Application of averaging technique for the numerical simulation of highly oscillatory problems

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We consider a highly oscillatory problem in a (functional) Banach space $X$:

$$(P_\varepsilon) \quad \frac{d}{dt} u^\varepsilon(t) = f_{t/\varepsilon}(u^\varepsilon(t)), \quad u^\varepsilon(t) \in X,$$

$u^\varepsilon(0) = u_0 \in X,$

where

- $\varepsilon$ is a possibly small parameter (scales as the inverse of a frequency).
- $(\theta, u) \mapsto f_\theta(u)$ is given, smooth and $P$-periodic with respect to $\theta$.

**Numerical difficulties:** Standard schemes lead to $\|u^\varepsilon - u^\varepsilon,\Delta t\| \leq C(\Delta t)^p\varepsilon^q$, $q > 0$, forcing $\Delta t \leq \varepsilon$ and thus formidable costs for small values of $\varepsilon$.

**Partial remedy:** Averaging methods lead to $\|u^\varepsilon - u^\varepsilon,\Delta t\| \leq C((\Delta t)^p + \varepsilon^q)$.

**Aim:** Construct a numerical method which is uniformly accurate with respect to $\varepsilon$, i.e. such that $\|u^\varepsilon - u^\varepsilon,\Delta t\| \leq C(\Delta t)^p$ with $C$ independent of $\varepsilon$. 
Our examples are of the form

\[ \frac{d}{dt} y^\varepsilon = \frac{1}{\varepsilon} Ay^\varepsilon + f(y^\varepsilon) \]

where \( \theta \mapsto e^{A\theta} \) is periodic with respect to \( \theta \).

To filter out the highly oscillatory dynamics, we introduce the unknown

\[ u^\varepsilon(t) = e^{-At/\varepsilon} y^\varepsilon(t) \]

which satisfies

\[ \frac{d}{dt} u^\varepsilon = e^{-At/\varepsilon} f \left( e^{At/\varepsilon} u^\varepsilon(t) \right) = f_{t/\varepsilon}(u^\varepsilon(t)) \]

Here we have

\[ f_\theta(u) = e^{-A\theta} f \left( e^{A\theta} u^\varepsilon(t) \right) \]
Examples (ii)

➤ Transport in graphene in semiclassical regime
➤ Schrödinger equation and Gross-Pitaevskii equation

\[ i\partial_t \psi^\varepsilon = -\frac{1}{\varepsilon} \Delta \psi^\varepsilon + \alpha |\psi^\varepsilon|^2 \psi^\varepsilon \text{ with periodic boundary conditions} \]

\[ i\partial_t \psi^\varepsilon = -\frac{1}{\varepsilon} \Delta \psi^\varepsilon + \frac{\omega}{\varepsilon} |x| \psi^\varepsilon + \alpha |\psi^\varepsilon|^2 \psi^\varepsilon \quad \text{on } \mathbb{R}^d \]

➤ The nonlinear Klein-Gordon equation in the nonrelativistic regime

\[ \varepsilon \partial_{tt} u^\varepsilon - \Delta u^\varepsilon + \frac{1}{\varepsilon} u^\varepsilon + f(u^\varepsilon) = 0, \quad x \in \mathbb{R}^d, \quad t > 0, \]

➤ Vlasov equation in a strong magnetic field

\[ \partial_t f^\varepsilon + v \cdot \nabla_x f^\varepsilon + E \cdot \nabla_v f^\varepsilon + \frac{v \times B}{\varepsilon} \cdot \nabla_v f^\varepsilon = 0 \]

➤ Non relativistic limit of nonlinear Dirac equation
Averaging methods assert that for all $k \in \mathbb{N}^*$ there exist

1. a $P$-periodic change of variables

   $$(\tau, u) \in \mathbb{T} \times X \mapsto \Phi^{[k]}_\tau(u) \in X$$

   such that

   $\Phi^{[k]}_0(u) = u$

2. a smooth, autonomous vector field $F^{[k]}$ and its flow-map $\Psi^{[k]}_t$

   - $u \in X \mapsto F^{[k]}(u) \in X$
   - $(t, u) \mapsto \Psi^{[k]}_t(u) \in X$

   such that

   $$\forall t \in [0, T], \quad \|u^\varepsilon(t) - \Phi^{[k]}_{\frac{t}{\varepsilon}} \circ \Psi^{[k]}_t(u_0)\|_X \leq C\varepsilon^{k+1}.$$
Averaging: an assessment

The standard use of averaging method consist in the simulation of

$$\frac{d}{dt} \Psi^k_t = F^k(\Psi^k_t)$$

generated with the computation of $\Phi^k_\theta$.

Pros of averaging

➤ models are non-stiff and do not suffer from severe constraints on the time step when $\epsilon$ is small
➤ preserve part or all geometric structures

Cons

➤ methods based on the (numerical or not) computation of the averaged vector field $F^k$ lead to an incompressible error term $O(\epsilon^{k+1})$ owing to the truncation of the series
➤ for values of $\epsilon$ away from 0 one needs to include many terms in the expansion leading to important costs
New approach: averaging with corrections (i)

Our approach, in the micro/macro spirit, consists in adding an equation to the averaged equation. The unknown is split as follows:

\[ u^\varepsilon(t) = \Phi_{t/\varepsilon}^{[k]} \left( \Psi_t^{[k]} \right) + w^\varepsilon(t) \]

where \( \Psi_t^{[k]} \) solves the macro (averaged) equation

\[ \frac{d}{dt} \Psi_t^{[k]} = F^{[k]}(\Psi_t^{[k]}), \quad \Psi_0^{[k]} = u_0. \]

The remainder \( w^\varepsilon \) solves the micro equation

\[ \frac{d}{dt} w^\varepsilon(t) = f_{t/\varepsilon} \left( \Phi_{t/\varepsilon}^{[k]} \left( \Psi_t^{[k]} \right) + w^\varepsilon(t) \right) - \left( \frac{1}{\varepsilon} \partial_\theta \Phi_{t/\varepsilon}^{[k]} - \partial_u \Phi_{t/\varepsilon}^{[k]} F^{[k]} \right) (\Psi_t^{[k]}), \]

\[ w^\varepsilon(0) = 0. \]

Theorem

\[ \forall \varepsilon \in ]0, 1], \quad \forall 0 \leq s \leq k + 1, \quad \forall t \in [0, T], \quad \left\| \frac{d^s}{dt^s} w^\varepsilon \right\| \leq C \varepsilon^{k+1-s} \]
It is clear that if $\Psi^\varepsilon$ and $w^\varepsilon$ satisfy the micro/macro equations, then $u^\varepsilon(t) = \Phi_{t/\varepsilon}^{[k]}(\Psi^\varepsilon(t_0)) + w^\varepsilon(t)$ satisfies the original equation

$$\frac{d}{dt}u^\varepsilon(t) = f_{t/\varepsilon}(u^\varepsilon(t)).$$

In contrast with usual averaging, our micro/macro method is not an approximation and contains whole the information of the original problem.

The fact that $w^\varepsilon$ has bounded time-derivatives with respect to $\varepsilon$ allows to use standard numerical methods for the micro/macro system with uniform accuracy with respect to $\varepsilon$.

**Take-away message:**

A $p$-th order standard scheme is uniformly accurate of order $p$ when applied to the micro-macro system provided $\Phi^{[p]}$ and $F^{[p]}$ are used.
Numerical tests for the Hénon-Heiles model

It is a Hamiltonian system, for the unknown \((q_1, q_2, p_1, p_2)\) with

\[
H(p, q) = \frac{p_1^2}{2\varepsilon} + \frac{p_2^2}{2} + \frac{q_1^2}{2\varepsilon} + \frac{q_2^2}{2} + q_1 q_2 - \frac{1}{3} q_3^3.
\]

When \(\varepsilon\) is small, the variables \((q_1^\varepsilon, p_1^\varepsilon)\) is highly oscillatory:

\[
\begin{align*}
\dot{q}_1^\varepsilon &= \frac{p_1^\varepsilon}{\varepsilon} \\
\dot{q}_2^\varepsilon &= p_2^\varepsilon \\
\dot{p}_1^\varepsilon &= -\frac{q_1^\varepsilon}{\varepsilon} - 2q_1^\varepsilon q_2^\varepsilon \\
\dot{p}_2^\varepsilon &= -q_2^\varepsilon - (q_1^\varepsilon)^2 + (q_2^\varepsilon)^2
\end{align*}
\]

We test the following numerical methods:

- Our second order method: UA of order 2
- A third order method constructed with \(\Phi^{[2]}\) and \(F^{[2]}\) by extrapolation: UA of order 3
- A fourth order method constructed with \(\Phi^{[3]}\) and \(F^{[3]}\) by extrapolation: UA of order 4
Our UA schemes (orders 2, 3 and 4)

(a) Error with respect to $\Delta t$

(b) Error with respect to $\varepsilon$, scheme of order 2
Thank you for your attention