})$ along the same lines as in Theorem 4.1. In the sequel, we shall refer to this scheme as the $(n+1)$-th exponential Adams-Bashforth micro-macro integrator **(AB-MM)**.

5. Numerical results

The goal of this section is to demonstrate on two examples that both numerical schemes **(AB-TSF)** and **(AB-MM)** in combination with the derivative-free change of variables $\widetilde{\Phi}_\theta^{[n]}$ are uniformly accurate.

5.1. **First example.** The Hénon-Heiles model [22] is a Hamiltonian system with energy

$$H(q_1,q_2,p_1,p_2) = \frac{p_1^2+q_1^2}{2\varepsilon} + \frac{p_2^2+q_2^2}{2} + q_1^2 q_2 - \frac{q_2^3}{3}, \quad 0<\varepsilon\leq 1.$$

Filtering with the stiff part, i.e. changing variables from (q_1,q_2,p_1,p_2) to (u_1,u_2,u_3,u_4) with

$$q_1 = \cos(t/\varepsilon)u_1(t) + \sin(t/\varepsilon)u_3, \quad p_1 = \cos(t/\varepsilon)u_3 - \sin(t/\varepsilon)u_1, \quad u_2 = q_2, \quad u_4 = p_2,$$

the problem takes the form (1.1)

$$\dot{u} = f_{\frac{t}{\varepsilon}}(u), \quad t>0, \tag{5.1}$$

with

$$f_\theta(u) = \begin{pmatrix} 2\sin(\theta)(u_1\cos(\theta)+u_3\sin(\theta))u_2 \\ u_4 \\ -2\cos(\theta)(u_1\cos(\theta)+u_3\sin(\theta))u_2 \\ -(u_1\cos(\theta)+u_3\sin(\theta))^2 + u_2^2 - u_2. \end{pmatrix}$$

The initial data of (5.1) is given by $u_0 = (0.12, 0.12, 0.12, 0.12)$.

Firstly, we consider the 3^{rd} order and 4^{th} order **(AB-TSF)** schemes (3.7) under respectively 3^{rd} order and 4^{th} order preparations. We take $N_\theta = 128$ and explore a wide range of values of ε in the interval $(0,1)$. For each value of ε, a very accurate reference solution is computed by the 4^{th} order micro-macro scheme from [10] using tiny values of the stepsize $\Delta t = 10^{-5}$ and a large number of Fourier modes $N_\theta = 256$. The error of the numerical solution $u(1) - u^J$ at time $t=1$ in maximum vector norm is presented in Figure 1. The corresponding errors for the 3^{rd} order and 4^{th} order **(AB-MM)** schemes (4.8) at time $t=1$ are presented on Figure 2.

Secondly, in order to test the long-time behaviour of the schemes, we plot the relative energy error

$$|H(u^n) - H(u_0)| \,/\, |H(u_0)|$$

of the 4^{th} order **(AB-TSF)** scheme with a restart every $T_0 = 3$ till $t = 120$ in Figure 3. The long-time behaviour of **(AB-MM)** is the same as **(AB-TSF)**, so that the corresponding experiment has been simply omitted. At last, the dependence of the error of **(AB-TSF)** schemes on N_θ is shown in Figure 4 with different values of ε. The corresponding error of **(AB-MM)** w.r.t. N_θ is very similar and the corresponding experiment has been again omitted.

According to Figures 1-3, it is apparent that:

(i) The two methods **(AB-TSF)** and **(AB-MM)** with the derivative-free change of variable have the expected order and uniform accuracy w.r.t. $\varepsilon \in]0,1]$. The error in the auxiliary variable θ decreases spectrally as N_θ increases and it is uniform in ε. The global errors of the two methods are similar. However, **(AB-MM)** is

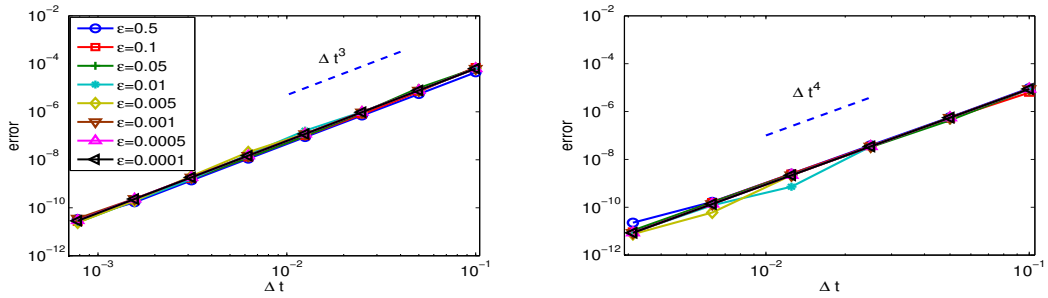

FIGURE 1. Error as Δt for different ε: the 3rd order (left) and the 4th order (right) AB-TSF methods in example 5.1.

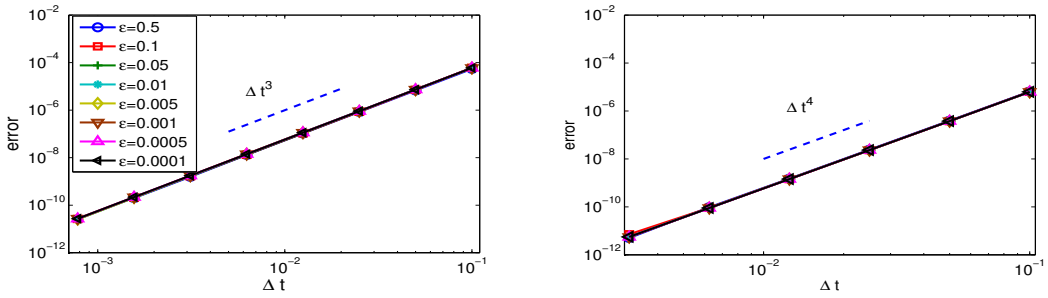

FIGURE 2. Error as Δt for different ε: the 3rd order (left) and the 4th order (right) AB-MM methods in example 5.1.

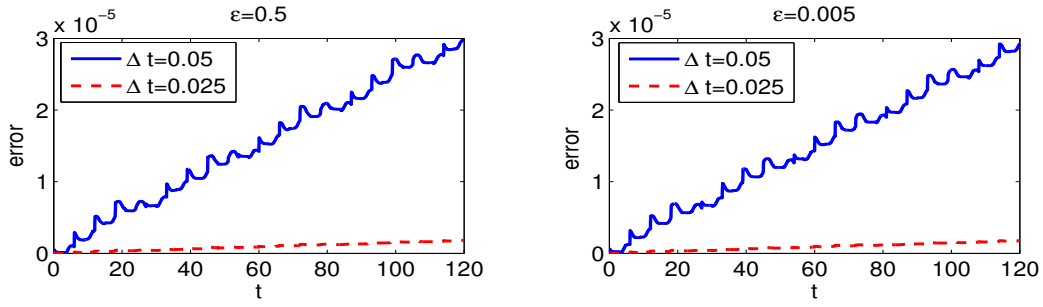

FIGURE 3. Energy error of the 4th order AB-TSF method with restart under $\varepsilon = 0.5$ and $\varepsilon = 0.005$ in example 5.1.

inherently less efficient than **(AB-TSF)**, as the micro-macro decomposition requires to evaluate the derivative-free change of variable at each step, whereas only one evaluation is necessary for the two-scale method (or at most a few if we take into account the refreshes).

(ii) Numerical approximations of the energy of **(AB-TSF)** and **(AB-MM)** converge (uniformly in ε) with the same order as the numerical solutions themselves. We can notice that method **(AB-TSF)** with restarts is stable on long-time intervals,

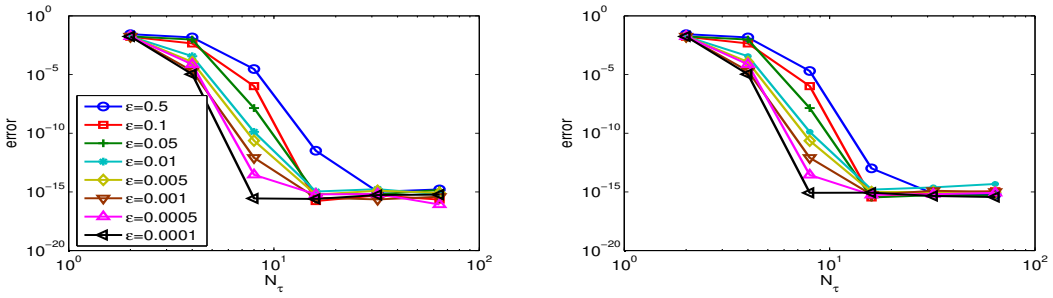

FIGURE 4. Error as N_θ under different ε: the 3rd order (left) and 4th order (right) AB-TSF methods in example 5.1.

even if the energy error drifts linearly, as is expected from a non-symplectic (and non-symmetric) method.

5.2. **Second example.** Our second example is the one-dimensional non-linear Klein-Gordon (KG) equation in the non-relativistic scaling [1, 2]

$$\begin{cases} \varepsilon \partial_{tt} a(x,t) - \partial_{xx} a(x,t) + \dfrac{1}{\varepsilon} a(x,t) + g(a(x,t)) = 0, \quad x \in \mathbb{T}, \quad t > 0, \\ a(x,0) = \phi_1(x), \quad \partial_t a(x,0) = \dfrac{1}{\varepsilon}\phi_2(x), \quad x \in \mathbb{T}, \end{cases} \tag{5.2}$$

where $0 < \varepsilon \leq 1$ is a scaled parameter inversely proportional to the square of the speed of light, a is the real-valued unknown, ϕ_1, ϕ_2 are the given initial data and $g : \mathbb{R} \to \mathbb{R}$ is a given non-linear function. By introducing [6]

$$b := b(x,t) = \mathrm{e}^{-it\sqrt{1-\varepsilon\partial_{xx}}/\varepsilon} \left[a(x,t) - i\varepsilon(1-\varepsilon\partial_{xx})^{-1/2} \partial_t a(x,t) \right] \quad x \in \mathbb{T},\ t \geq 0,$$

the equation (5.2) becomes

$$\begin{cases} \partial_t b = i(1-\varepsilon\partial_{xx})^{-1/2} \mathrm{e}^{-i(t/\varepsilon + tA_\varepsilon)} g\left(\dfrac{1}{2}\left(\mathrm{e}^{i(t/\varepsilon+tA_\varepsilon)} b + \mathrm{e}^{-i(t/\varepsilon+tA_\varepsilon)} \bar{b} \right) \right), \quad x \in \mathbb{T},\ t > 0, \\ b(x,0) = \phi_1(x) - i(1-\varepsilon\partial_{xx})^{-1/2}\phi_2(x), \qquad x \in \mathbb{T}, \end{cases} \tag{5.3}$$

with $A_\varepsilon := \frac{1}{\varepsilon}\left[\sqrt{1-\varepsilon\partial_{xx}} - 1\right]$ Note that the operator $0 \leq A_\varepsilon \leq \frac{-\partial_{xx}}{2}$, so that (5.3) belongs to the class of highly-oscillatory problems of the form (1.1) after discretisation of the variable x. Hereafter, we take

$$g(u) = \sin(u)/2, \quad \phi_1(x) = \frac{2\sin(2x)}{2+\cos(x)}, \quad \phi_2(x) = \cos(x),$$

and solve (5.3) on the time-interval $(0, 1)$. The reference solution is obtained by the two-scale method from [6] with a very small step-size $\Delta t = 10^{-6}$ and a large number of Fourier modes $N_\theta = 128$. Global errors in H^1-norm of **(AB-TSF)** versus Δt or ε are plotted on Figure 5. The error w.r.t. N_θ is represented in Figure 6. Corresponding results for **(AB-MM)** are very similar and are therefore omitted.

Based on the numerical results in Figures 5, we can see that the proposed AB-TSF (also AB-MM) reaches the desired high order uniform accuracy.

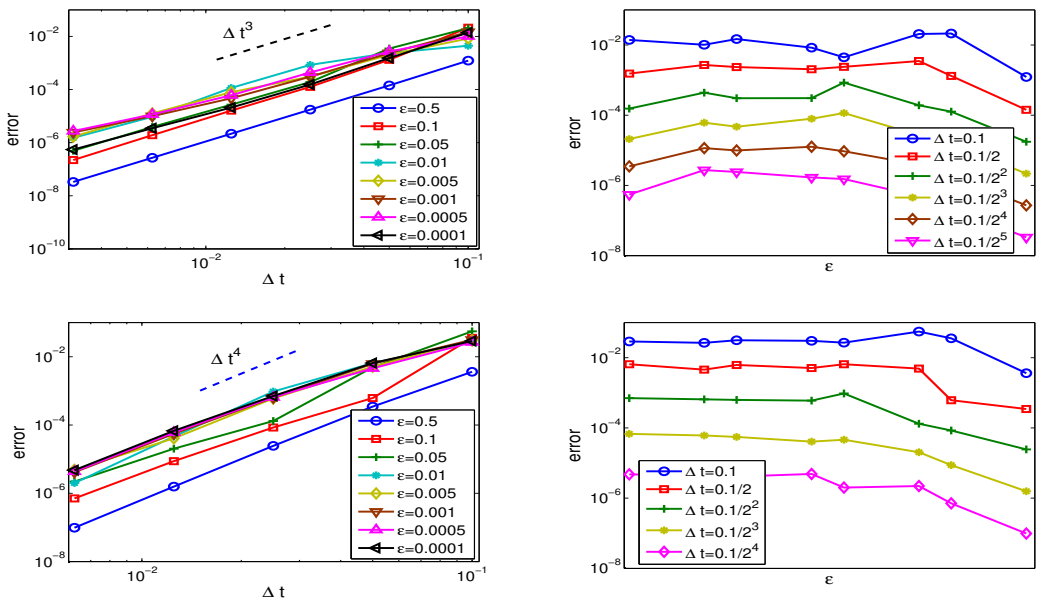

FIGURE 5. Temporal error of AB-TSF methods as Δt or ϵ for KG in example 5.2: the 3rd order (up) and the 4th order (down).

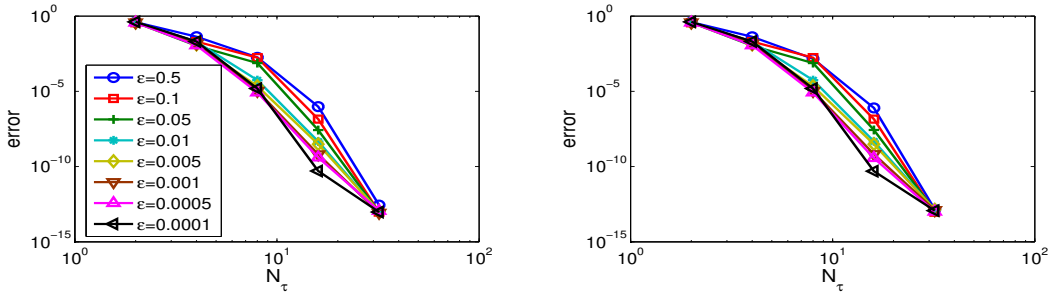

FIGURE 6. Error of AB-TSF methods as N_θ for KG in example 5.2: the 3rd order (left) and the 4th order (right).

5.3. **Third example.** Our last experiment is concerned with the three-dimensional Vlasov equation i with a strong external magnetic field, which is a model of plasma dynamics [13]:

$$\partial_t h^\varepsilon(t,\mathbf{x},\mathbf{v})+\mathbf{v}\cdot\nabla_{\mathbf{x}}h^\varepsilon(t,\mathbf{x},\mathbf{v})+\left(\mathbf{E}(t,\mathbf{x})+\frac{1}{\varepsilon}\mathbf{v}\times\mathbf{B}(\mathbf{x})\right)\cdot\nabla_{\mathbf{v}}h^\varepsilon(t,\mathbf{x},\mathbf{v})=0,\ t>0,\ \mathbf{x},\mathbf{v}\in\mathbb{R}^3,$$

where h^ε is the unknown distribution function, $\varepsilon\in]0,1]$ is inversely proportional to the strength of the magnetic field, and $\mathbf{E}$ and $\mathbf{B}$ denote the electrical and magnetic fields. In this paper, we consider the situation where the magnetic field has constant intensity at leading order, i.e.

$$\mathbf{B}=\mathbf{B}_0+\mathcal{O}(\varepsilon)$$

with $|\mathbf{B}_0(\mathbf{x})|=const$ for all $\mathbf{x}\in\mathbb{R}^3$. In this case, the stiff part of the above equation gives rise to a periodic motion in time [13] so that, once again, the problem belongs to the class (1.1). As one of the most popular spatial discretization techniques for the Vlasov equation

in high dimension, the Particle-In-Cell method approximates the distribution function by many ($N_p \gg 1$) Dirac mass

$$h^\varepsilon(t,\mathbf{x},\mathbf{v}) \approx \sum_{k=1}^{N_p} \omega_k \delta(\mathbf{x}-\mathbf{x}_k(t))\delta(\mathbf{v}-\mathbf{v}_k(t)), \quad t \geq 0,\ \mathbf{x},\mathbf{v} \in \mathbb{R}^2. \tag{5.4}$$

and reduces the problem to the characteristics:

$$\dot{\mathbf{x}}_k(t) = \mathbf{v}_k(t), \tag{5.5a}$$

$$\dot{\mathbf{v}}_k(t) = \mathbf{E}(t,\mathbf{x}_k(t)) + \frac{1}{\varepsilon}\mathbf{v}_k(t) \times \mathbf{B}(\mathbf{x}_k(t)), \quad t > 0, \tag{5.5b}$$

$$\mathbf{x}_k(0) = \mathbf{x}_{k,0}, \quad \mathbf{v}_k(0) = \mathbf{v}_{k,0}. \tag{5.5c}$$

To illustrate the performance of our proposed numerical methods, we here consider the approximation of one characteristic equation (5.5) with initial data

$$\mathbf{x}_{k,0} = (1/3, -1/2, \sqrt{\pi}/2), \quad \mathbf{v}_{k,0} = (1/2, \mathrm{e}/4, -1/3).$$

Hereafter, the vector fields $\mathbf{E}$ and $\mathbf{B}$ are given as

$$\mathbf{E}(\mathbf{x}) = \begin{pmatrix} \cos(x_1/2)\sin(x_2)\sin(x_3)/2 \\ \sin(x_1/2)\cos(x_2)\sin(x_3) \\ \sin(x_1/2)\sin(x_2)\cos(x_3) \end{pmatrix}, \quad \mathbf{B}(\mathbf{x}) = \frac{1}{\sqrt{1+\alpha^2x_1^2+\alpha^2x_2^2}} \begin{pmatrix} \alpha x_2 \\ -\alpha x_1 \\ 1 \end{pmatrix},$$

with $\mathbf{x} = (x_1, x_2, x_3)^T$ and $\alpha = 0.5$. This choice of $\mathbf{B}$ is known as the screw-pinch case [23] with $|\mathbf{B}(\mathbf{x})| = 1$.

We apply our 3^{rd} order and 4^{th} order **(AB-MM)** methods to (5.5) with$N_\tau = 128$. The reference solution is obtained by the 4^{th} order **(AB-MM)** with step-size$\Delta t = 10^{-4}$. Global errors at time $t = 1$ for different values of ε are represented on Figure 7. Clear-cut convergence 3^{rd} order and 4^{th} order are observed for all ε in the interval $(0, 1]$ in both position and velocity variables. Owing to the uniform accuracy of our methods, very few grids points are necessary for a realistic simulation, as one can see on Figure 8 where the numerical solution does not oscillate while still lying on the correct trajectory. Moreover, the **(AB-MM)** approach allows for accurate interpolations. As a matter of fact, quadratic interpolations of v^j and w^j can be obtained from (4.8) for arbitrary $t > 0$, $t_j < t < t_{j+2}$, by computing

$$v_I^j(t) = \frac{(t-t_{j+1})(t-t_{j+2})}{\Delta t^2}v^j - \frac{(t-t_j)(t-t_{j+2})}{\Delta t^2}v^{j+1} + \frac{(t-t_j)(t-t_{j+1})}{\Delta t^2}v^{j+2},$$
$$w_I^j(t) = \frac{(t-t_{j+1})(t-t_{j+2})}{\Delta t^2}w^j - \frac{(t-t_j)(t-t_{j+2})}{\Delta t^2}w^{j+1} + \frac{(t-t_j)(t-t_{j+1})}{\Delta t^2}j^{n+2},$$

and the interpolated numerical solution then reads

$$u_I^j(t) = \widetilde{\Phi}_{t/\varepsilon}^{[2]}(v_I^j(t)) + w_I^n(t), \quad t_n \leq t \leq t_{j+2}.$$

Since $v(t)$ and $w(t)$ are smooth with bounded derivatives $\partial_t^3 v(t) = \mathcal{O}(1)$, and $\partial_t^3 w(t) = \mathcal{O}(1)$, it is clear that the above formulas give uniform third-order approximations to $v(t)$ and $w(t)$. Hence, the full trajectory can also be recovered uniformly . This is also shown in Figures 8 and Figure 9.

Acknowledgements

This work is supported by the French ANR project MOONRISE ANR-14-CE23-0007-01. X. Zhao is partially supported by the Natural Science Foundation of Hubei Province No. 2019CFA007 and the NSFC 11901440.

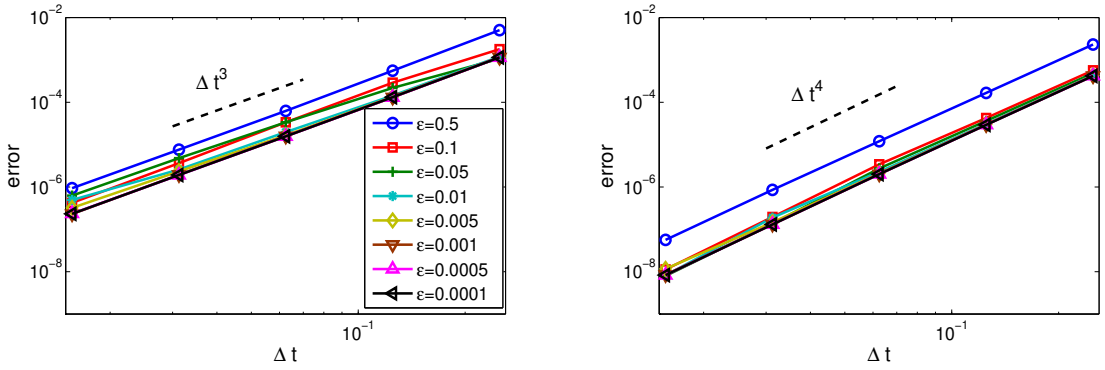

FIGURE 7. Error $|\mathbf{x}(t_n)-\mathbf{x}^n|/|\mathbf{x}(t_n)|+|\mathbf{v}(t_n)-\mathbf{v}^n|/|\mathbf{v}(t_n)|$ as Δt for different ε: the 3rd order (left) and the 4th order (right) AB-MM in example 5.2.

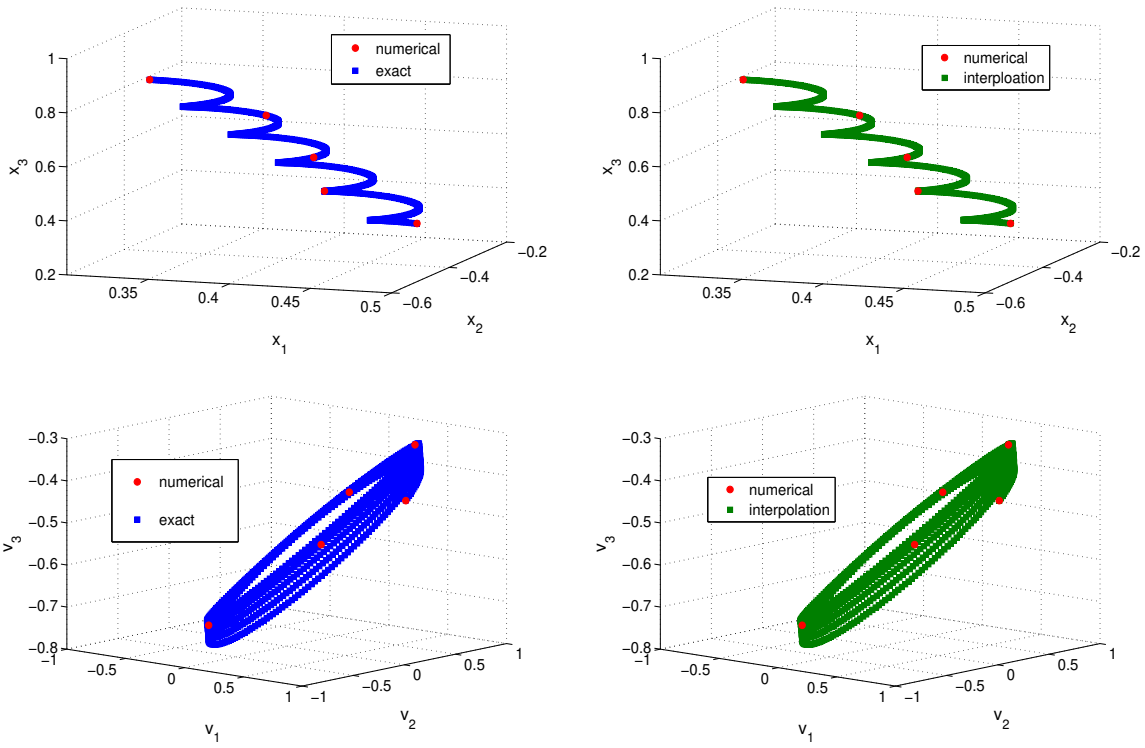

FIGURE 8. Left column: exact trajectory of the particle (blue squares) and the numerical solution of AB-MM with time step $\Delta t = 1/4$ till $t = 1$ under $\varepsilon = 1/2^5$ (red dots, ratio $\Delta t/\varepsilon = 8$). Right column: the numerical solution under $\Delta t = 1/4$ and the fully recovered trajectory with quadratic interpolation at fine mesh.

APPENDIX

Proof of Theorem 3.1. We decompose the solution of (3.1) into a macro and a micro part as follows

$$U(t,\theta) = \Phi_\theta^{[n]}(v(t)) + W(t,\theta), \tag{5.6}$$

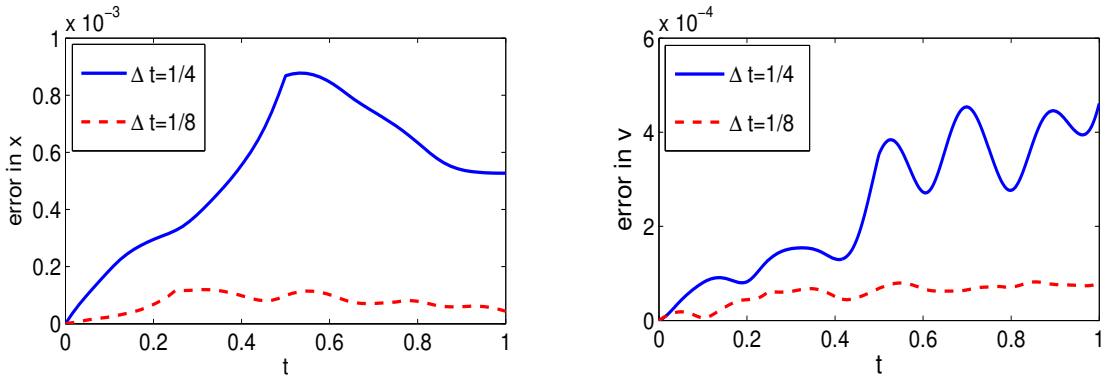

FIGURE 9. Error of the quadratic interpolation based on the numerical solution of AB-MM with $\Delta t = 1/4$ till $t = 1$ under $\varepsilon = 1/2^5$ in position $\mathbf{x}$ (left) and in velocity $\mathbf{v}$ (right).

where v is the solution of the averaged equation (4.2)

$$\dot{v}(t) = F^{[n]}(v(t)), \quad v(0) = \widetilde{u}_0.$$

All we have to show is that the derivatives of W are bounded independently of ε, as this is clearly the case for $\Phi_\theta^{[n]}(v(t))$ (see Proposition 3.2. in [10]). It is straightforward to see that $W(t,\theta)$ is then solution of the transport equation

$$\partial_t W(t,\theta) + \frac{1}{\varepsilon}\partial_\theta W(t,\theta) = f_\theta\Big(\Phi_\theta^{[n]}(v(t)) + W(t,\theta)\Big) - f_\theta\Big(\Phi_\theta^{[n]}(v(t))\Big) - \delta_\theta^{[n]}(v(t)) \tag{5.7}$$

with initial condition $W(0,\theta) = 0$ and where $\delta_\theta^{[n]}$ is given by equation (2.2)

$$\delta_\theta^{[n]} = \frac{1}{\varepsilon}\partial_\theta \Phi_\theta^{[n]} + \partial_u \Phi_\theta^{[n]}\ F^{[n]} - f_\theta \circ \Phi_\theta^{[n]}.$$

Written in compact form, we have

$$\partial_t W + \frac{1}{\varepsilon}\partial_\theta W = L^{[n]}(\theta,t,W)W + b^{[n]}(\theta,t) \tag{5.8}$$

where we have denoted

$$\begin{aligned} L^{[n]}(\theta,t,W)W &= f_\theta\Big(\Phi_\theta^{[n]}(v(t)) + W\Big) - f_\theta\Big(\Phi_\theta^{[n]}(v(t))\Big) \\ &= \left(\int_0^1 \partial_u f_\theta\Big(\Phi_\theta^{[n]}(v(t)) + \mu W\Big) d\mu\right) W, \\ b^{[n]}(\theta,t) &= -\delta_\theta^{[n]}(v(t)). \end{aligned}$$

Under the assumptions of Theorem 2.1, both the operator $L^{[n]}(\theta,t,W)$ and the source term $b^{[n]}(\theta,t)$ are of class C^p w.r.t. $\theta \in \mathbb{T}$, of class C^∞ w.r.t. $t \in [0,T]$ and real-analytic w.r.t. W. In particular, according to Theorem 3.5. in [10], we have the following bounds for all $(\nu,\mu,\xi) \in \mathbb{N}^3$ such that $\nu+\mu+\xi \le p$ and for all $(\theta,t) \in [0,2\pi]\times[0,1]$

$$\forall (W, Y_1, \ldots, Y_\xi) \in \mathcal{K}^{1+\xi}, \quad \|\partial_\theta^\nu \partial_t^\mu \partial_w^\xi L^{[n]}(\theta,t,W)\,(Y_1,\ldots,Y_\xi)\| \le C_n^L \|Y_1\| \ldots \|Y_\xi\| \tag{5.9}$$

and

$$\forall W \in \mathcal{K},\ \|\partial_\theta^\nu \partial_t^\mu b^{[n]}(\theta,t)\| \le C_n^b\, \varepsilon^n, \tag{5.10}$$

for some positive constants C_n^L and C_n^b independent of ε. We now observe that the derivatives of W w.r.t. θ may be easily bounded independently of ε given that, on the one-hand, the right-hand side of (5.7) and its derivatives w.r.t. θ are all bounded themselves, and on the other hand, $(\partial_\theta^k W)(0,\theta) = 0$ for all $k \geq 0$. As for derivatives w.r.t. t, we introduce $W_k(t,\theta) = \partial_t^k W(t,\theta)$ and write

$$\begin{aligned}\partial_t W_k + \frac{1}{\varepsilon}\partial_\theta W_k &= \frac{d^k}{dt^k}\left(L^{[n]}(\theta,t,W)W + b^{[n]}(\theta,t)\right)\\ &= \partial_t^k b^{[n]} + \sum_{\alpha+\beta\leq k}\sum_{\mathbf{i}} c_{\mathbf{i}}\left(\partial_t^\alpha \partial_W^\beta L\right)\left(W_{i_0}, W_{i_1}, \ldots, W_{i_\beta}\right) \end{aligned} \tag{5.11}$$

where the second sum is extended over multi-indices $\mathbf{i} = (i_0, \ldots, i_\beta) \in \mathbb{N}^{\beta+1}$ such that

$$i_0 \geq 0,\ i_1 \geq 1, \ldots, i_\beta \geq 1, \quad i_0 + i_1 + \ldots + i_\beta + \alpha = k$$

and where the $c_{\mathbf{i}}$ are fixed coefficients. Equation (5.11) prescribes the initial condition $W_k^0(\theta)$ for W_k recursively. As a matter of fact, we have at $t = 0$

$$\begin{aligned} W_1^0 &= -\frac{1}{\varepsilon}\partial_\theta W^0 + L^{[n]}W^0 + b^{[n]} = b^{[n]},\\ W_2^0 &= -\frac{1}{\varepsilon}\partial_\theta W_1^0 + \partial_t b^{[n]} + (\partial_t L^{[n]})W^0 + (\partial_u L^{[n]})(W^0, W_1^0) + L^{[n]}W_1^0\\ &= -\frac{1}{\varepsilon}\partial_\theta b^{[n]} + \partial_t b^{[n]} + L^{[n]}b^{[n]}, \end{aligned}$$

and more generally

$$W_{k+1}^0 = -\frac{1}{\varepsilon}\partial_\theta W_k^0 + \partial_t^k b^{[n]} + \sum_{\alpha+\beta\leq k}\sum_{\mathbf{i}} c_{\mathbf{i}}\left(\partial_t^\alpha \partial_W^\beta L\right)\left(W_{i_0}^0, W_{i_1}^0, \ldots, W_{i_\beta}^0\right).$$

Using (5.9) and (5.10), it is easy to obtain by induction

$$\forall \nu \leq p,\ \forall k \leq \min(p, n+1),\ \forall \theta \in \mathbb{T}, \quad \|\partial_\theta^\nu W_k^0(\theta)\| \leq \mathcal{C}_k \varepsilon^{n+1-k} \tag{5.12}$$

where the constant depends only on the constants in (5.9) and (5.10) but not on ε. By solving the characteristics of (5.11) and taking into account (5.12) and the fact that its right-hand side together with all its derivatives are bounded independently of ε, the statement of the theorem follows. □

Acknowledgements

This work has been carried out within the framework of the EUROfusion Consortium and has received funding from the Euratom Research and Training Programme 2019-2020. The views and opinions expressed herein do not necessarily reflect those of the European Commission. It is furthermore supported by the French ANR project MOONRISE ANR-14-CE23-0007-01. X. Zhao is partially supported by the Natural Science Foundation of Hubei Province No. 2019CFA007 and the NSFC 11901440.

References

[1] W. Bao, Y. Cai, X. Zhao, A uniformly accurate multiscale time integrator pseudospectral method for the Klein-Gordon equation in the nonrelativistic limit regime, SIAM J. Numer. Anal. 52 (2014) pp. 2488-2511.

[2] W. Bao, X. Zhao, Comparison of numerical methods for the nonlinear Klein-Gordon equation in the nonrelativistic limit regime, J. Comput. Phys. 398 (2019) pp. 108886.

[3] S. Baumstark, E. Faou, K. Schratz, Uniformly accurate exponential-type integrators for Klein-Gordon equations with asymptotic convergence to classical splitting schemes in the NLS splitting, Math. Comp. 87 (2018) pp. 1227-1254.

[4] Y. Cai, Y. Wang, Uniformly accurate nested Picard iterative integrators for the Dirac equation in the nonrelativistic limit regime, SIAM J. Numer. Anal. 57 (2019) pp. 1602-1624.
[5] F. Castella, Ph. Chartier, F. Méhats, A. Murua, Stroboscopic Averaging for the Nonlinear Schrödinger Equation, Found. Comput. Math. 15 (2015) pp. 519-559.
[6] Ph. Chartier, N. Crouseilles, M. Lemou, F. Méhats, Uniformly accurate numerical schemes for highly oscillatory Klein-Gordon and nonlinear Schrödinger equations, Numer. Math. 129 (2015), pp. 211-250.
[7] M. P. Calvo, Ph. Chartier, A. Murua, and J. M. Sanz-Serna, Numerical stroboscopic averaging for ODEs and DAEs. Appl. Numer. Math., 61(10):1077–1095, 2011.
[8] Ph. Chartier, J. Makazaga, A. Murua, and G. Vilmart, Multi-revolution composition methods for highly oscillatory differential equations, Numer. Math., Vol. 128, No. 1, pp 167-192, 2014.
[9] Ph. Chartier, M. Lemou, and F. Méhats, Highly-oscillatory evolution equations with multiple frequencies: averaging and numerics, Numer. Math., 136(4):907–939, 2017.
[10] Ph. Chartier, M. Lemou, F. Méhats, G. Vilmart, A new class of uniformly accurate methods for highly oscillatory evolution equations, to appear on Found. Comput. Math. 2019.
[11] Ph. Chartier, M. Lemou, F. Méhats, G. Vilmart, Highly-oscillatory problems with time-dependent vanishing frequency, to appear on SIAM J. Numer. Anal. 2019.
[12] Ph. Chartier, N. Crouseilles, M. Lemou, F. Méhats, X. Zhao, Uniformly accurate methods for Vlasov equations with non-homogeneous strong magnetic field, Math. Comp. 88 (2019), pp. 2697-2736.
[13] Ph. Chartier, N. Crouseilles, M. Lemou, F. Méhats, X. Zhao, Uniformly accurate methods for three dimensional Vlasov equations under strong magnetic field with varying direction, preprint, arXiv:1907.04851.
[14] Ph. Chartier, N. Crouseilles, X. Zhao, Numerical methods for the two-dimensional Vlasov-Poisson equation in the finite Larmor radius approximation regime, J. Comput. Phys. 375 (2018), pp. 619-640.
[15] N. Crouseilles, M. Lemou, F. Méhats, Asymptotic preserving schemes for highly oscillatory Vlasov-Poisson equations, J. Comput. Phys. 248 (2013), pp. 287-308.
[16] N. Crouseilles, M. Lemou, F. Méhats, X. Zhao, Uniformly accurate forward semi-Lagrangian methods for highly oscillatory Vlasov-Poisson equations, SIAM J. Multiscale Model. Simul. 15 (2017), pp. 723-744.
[17] N. Crouseilles, S.A. Hirstoaga, X. Zhao, Multiscale Particle-In-Cell methods and comparisons for long time two-dimensional Vlasov-Poisson equation with strong magnetic field, Comput. Phys. Commun. 222 (2018), pp. 136-151.
[18] N. Crouseilles, M. Lemou, F. Méhats, X. Zhao, Uniformly accurate Particle-in-Cell method for the long time two-dimensional Vlasov-Poisson equation with uniform strong magnetic field, J. Comput. Phys. 346 (2017), pp. 172-190.
[19] E. Frénod, F. Salvarani, E. Sonnendrücker, Long time simulation of a beam in a periodic focusing channel via a two-scale PIC-method, Math. Models Methods Appl. Sci. 19 (2009), pp. 175-197.
[20] E. Frénod, E. Sonnendrücker, Long time behavior of the two-dimensional Vlasov equation with a strong external magnetic field, Math. Models Methods Appl. Sci. 10 (2000), pp. 539-553.
[21] B. García-Archilla, J.M. Sanz-Serna, R.D. Skeel, Long-time-step methods for oscillatory differential equations. SIAM J. Sci. Comput. 20 (1999), pp. 930-963.
[22] E. Hairer, Ch. Lubich, G. Wanner, Geometric Numerical Integration: Structure-Preserving Algorithms for Ordinary Differential Equations, Springer, Berlin, 2006
[23] G. Latu, M. Mehrenberger, Y. Güçlü, M. Ottaviani, E. Sonnendrücker, Field-Aligned Interpolation for Semi-Lagrangian Gyrokinetic Simulations, J. Sci. Comput. 74 (2018), pp. 1601-1650.
[24] L. M. Perko, Higher order averaging and related methods for perturbed periodic and quasi-periodic systems, SIAM J. Applied. Math., **17**, 698-724, 1969.
[25] K. Schratz, X. Zhao, On the comparison of asymptotic expansion techniques for the nonlinear Klein-Gordon equation in the nonrelativistic limit regime, to appear on Discrete Contin. Dyn. Syst. Ser. B. 2020.
[26] J.A. Sanders, F. Verhulst, Averaging methods in nonlinear dynamical systems, volume 59 of Applied Mathematical Sciences. Springer-Verlag, New York, 1985.
[27] E. Sonnendrücker, Numerical Methods for Vlasov Equations, Lecture notes, 2016.

Ph. Chartier: Univ Rennes, INRIA-MINGuS, CNRS, IRMAR-UMR 6625, F-35000 Rennes, France
Email address: Philippe.Chartier@inria.fr

M. Lemou: Univ Rennes, CNRS, INRIA-MINGuS, IRMAR-UMR 6625, F-35000 Rennes, France
Email address: mohammed.lemou@univ-rennes1.fr

F. Méhats: Univ Rennes, CNRS, INRIA-MINGuS, IRMAR-UMR 6625, F-35000 Rennes, France
Email address: florian.mehats@univ-rennes1.fr

X. Zhao: School of Mathematics and Statistics & Hubei Key Laboratory of Computational Science, Wuhan University, Wuhan, 430072, China
Email address: matzhxf@whu.edu.cn