HIGH ORDER NUMERICAL HOMOGENIZATION FOR DISSIPATIVE ORDINARY DIFFERENTIAL EQUATIONS

ZEYU JIN∗ AND RUO LI†

Abstract. We propose a high order numerical homogenization method for dissipative ordinary differential equations (ODEs) containing two time scales. Essentially, only first order homogenized model globally in time can be derived. To achieve a high order method, we have to adopt a numerical approach in the framework of the heterogeneous multiscale method (HMM). By a successively refined microscopic solver, the accuracy improvement up to arbitrary order is attained providing input data smooth enough. Based on the formulation of the high order microscopic solver we derived, an iterative formula to calculate the microscopic solver is then proposed. Using the iterative formula, we develop an implementation to the method in an efficient way for practical applications. Several numerical examples are presented to validate the new models and numerical methods.

Key words. Multiscale methods; Dissipative systems; Homogenization; Correction model

AMS subject classifications. 34E13, 65L04

1. Introduction. Multiple-time-scale problems are often encountered in many disciplines such as chemical kinetics [23], molecular dynamics [4, 32] and celestial mechanics [21]. There are many studies concerning stiff systems of ordinary differential equations (ODEs), especially those with two time scales. In general, these systems can be divided into two categories [9]. One is dissipative systems where fast variables tend to the stationary state at an exponential rate. The other one is oscillatory systems where fast variables oscillate in some orbits.

It is impossible to resolve all the time scales and capture all the variables numerically due to limited computing power. In many problems, we are only interested in the dynamics of slow macroscopic variables. There is some work on designing efficient numerical algorithms for stiff ODEs, such as implicit Runge-Kutta methods [30], backward differentiation formulas [2], Rosenbrock methods [20] and projective methods [14].

It is well known [24] that, as $\varepsilon \to 0$, the dynamics of slow variables satisfy a limiting equation, which can be obtained by averaging methods. For simple systems, the limiting equation can be derived by analytical tools. For complex systems, however, we have to sample the fast variables to approximate the limiting equation. A famous method of this type is the heterogeneous multiscale method [10, 1, 11]. In HMM, there is a microscopic solver to sample the fast variables, and a macroscopic solver to evolve the slow variables. Some results of numerical analysis on this method can be found in [9]. There are three main sources of errors of HMM, including modeling error, sampling error and truncation error of the macroscopic solver. The modeling error is of order $O(\varepsilon)$. When $\varepsilon$ is sufficiently small, the modeling error is small enough. However, when $\varepsilon$ is relatively but not extremely small, the modeling error is not ignorable. Therefore, it is necessary to propose a correction model to reduce the modeling error in this situation.

There have been several attempts to reduce modeling error in multiscale method. For example, in [6], they use B-series to derive a high-order stroboscopic averaged equations for a kind of highly oscillatory systems. In [19, 31], they develop a first order correction model for sediment transport in sub-critical case, where the modeling error can be reduced to $O(\varepsilon^2)$.

In this paper, we develop a novel high-order correction model and the corresponding numerical algorithms for stiff dissipative system of ODEs. Our studies begin with the theory of invariant manifold for ODEs [15, 25]. It can be proved that the invariant manifold is a global attractor. Actually, the microscopic solver of HMM is designed to find an approximation to the invariant manifold with an error of $O(\varepsilon)$. In order to derive the correction models, we need to find high-order approximations to the invariant manifold. By the asymptotic approximation method, the analytical expressions of the first several terms in the formal expansion can be obtained. We can prove that this approximation shares similar properties to the invariant manifold. In other words, the trajectories tend to this approximation to invariant manifold at an exponential rate. Once the trajectories are close to this approximation, then they can be approximated by a reduced model over a finite time horizon. However, the terms obtained by the formal expansion are too complicated.

∗Yuanpei College & School of Mathematical Sciences, Peking University (jinzy@pku.edu.cn).
†CAPT, LMAM & School of Mathematical Sciences, Peking University (rli@math.pku.edu.cn).
to be implemented, especially for higher-order methods. In addition, it requires the evaluation of high-order derivatives. We design an iterative formula for the sake of practicality. We can prove that the iterative method matches with the formal expansion in some sense. We can also prove that the approximation accuracy reaches $O(\varepsilon^{k+1})$ after $k$ iteration steps. By the technology of numerical derivatives, we design a recursion method using the iterative scheme. We also present some numerical analysis on our algorithms.

The rest of this paper is arranged as follows. In Section 2, we briefly introduce the multiscale dissipative systems and the heterogeneous multiscale methods. In Section 3, we present our models for high-order homogenization and analyze their properties. In Section 4, we develop two types of algorithms in the framework of HMM. Some numerical analysis is presented in Section 5. Numerical results are shown in Section 6 and the paper ends with a brief summary and conclusion in Section 7.

2. Preliminaries.

2.1. Dissipative systems. Let us consider the following ODEs with scale separation [25]:

$$\begin{cases}
\frac{dx}{dt} = f(x, y), \\
\frac{dy}{dt} = \frac{1}{\varepsilon} g(x, y), \\
x|_{t=0} = x_0, \ y|_{t=0} = y_0,
\end{cases}
$$

(2.1)

where $x \in \mathbb{R}^{n_x}$ is the slow variable and $y \in \mathbb{R}^{n_y}$ is the fast variable, $n_x$ and $n_y$ are the dimension of $x$ and $y$, respectively. The parameter $0 < \varepsilon \leq \varepsilon_0 \ll 1$ characterizes the separation of time scales. Let $y^\varepsilon$ be the solution of

$$\begin{cases}
\frac{dy^\varepsilon}{dt} = \frac{1}{\varepsilon} g(x, y^\varepsilon), \\
y^\varepsilon|_{t=0} = y_0,
\end{cases}
$$

(2.2)

for any $x$ fixed. Suppose that $d\mu^\varepsilon(y)$ is the corresponding invariant measure of (2.2) satisfying that for any $\phi \in L^1(\mathbb{R}^{n_y}; d\mu^\varepsilon)$,

$$\lim_{T \to +\infty} \frac{1}{T} \int_0^T \phi(y^\varepsilon(t)) \, dt = \int_{\mathbb{R}^{n_y}} \phi(y) \, d\mu^\varepsilon(y), \quad \text{for } \mu^\varepsilon - \text{a.e. } y_0 \in \mathbb{R}^{n_y}.$$

Let

$$F(x) = \lim_{T \to +\infty} \frac{1}{T} \int_0^T f(x, y^\varepsilon(t)) \, dt = \int_{\mathbb{R}^{n_y}} f(x, y) \, d\mu^\varepsilon(y).$$

Under some appropriate assumptions [24], the trajectory of $x(t)$ tends to a solution of the limiting equation

$$\frac{dX_0}{dt} = F(X_0),
$$

(2.3)

as $\varepsilon \to 0$ in some sense.

Since now on, we assume the regularity of the functions $f$ and $g$. Precisely, we assume that

**Assumption 2.1.** The functions $f$ and $g$ are sufficiently smooth. In addition, there exists $K \in \mathbb{N} \setminus \{0\}$ such that \(^1\)

$$f \in W^{K, \infty}(\mathbb{R}^{n_x} \times \mathbb{R}^{n_y}, \mathbb{R}^{n_x}), \quad \nabla g \in W^{K, \infty}(\mathbb{R}^{n_x} \times \mathbb{R}^{n_y}, \mathbb{R}^{n_x \times (n_x + n_y)}).$$

\(^1\)Here we adopt standard notations of Sobolev spaces. The space $W^{k, \infty}(\mathbb{R}^n, \mathbb{R}^m)$ is equipped with the norm defined by

$$\|\xi\|_{W^{k, \infty}(\mathbb{R}^n, \mathbb{R}^m)} := \max_{j=0,1,...,k} \|\nabla^j \xi\|_{L^\infty}, \quad \xi \in W^{k, \infty}(\mathbb{R}^n, \mathbb{R}^m).$$

When no ambiguity is possible, $\|\xi\|_{W^{k, \infty}(\mathbb{R}^n, \mathbb{R}^m)}$ and $W^{k, \infty}(\mathbb{R}^n, \mathbb{R}^m)$ are abbreviated as $\|\xi\|_{k, \infty}$ and $W^{k, \infty}$, respectively. Let $| \cdot |_{k, \infty}$ defined by

$$|\xi|_{k, \infty} := \|\nabla^k \xi\|_{L^\infty}$$

be the Sobolev semi-norm.
Furthermore, we always have the following assumption for $g$.

**Assumption 2.2.** For each $x \in \mathbb{R}^{n_x}$, there exists $\gamma(x) \in \mathbb{R}^{n_y}$ such that

$$
(2.4) \quad g(x, \gamma(x)) = 0.
$$

In addition, there exists $\beta > 0$ such that

$$
(2.5) \quad (g(x, y) - g(x, \tilde{y}), y - \tilde{y}) \leq -\beta|y - \tilde{y}|^2, \quad \forall x \in \mathbb{R}^{n_x}, \forall y, \tilde{y} \in \mathbb{R}^{n_y}.
$$

By Assumption 2.2, one can see that the dynamic for $y$ with $x$ fixed has a unique, globally exponentially attracting point [25]. At this time, the system (2.1) is called a dissipative system. It is clear that the invariant measure $\mu(x)$ at fixed $x$ is a one-point distribution at $y = \gamma(x)$. In addition, one has that $F(x) = f(x, \gamma(x))$. It was pointed out in [25] that, under some appropriate assumptions, the modeling error between the solutions of (2.1) and (2.3) is of order $O(\varepsilon)$ in a finite time horizon.

**Remark 2.3.** Let $\tilde{g}_x = g(x, \cdot) : \mathbb{R}^{n_x} \to \mathbb{R}^{n_y}$. If $g(x, y)$ satisfies (2.5), then we say that $\tilde{g}_x$ is a $\beta$-strongly dissipative operator or $-\tilde{g}_x$ is a $\beta$-strongly monotonic operator on $\mathbb{R}^{n_y}$ by the definitions in [27, 3]. It can be deduced [17] that, if $\tilde{g}_x$ is $L$-Lipschitz continuous, and $\beta$-strongly dissipative, then $\tilde{g}_x$ is a bijection on $\mathbb{R}^{n_y}$, $\tilde{g}_x^{-1} : \mathbb{R}^{n_y} \to \mathbb{R}^{n_y}$ is $\frac{1}{\beta}$-Lipschitz continuous, and $\beta^2$-strongly dissipative.

### 2.2. Heterogeneous multiscale method.

The heterogeneous multiscale method (HMM) is a general strategy for multiscale problems [1, 9]. It makes use of two solvers: a macroscopic solver and a microscopic solver. Let us consider the system (2.1). As a macroscopic solver, a conventional explicit ODE solver is chosen to evolve (2.3). For example, take the forward Euler method with a time step $\Delta t$ as the macroscopic solver, which can be expressed as

$$
\begin{align*}
 x_{n+1} &= x_n + \Delta t F(x_n).
\end{align*}
$$

To evaluate $F(x_n)$, a microscopic solver is chosen to resolve the microscopic scale. In the case of the forward Euler method with a time step $\delta t$, one gets that

$$
\begin{align*}
 (2.6a) \quad y_{n,m+1} &= y_{n,m} + \frac{\delta t}{\varepsilon} g(x_n, y_{n,m}), \quad m = 0, 1, \ldots, M - 1, \\
 (2.6b) \quad y_{n,0} & \text{ suitably chosen.}
\end{align*}
$$

Then one can estimate $F(x_n)$ by

$$
F(x_n) \approx \sum_{m=0}^{M} K_{m,M} f(x_n, y_{n,m}),
$$

where the weights $\{K_{m,M}\}$ should satisfy the constraint $\sum_{m=0}^{M} K_{m,M} = 1$. As suggested in [9], for dissipative systems, one can choose the weights as

$$
K_{m,M} = 0, \quad m = 0, 1, \ldots, M - 1, \\
K_{M,M} = 1.
$$

In other words, one may estimate that $F(x_n) = f(x_n, \gamma(x_n)) \approx f(x_n, y_{n,M})$. In this situation, the microscopic solver (2.6) can be regarded as a nonlinear solver for the equation $g(x_n, y) = 0$ with respect to $y$.

### 3. Models.

In this section, we present our high-order correction models of the limiting equation (2.3) and analyze their properties. We begin with asymptotic approximation to the invariant manifold and then design an iterative formula to generate high-order correction models automatically. The modeling error can be reduced to $O(\varepsilon^{k+1})$ in the $k$th-order correction model.
3.1. Invariant manifold. To begin with, we introduce the concept of invariant manifold [25]. Assuming that there exists an invariant set $S_{\varepsilon}$ of (2.1), and that it can be represented as a smooth graph over $x$, namely, there exists a function $\Gamma: \mathbb{R}^{n_x} \times (0, \varepsilon_0] \to \mathbb{R}^{n_x}$ that is differentiable with respect to $x$, such that
\[ S_{\varepsilon} = \{(x, y): y = \Gamma(x, \varepsilon), \ x \in \mathbb{R}^{n_x}\}, \ \forall \varepsilon \in (0, \varepsilon_0]. \]
This implies that
\[ g(x, \Gamma(x, \varepsilon)) = \varepsilon \nabla_x \Gamma(x, \varepsilon) f(x, \Gamma(x, \varepsilon)), \ \forall x \in \mathbb{R}^{n_x}. \]
The equation (3.1) plays a central role in our discussions. It can be proved under some appropriate conditions that $S_{\varepsilon}$ is a global attractor of the system (2.1), that is, for any initial values,
\[ \lim_{t \to +\infty} |y(t) - \Gamma(x(t), \varepsilon)| = 0. \]

**Proposition 3.1.** Suppose that $\nabla_y f(x, y)$ and $\nabla_x \Gamma(x, \varepsilon)$ are bounded, then $S_{\varepsilon}$ is a global attractor of the system (2.1) for sufficiently small $\varepsilon$.

**Proof.** Assuming that $|\nabla_y f(x, y)| \leq C$ and $|\nabla_x \Gamma(x, \varepsilon)| \leq C$. Let $z(t) = y(t) - \Gamma(x(t), \varepsilon)$. By Assumption 2.2, one gets that
\[
\frac{1}{2} \frac{d|z|^2}{dt} = \langle z, \frac{dz}{dt} \rangle = \left\langle y - \Gamma(x, \varepsilon), \frac{1}{\varepsilon} g(x, y) - \nabla_x \Gamma(x, \varepsilon) f(x, y) \right\rangle
\]
\[
= \left\langle y - \Gamma(x, \varepsilon), \frac{1}{\varepsilon} g(x, y) - \frac{1}{\varepsilon} g(x, \Gamma(x, \varepsilon)) \right\rangle
\]
\[
+ \left( y - \Gamma(x, \varepsilon), \nabla_x \Gamma(x, \varepsilon) f(x, \Gamma(x, \varepsilon)) - \nabla_x \Gamma(x, \varepsilon) f(x, y) \right) \leq \left( -\frac{\beta}{\varepsilon} + C^2 \right) |z|^2.
\]
This implies that $|z(t)|^2 \leq e^{-\frac{\beta}{2\varepsilon}t}|z(0)|^2$ when $0 < \varepsilon \leq \min \left\{ \frac{\beta}{2C^2}, \varepsilon_0 \right\}$, and then the proof is completed. \[ \square \]

Proposition 3.1 says that the trajectory of $(x(t), y(t))$ tends to the set $S_{\varepsilon}$ at an exponential rate. Later we refer to this type of properties as the attractive property. Since $S_{\varepsilon}$ is invariant, one obtains that, if the initial values lie on $S_{\varepsilon}$, then the trajectory of $(x(t), y(t))$ stays on $S_{\varepsilon}$ for any $t > 0$. At this time, one may use
\[ \frac{dX}{dt} = f(X, \Gamma(X, \varepsilon)) \]
rather than (2.1) to calculate the trajectory of $x(t)$. In other words, the system (2.1) can be decoupled. We refer to this type of properties as the decouplable property. It should be emphasized that Proposition 3.1 depends on the existence of $\Gamma(x, \varepsilon)$, however, the rest of this article does not depend on it.

As an example, we study the invariant manifold of the linearized equation of the system (2.1).

**Example 3.2.** We consider the following linear equation as a special case of the system (2.1):
\[
\begin{align*}
\begin{cases}
\frac{dx}{dt} = A_{11}x + A_{12}y + b_1, \\
\frac{dy}{dt} = \frac{1}{\varepsilon}(A_{21}x + A_{22}y + b_2),
\end{cases}
\end{align*}
\]
where $A_{11} \in \mathbb{R}^{n_x \times n_x}$, $A_{12} \in \mathbb{R}^{n_x \times n_y}$, $A_{21} \in \mathbb{R}^{n_y \times n_x}$, $A_{22} \in \mathbb{R}^{n_y \times n_y}$, $b_1 \in \mathbb{R}^{n_x}$, $b_2 \in \mathbb{R}^{n_y}$. We assume that $A_{22}$ is a negative definite matrix to satisfy Assumption 2.2.

Suppose that the function $\Gamma(x, \varepsilon)$ has a form of $\Gamma(x, \varepsilon) = Cx + d$, where $C = C(\varepsilon) \in \mathbb{R}^{n_x \times n_x}$ and $d = d(\varepsilon) \in \mathbb{R}^{n_y}$. By (3.1), one gets the following equations:
\[
\begin{align*}
\varepsilon CA_{12}C + \varepsilon CA_{11} - A_{22}C - A_{21} &= 0, \\
(A_{22} - \varepsilon CA_{12})d &= \varepsilon Cb_1 - b_2.
\end{align*}
\]
It is known that (3.5a) is an algebraic matrix Riccati equation [13, 28]. We can prove the well-posedness of (3.5) when $\varepsilon$ is sufficiently small. See Theorem A.1 in Appendix A.
3.2. Asymptotic approximation. In this part, we consider the asymptotic approximation to \( \Gamma(x, \varepsilon) \).

We calculate the first several terms in the formal asymptotic expansion, and then prove the attractive property and the decouplable property of this approximation.

3.2.1. Formal expansions. Suppose that \( \Gamma(x, \varepsilon) \) satisfies (3.1). We try formal expansions of the form

\begin{align}
(3.6a) & \quad \Gamma(x, \varepsilon) = \gamma_0(x) + \varepsilon \gamma_1(x) + \varepsilon^2 \gamma_2(x) + O(\varepsilon^3), \\
(3.6b) & \quad \nabla_x \Gamma(x, \varepsilon) = \nabla \gamma_0(x) + \varepsilon \nabla \gamma_1(x) + \varepsilon^2 \nabla \gamma_2(x) + O(\varepsilon^3).
\end{align}

By Assumption 2.2, we specify that \( \gamma_0(x) = \gamma(x) \). By Taylor’s expansion of \( g(x, y) \) at \( (x, \gamma(x)) \) and the formal expansion in (3.6a), one notices that the left-hand side of (3.1) can be written as

\[
(3.7) \quad g(x, \Gamma(x, \varepsilon)) = g(x, \gamma(x) + \varepsilon \gamma_1(x) + \varepsilon^2 \gamma_2(x) + O(\varepsilon^3))
\]

Similarly, by Taylor’s expansion of \( f(x, y) \) at \( (x, \gamma(x)) \) and the formal expansions in (3.6), one obtains that the right-hand side of (3.1) can be written as

\[
(3.8) \quad \varepsilon \nabla_x \Gamma(x, \varepsilon) f(x, \Gamma(x, \varepsilon))
\]

where \( G_y(x) = [G_y^i(x)]_{i,j=1}^{n_y} = \frac{\partial g}{\partial y^i}(x, \gamma(x)) \) and \( G_{yy}(x) = [G_{yy}^{i,j,k}(x)]_{i,j,k=1}^{n_y} = \frac{\partial^2 g}{\partial y^i \partial y^j}(x, \gamma(x)) \).

Remark 3.3. By taking gradient of both sides of (2.4), one obtains that

\[
(3.10) \quad G_x(x) + G_y(x) \nabla \gamma(x) = 0,
\]

where \( G_x(x) = [G_x^i(x)]_{i=1}^{n_x} = \frac{\partial f}{\partial x^i}(x, \gamma(x)) \) and \( G_{yy}(x) = [G_{yy}^{i,j,k}(x)]_{i=1}^{n_y} = \frac{\partial^2 f}{\partial x^i \partial x^j}(x, \gamma(x)) \). Therefore, one can obtain that

\[
\nabla \gamma(x) = -G_y(x)^{-1} G_x(x).
\]

This implies that \( \gamma_1, \nabla \gamma_1(x) \) and \( \gamma_2(x) \) can be rewritten as algebraic expressions of function values and derivatives of \( f(x, y) \) and \( g(x, y) \) at \( (x, \gamma(x)) \). Therefore, one can obtain that \( \gamma, \gamma_1 \) and \( \gamma_2 \) are sufficiently smooth. In addition, by Assumptions 2.1 and 2.2, and the expressions in (3.9), one can deduce that \( \nabla \gamma \in W^{K,\infty}, \gamma_1 \in W^{K,\infty} \) and \( \gamma_2 \in W^{K-1,\infty} \). (See Lemmas in Appendix C.1).
3.2.2. Properties. As an approximation to \( \Gamma(x, \varepsilon) \), the function \( \tilde{\Gamma}_2(x, \varepsilon) := \gamma(x) + \varepsilon \gamma_1(x) + \varepsilon^2 \gamma_2(x) \) should share similar properties with \( \Gamma(x, \varepsilon) \). Now we make the above statement rigorous. In this part, we let \( S^{(2)}_\varepsilon := \{(x, y) : y = \tilde{\Gamma}_2(x, \varepsilon), \ x \in \mathbb{R}^{n_x}\} \) and \( z(t) = y(t) - \tilde{\Gamma}_2(x(t), \varepsilon) \).

The attractive property that is parallel to Proposition 3.1 can be formulated as in Theorem 3.4, which says that the system goes quickly from arbitrary initial values into a small vicinity of the approximate invariant manifold \( S^{(2)}_\varepsilon \).

**Theorem 3.4.** There exists a constant \( C > 0 \) independent of \( \varepsilon \) such that
\[
|z(t)|^2 \leq C\varepsilon^6 + e^{-\frac{2\varepsilon t}{3}}|z(0)|^2,
\]
for sufficiently small \( \varepsilon \). In particular, as long as \( t \) is sufficiently large, then \( |z(t)| = O(\varepsilon^3) \).

**Proof.** By Taylor’s expansion of \( f(x, y) \) and \( g(x, y) \) at \( (x, \gamma(x)) \), one gets that
\[
\begin{align*}
\frac{1}{\varepsilon}g(x, \tilde{\Gamma}_2(x, \varepsilon)) - \nabla_x \tilde{\Gamma}_2(x, \varepsilon)f(x, \tilde{\Gamma}_2(x, \varepsilon)) & = G_y(x) (\gamma_1(x) + \varepsilon \gamma_2(x)) + \frac{1}{2} \varepsilon \sum_{j,k=1}^{n_y} \left( G^{i,j,k}_{yy} \gamma^i_1(x) \gamma^j_1(x) \right)_{i=1}^{n_y} \\
& - (\nabla \gamma(x) + \varepsilon \nabla \gamma_1(x)) (F(x) + \varepsilon F_y(x) \gamma_1(x)) + O(\varepsilon^2) \\
& = (G_y(x) \gamma_1(x) - \nabla \gamma(x) F(x)) \\
& + \varepsilon \left( G_y(x) \gamma_2(x) + \frac{1}{2} \sum_{j,k=1}^{n_y} \left( G^{i,j,k}_{yy} \gamma^i_1(x) \gamma^j_1(x) \right)_{i=1}^{n_y} \\
& - \nabla \gamma(x) F_y(x) \gamma_1(x) - \nabla \gamma_1(x) F(x) \right) + O(\varepsilon^2)
\end{align*}
\]
(3.11)

where \( O(\varepsilon^2) \) can be controlled uniformly thanks to Assumption 2.1. By Assumption 2.2, Remark 3.3 and (3.11), there exists a constant \( C_1 > 0 \) such that
\[
\begin{align*}
\frac{1}{2} \frac{d|z|^2}{dt} & = \left\langle z, \frac{dz}{dt} \right\rangle = \left\langle y - \tilde{\Gamma}_2(x, \varepsilon), \frac{1}{\varepsilon}g(x, y) - \nabla_x \tilde{\Gamma}_2(x, \varepsilon)f(x, y) \right\rangle \\
& = \left\langle y - \tilde{\Gamma}_2(x, \varepsilon), \frac{1}{\varepsilon}g(x, y) - \frac{1}{\varepsilon}g(x, \tilde{\Gamma}_2(x, \varepsilon)) \right\rangle \\
& + \left\langle y - \tilde{\Gamma}_2(x, \varepsilon), \frac{1}{\varepsilon}g(x, \tilde{\Gamma}_2(x, \varepsilon)) - \nabla_x \tilde{\Gamma}_2(x, \varepsilon)f(x, \tilde{\Gamma}_2(x, \varepsilon)) \right\rangle \\
& + \left\langle y - \tilde{\Gamma}_2(x, \varepsilon), \nabla_x \tilde{\Gamma}_2(x, \varepsilon)f(x, \tilde{\Gamma}_2(x, \varepsilon)) - f(x, y) \right\rangle \\
& \leq \left( -\frac{\beta}{\varepsilon} + C_1 \right)|z|^2 + C_1 \varepsilon^2 |z| \leq -\frac{\beta}{2\varepsilon} |z|^2 + \frac{C_1^2}{\beta} \varepsilon^5,
\end{align*}
\]
where \( 0 < \varepsilon \leq \min \left\{ \frac{\beta}{2\gamma^2}, \varepsilon_0 \right\} \). Here the last inequality is due to the Cauchy-Schwarz inequality. By Gronwall’s inequality, one gets that
\[
|z(t)|^2 \leq \frac{2C_1^2}{\beta^2} \varepsilon^6 (1 - e^{-\frac{2\varepsilon t}{3}}) + e^{-\frac{2\varepsilon t}{3}}|z(0)|^2,
\]
which completes the proof.

Now we consider the decouplable property. Substituting \( \tilde{\Gamma}_2(x, \varepsilon) \) for \( \Gamma(x, \varepsilon) \) in (3.3), one obtains the following equation:
\[
\frac{dX_2}{dt} = f(X_2, \tilde{\Gamma}_2(X_2, \varepsilon)).
\]
(3.12)
One may surmise that, if the initial values are sufficiently close to $S^{(2)}_k$, then one may use (3.12) to approximate the trajectory of $x(t)$ in some sense. To be rigorous, we have Theorem 3.5.

**Theorem 3.5.** There exists a constant $C > 0$ independent of $\varepsilon$ such that

$$|x(t) - X_2(t)|^2 \leq e^{Ct} \left( |x(0) - X_2(0)|^2 + \varepsilon^6 + \frac{\varepsilon}{3} |z(0)|^2 \right),$$

for sufficiently small $\varepsilon$. In particular, if $|x(0) - X_2(0)| = O(\varepsilon^3)$ and $|z(0)| = O(\varepsilon^2)$, then $|x(t) - X_2(t)| = O(\varepsilon^3)$ for $t \sim O(1)$.

**Proof.** Since $\nabla_x f(x, y), \nabla_y f(x, y)$ and $\nabla_x \tilde{\Gamma}_2(x, \varepsilon)$ are all bounded, then there exists a constant $C_1 > 0$ such that

$$\left| \frac{d(x - X_2)}{dt} \right| = |f(x, y) - f(X_2, \tilde{\Gamma}_2(X_2, \varepsilon))|$$

$$\leq |f(x, z + \tilde{\Gamma}_2(x, \varepsilon)) - f(x, \tilde{\Gamma}_2(X_2, \varepsilon))| + |f(x, \tilde{\Gamma}_2(X_2, \varepsilon)) - f(X_2, \tilde{\Gamma}_2(X_2, \varepsilon))|$$

$$\leq C_1 |z| + C_1 |x - X_2|.$$ 

Then one obtains that

$$\frac{1}{2} \frac{d|x - X_2|^2}{dt} = \left< x - X_2, \frac{d(x - X_2)}{dt} \right>$$

$$\leq |x - X_2| \cdot \left| \frac{d(x - X_2)}{dt} \right| \leq C_1 |z| \cdot |x - X_2| + C_1 |x - X_2|^2.$$ 

Therefore, by Theorem 3.4 and Cauchy-Schwarz inequality, there exists a constant $C > 0$ such that

$$\frac{d|x - X_2|^2}{dt} \leq C( |x - X_2|^2 + \varepsilon^6 ) + e^{-\frac{2}{\varepsilon}} |z(0)|^2.$$ 

By Gronwall’s inequality,

$$|x(t) - X_2(t)|^2 \leq e^{Ct} |x(0) - X_2(0)|^2 + \varepsilon^6 e^{Ct - 1} + \frac{e^{Ct} - e^{-\frac{2}{\varepsilon} t}}{\frac{2}{\varepsilon} + C} |z(0)|^2,$$

which completes the proof.

**Remark 3.6.** Now we look back on what Theorems 3.4 and 3.5 tell us. Theorem 3.4 says that, no matter what the initial values are, the trajectory of $(x(t), y(t))$ always tends to a state where $|y - \tilde{\Gamma}_2(x, \varepsilon)| = O(\varepsilon^3)$ at an exponential rate. Theorem 3.5 says that, once the trajectory arrives at this state, one may use (3.12), which is not stiff, to approximate the trajectory of $x(t)$ in a finite time horizon with an accuracy of $O(\varepsilon^3)$. In the literature, this phenomenon is referred as an initial layer or a boundary layer [25, 26, 29, 8, 22]. This remark plays a guiding role in designing our numerical algorithms later.

**Remark 3.7.** The properties of $\tilde{\Gamma}_2(x, \varepsilon)$ are studied in this part. One may guess that $\tilde{\Gamma}_k(x, \varepsilon) := \sum_{j=0}^{k} \varepsilon^j \gamma_j(x)$ should have similar properties. However, it is expected that the expression of $\gamma_k(x)$ is very complex when $k$ is large. In addition, the evaluation of high-order derivatives is involved in the expressions of $\gamma_k(x)$. It is not convenient to conduct theoretical analysis or to design numerical algorithms at this time.

### 3.3. An iterative method

In this part, an iterative method is presented to approximate the invariant manifold $S_k$. We put forward an iterative formula, which can be used to produce a series of successively refined approximations to $\Gamma(x, \varepsilon)$. This method overcomes the difficulties in Remark 3.7 due to its concise form. It can be proved theoretically that this method is consistent with asymptotic approximation in some sense, and that the approximation accuracy reaches $O(\varepsilon^{k+1})$ after $k$ iteration steps.
3.3.1. An iterative formula. Inspired by (3.1), we propose the following fixed-point iterative formula to approximate \( \Gamma(x, \varepsilon) \):

\[
\begin{align*}
\Gamma_0(x, \varepsilon) &= \gamma(x), \\
g(x, \Gamma_{k+1}(x, \varepsilon)) &= \varepsilon \nabla_x \Gamma_k(x, \varepsilon) f(x, \Gamma_k(x, \varepsilon)), \quad k = 0, 1, 2, \ldots
\end{align*}
\]

Remark 2.3 implies the existence and uniqueness of the solution \( \Gamma_{k+1}(x, \varepsilon) \) of (3.13b), since \( g(x, \cdot) \) is Lipschitz continuous and strongly dissipative. Using the notations in Remark 2.3, one can write (3.13b) as

\[
\Gamma_{k+1}(x, \varepsilon) = \tilde{g}_k^{-1}(\varepsilon \nabla_x \Gamma_k(x, \varepsilon) f(x, \Gamma_k(x, \varepsilon))).
\]

3.3.2. Relationships with asymptotic approximation. In this part, we study the relationships between the iterative formula (3.13) and asymptotic approximation. It can be proved that the iterative formula can produce approximations in (3.9) in the first two iteration steps. The proof of Theorem 3.8 can be found in Appendix B.

Theorem 3.8. We have the following conclusions:

\[
\begin{align*}
|\Gamma_1(x, \varepsilon) - \gamma(x) - \varepsilon \gamma_1(x)| &= O(\varepsilon^2), \\
|\nabla_x \Gamma_1(x, \varepsilon) - \nabla \gamma(x) - \varepsilon \nabla \gamma_1(x)| &= O(\varepsilon^2), \\
|\Gamma_2(x, \varepsilon) - \gamma(x) - \varepsilon \gamma_1(x) - \varepsilon^2 \gamma_2(x)| &= O(\varepsilon^3),
\end{align*}
\]

where the bounds can be uniformly controlled in \( x \in \mathbb{R}^{n_*} \). In other words,

\[
\begin{align*}
\|\Gamma_1(\cdot, \varepsilon) - \gamma - \varepsilon \gamma_1\|_{1, \infty} &= O(\varepsilon^2), \\
\|\Gamma_2(\cdot, \varepsilon) - \gamma - \varepsilon \gamma_1 - \varepsilon^2 \gamma_2\|_{0, \infty} &= O(\varepsilon^3).
\end{align*}
\]

3.3.3. High-order approximation and convergence. We prove in Theorem 3.8 that the iterative formula (3.13) matches the formal expansions in the first two iteration steps. As for high-order approximation, it should be tedious to prove similar results due to the complex expressions of \( \gamma_k(x) \) when \( k \) is large. However, we can get rid of the specific expressions of \( \gamma_k(x) \) and prove the attractive property and the decouplable property that are parallel to Theorems 3.4 and 3.5. Proofs of the following two theorems can be found in Appendix C. The interpretations for these properties are similar to Remark 3.6. In this part, we let \( z_k(t) = y(t) - \Gamma_k(x(t), \varepsilon) \) and let \( X_k \) be defined as the solution of

\[
\frac{dX_k}{dt} = f(X_k, \Gamma_k(X_k, \varepsilon)).
\]

Theorem 3.9. For any \( k = 0, 1, \ldots, K \) and for any \( A \in (0, 2\beta) \), there exists a constant \( C_k > 0 \) such that

\[
|z_k(t)|^2 \leq C_k \varepsilon^{2k+2} e^{-\frac{\beta}{4} |z_k(0)|^2},
\]

where \( C_k \) is dependent on \( k \) and independent of \( \varepsilon \). In particular, as long as \( t \) is sufficiently large, then \( |z_k(t)| = O(\varepsilon^{k+1}) \).

Theorem 3.10. For any \( k = 0, 1, \ldots, K \), there exists a constant \( C_k > 0 \) dependent on \( k \) and independent of \( \varepsilon \) such that

\[
|x(t) - X_k(t)|^2 \leq e^{C_k t} \left( |x(0) - X_k(0)|^2 + \varepsilon^{2k+2} + \frac{C_k \varepsilon}{\beta} |z_k(0)|^2 \right).
\]

In particular, if \( |x(0) - X_k(0)| = O(\varepsilon^{k+1}) \) and \( |z_k(0)| = O(\varepsilon^{k+1}) \), then \( |x(t) - X_k(t)| = O(\varepsilon^{k+1}) \) for \( t \sim O(1) \).

Now we consider using the iterative formula (3.13) on the linearized equation (3.4). One may notice that (3.4) does not satisfy Assumption 2.1 since \( f(x, y) \) in this case is not bounded. However, we can still prove similar results that the iterative formula (3.13) improves the approximation accuracy. Actually, we can also prove the convergence of (3.13) in this case.
Example 3.11. We continue considering the linear equation (3.4) in Example 3.2. By Theorem A.1, there exist uniform bounded solutions \((C^*, d^*)\) to (3.5) for sufficiently small \(\varepsilon\). Suppose that \(\Gamma_k(x, \varepsilon) = C_k x + d_k\), where \(C_k = C_k(\varepsilon) \in \mathbb{R}^{n_x \times n_x}\) and \(d_k = d_k(\varepsilon) \in \mathbb{R}^{n_x}\). By (3.13), the iterative formula for \(C_k\) and \(d_k\) can be given as

\[
\begin{align*}
C_0 &= -A_{22}^{-1} A_{21}, \quad d_0 = -A_{22}^{-1} b_2, \\
C_{k+1} &= -A_{22}^{-1} A_{21} + \varepsilon A_{22}^{-1} C_k A_{11} + \varepsilon A_{22}^{-1} C_k A_{12} C_k, \\
d_{k+1} &= -A_{22}^{-1} b_2 + \varepsilon A_{22}^{-1} C_k b_1 + \varepsilon A_{22}^{-1} C_k A_{12} d_k.
\end{align*}
\]

Therefore, one can deduce that

\[
\begin{align*}
C_{k+1} - C^* &= \varepsilon A_{22}^{-1} C_k(\varepsilon - C^*) A_{11} + \varepsilon A_{22}^{-1} C_k A_{12}(C_k - C^*) + \varepsilon A_{22}^{-1}(C_k - C^*) A_{12} C^*, \\
d_{k+1} - d^* &= \varepsilon A_{22}^{-1}(C_k - C^*) b_1 + \varepsilon A_{22}^{-1} C_k A_{12}(d_k - d^*) + \varepsilon A_{22}^{-1}(C_k - C^*) A_{12} d^*.
\end{align*}
\]

First, we consider (3.16a). By the uniform boundedness of \(C^*\), there exists a constant \(M_1 > 0\) independent of \(\varepsilon\) and \(k\) such that

\[
\|C_{k+1} - C^*\| \leq \varepsilon M_1 \|C_k - C^*\| + \varepsilon M_1 \|C_k - C^*\|^2.
\]

If we take \(\varepsilon\) sufficiently small, for example, such that \(\varepsilon M_1(1 + \|C_0 - C^*\|) \leq \frac{1}{2}\), then one can obtain by (3.17) that

\[
\|C_{k+1} - C^*\| \leq \frac{1}{2} \|C_k - C^*\|, \quad \forall k = 0, 1, 2, \ldots.
\]

Therefore, the sequence \(\{C_k\}\) converges to \(C^*\) and is uniformly bounded in \(k\) and sufficiently small \(\varepsilon\). By (3.16a), there exists a constant \(M_2 > 0\) independent of \(\varepsilon\) and \(k\) such that

\[
\|C_{k+1} - C^*\| \leq \varepsilon M_2 \|C_k - C^*\|.
\]

By Theorem A.1, \(\|C_0 - C^*\| = O(\varepsilon)\). Therefore, \(\|C_k - C^*\| = O(\varepsilon^{k+1})\) for fixed \(k\).

By (3.16b), there exists a constant \(M_3 > 0\) independent of \(\varepsilon\) and \(k\) such that

\[
|d_{k+1} - d^*| \leq \varepsilon M_3 \|C_k - C^*\| + \varepsilon M_3 |d_k - d^*|,
\]

which indicates that \(|d_k - d^*|\) is uniformly bounded when \(\varepsilon\) is sufficiently small. Thus, \(\lim_{k \to \infty} |d_k - d^*| < +\infty\).

By taking upper limit of (3.18), one gets that

\[
(1 - \varepsilon M_3) \lim_{k \to \infty} |d_k - d^*| \leq 0.
\]

Therefore, when \(\varepsilon\) is sufficiently small, the sequence \(\{d_k\}\) converges to \(d^*\). By Theorem A.1, \(|d_0 - d^*| = O(\varepsilon)|\). Therefore, by (3.18), one obtains that \(|d_k - d^*| = O(\varepsilon^{k+1})\) for fixed \(k\).

In conclusion, we have already proven that \(C_k \to C^*\) and \(d_k \to d^*\) as \(k \to \infty\). Furthermore, for fixed \(k\), we have that \(\|C_k - C^*\| = O(\varepsilon^{k+1})\) and \(|d_k - d^*| = O(\varepsilon^{k+1})\).

4. Numerical Scheme. In this section, we develop numerical algorithms to implement the models in Section 3.

4.1. Basic framework and notations. Basically, our numerical scheme falls into the framework of HMM, which contains a microscopic solver to compute the steady state, and a macroscopic solver to evaluate the slow variables. As seen in Remark 3.6, the numerical simulations can be divided into two stages:

- the first stage: solving the coupled system (2.1) in the initial layer by a coupled solver until \(|z_k(t) - y_k(x(t), \varepsilon)|\) is sufficiently small;
- the second stage: using the HMM-type algorithms developed later to solve the decoupled system (3.15).

Briefly, the HMM-type algorithms contain two parts:

- approximating the invariant manifold, i.e., calculating \(\Gamma_k(x, \varepsilon)\) by a microscopic solver;

...
• solving the decoupled system of the slow variables by a macroscopic solver.

In our numerical scheme, we need to calculate $\Gamma_k(x, \varepsilon)$, as mentioned before. Let $\hat{\Gamma}_k(x, \varepsilon)$ be the numerical approximation to $\Gamma_k(x, \varepsilon)$. Hereinafter, we denote the algorithms, where $\Gamma_k(x, \varepsilon)$ is needed, by HMMk. Given a grid \{t_n\}, let $(x_n, y_n)$ be the numerical approximation to $(x(t_n), y(t_n))$.

In the first stage, we solve the coupled system (2.1) numerically on the grid \(\{t_n = n\Delta t_c\}_{n=0}^{N_c}\) with $N_c\Delta t_c = T_c$, where $\Delta t_c$ is the time step size of the coupled solver and $N_c$ can be determined by the criterion in Remark 4.1. One may choose an explicit one-step scheme as the coupled solver, which can be written as 2

\[
(x_{n+1}, y_{n+1}) = (x_n, y_n) + \Delta t_c \phi_c ((x_n, y_n), (f, g/\varepsilon), \Delta t_c), \quad n = 0, 1, \ldots, N_c - 1.
\]

In the second stage, we solve the decoupled system (3.15) numerically with initial value $x_{N_c}$ on the grid \(\{t_n = T_c + (n - N_c)\Delta t\}_{n=N_c}^{N}\) with $(N - N_c)\Delta t = T - T_c$, where $\Delta t$ is the time step size of the macroscopic solver. Similarly, we may choose an explicit one-step scheme as the macroscopic solver:

\[
x_{n+1} = x_n + \Delta t \phi_d(x_n, f(\cdot, \hat{\Gamma}_k(\cdot, \varepsilon)), \Delta t), \quad n = N_c, N_c + 1, \ldots, N - 1.
\]

In our numerical scheme, we may need to solve the equation

\[
g(\bar{x}, \bar{y}) = \varepsilon h
\]

with respect to $\bar{y}$, where $h$ is a given quantity which may depend on $\bar{x}$. Remark 2.3 ensures the existence and uniqueness of the solution of (4.1). Let us denote the solution by $\tilde{y}_\varepsilon^{-1}(\varepsilon h)$. Consider the following ODE with respect to $\bar{y}$

\[
\frac{d\bar{y}}{dt} = \frac{1}{\varepsilon} g(\bar{x}, \bar{y}) - h,
\]

whose stationary point is exactly $\tilde{y}_\varepsilon^{-1}(\varepsilon h)$. The microscopic solver solves (4.2) numerically:

\[
y_{m+1} = \tilde{y}_m + \delta t \phi_m(\tilde{y}_m, g(\bar{x}, \cdot)/\varepsilon - h, \delta t), \quad m = 0, 1, \ldots, M - 1,
\]

$\tilde{y}_0$ suitably chosen,

where $\tilde{y}_m$ is short for $\tilde{y}_m(\bar{x}, h)$, $\delta t$ is the time step size and $M$ is number of steps in the microscopic solver. One may estimate $\tilde{y}_\varepsilon^{-1}(\varepsilon h)$ by $\tilde{y}_M(\bar{x}, h)$. We will discuss the selection of the initial value $\tilde{y}_0$ in Remark 4.4.

4.2. Initial layer. In the initial layer $[0, T_c]$, i.e., the first stage of simulation, the system tends to the invariant manifold quickly. According to Theorem 3.10, the terminal time $T_c$ of the coupled solver should be taken such that

\[
|g(T_c) - \Gamma_k(x(T_c), \varepsilon)| = O(\varepsilon^{k+\frac{1}{2}}).
\]

By Theorem 3.9, $T_c$ should be of order $O(\varepsilon \log \frac{1}{\varepsilon})$ for fixed initial value and $k$. This indicates that the coupled solver is only needed for a short time.

Remark 4.1. It is a subtle problem to determine $T_c$ in numerical simulations. Here we present a possible empirical criterion inspired by Theorem 3.9: if

\[
n \equiv 0 \mod n_p
\]

\[
|y_n - \hat{\Gamma}_k(x_n, \varepsilon)| \geq \mu |y_{n-n_p} - \hat{\Gamma}_k(x_{n-n_p}, \varepsilon)|,
\]

for some positive integer $n$, where $n_p \in \mathbb{N} \setminus \{0\}$ are given beforehand, then terminate the coupled solver and let $N_c$ be $n$. We let $\mu = \exp \left(-\frac{\beta}{\varepsilon} n_p \Delta t_c\right)$, where $-\beta < 0$ is an estimation of the upper bound of the eigenvalues of $\frac{\partial g}{\partial y}(x, y)$. We calculate $\hat{\Gamma}_k$ per $n_p$ steps in order to reduce computational cost. In our numerical experiments, we set $n_p = 10$.

\[\text{Notice that an explicit one-step scheme for the ODE: } \frac{dz}{dt} = h(z) \text{ can be written in the form of } z_{n+1} = z_n + \Delta t \phi(z_n, h, \Delta t).\]
4.3. Approximation to the invariant manifold. In this part, we present several numerical approaches to approximating \( \Gamma_k(x, \varepsilon) \).

4.3.1. A naive approach. Remark 3.3 tells us that \( \gamma_1(x) \) and \( \gamma_2(x) \) can be rewritten as expressions of function values and derivatives of \( f(x, y) \) and \( g(x, y) \) at \((x, \gamma(x))\). In addition, \( \gamma(x) \) can be approximated by

\[
\gamma(x) \approx \tilde{y}_{MM}(x, 0).
\]

Therefore, \( \Gamma_k(x, \varepsilon) \) can be approximated according to the expressions (3.9) when \( k = 0, 1, 2 \). However, these expressions are too complicated. In this part, we would like to design an algorithm that is easy to implement. The algorithm is based on the analytical expressions in (3.9) and it requires to evaluate the Jacobian matrix of \( g(x, y) \).

First, we notice by (3.9b) and (3.10) that

\[
\gamma_1(x) = -G_y(x)^{-2}G_x(x)F(x).
\]

By (3.9), one can obtain that

\[
\Gamma_2(x, \varepsilon) = \gamma_0(x) + \varepsilon \gamma_1(x) + \varepsilon^2 \gamma_2(x) + \mathcal{O}(\varepsilon^3)
\]

\[
= \gamma(x) + \varepsilon G_y(x)^{-1} (\nabla \gamma(x) + \varepsilon \nabla \gamma_1(x)) f(x, \gamma(x) + \varepsilon \gamma_1(x))
\]

\[
- \frac{1}{2} \varepsilon^2 G_y(x)^{-1} \left[ \sum_{j,k=1}^{n_y} G_{yy}^{j,k} \gamma'_1(x)^j \gamma'_1(x)^k \right]_{i=1}^{n_y} + \mathcal{O}(\varepsilon^3).
\]

Now we consider how the terms in (4.5) are evaluated. One can notice that

\[
(\nabla \gamma(x) + \varepsilon \nabla \gamma_1(x)) f(x, \gamma(x) + \varepsilon \gamma_1(x))
\]

\[
= \lim_{\tau \to 0} \frac{\gamma(x + F_1(x)\tau, \gamma_1(x) + \varepsilon \gamma_1(x)) - \gamma(x) - \varepsilon \gamma_1(x)}{\tau},
\]

where \( F_1(x) := f(x, \gamma(x) + \varepsilon \gamma_1(x)) \). Therefore, numerical derivatives can be used to approximate this term, that is,

\[
(\nabla \gamma(x) + \varepsilon \nabla \gamma_1(x)) f(x, \gamma(x) + \varepsilon \gamma_1(x)) \approx \frac{\Delta_y \gamma_1(x)}{\tau},
\]

where \( \Delta_y \gamma = \gamma(x + F_1(x)\tau, \gamma_1(x) + \varepsilon \gamma_1(x)) - \gamma(x) - \varepsilon \gamma_1(x) \) with \( \tau \) suitably chosen. Besides, Taylor’s expansion of \( g(x, y) \) at \((x, \gamma(x))\) yields that

\[
g(x, \gamma(x) + \varepsilon \gamma_1(x)) = \varepsilon G_y(x) \gamma_1(x) + \frac{1}{2} \varepsilon^2 \left[ \sum_{j,k=1}^{n_y} G_{yy}^{j,k} \gamma'_1(x)^j \gamma'_1(x)^k \right]_{i=1}^{n_y} + \mathcal{O}(\varepsilon^3).
\]

By (4.5), (4.6) and (4.7), one can obtain that

\[
\Gamma_2(x, \varepsilon) \approx \gamma(x) + \varepsilon \gamma_1(x) + G_y(x)^{-1} \left( \frac{\Delta_y \gamma_1(x)}{\tau} - g(x, \gamma(x) + \varepsilon \gamma_1(x)) \right),
\]

where \( \gamma(x) \) and \( \gamma_1(x) \) can be approximated by (4.3) and (4.4), respectively.

4.3.2. Based on the iterative formula. Now we would like to utilize the iterative formula (3.13) to design an high-order HMM-type algorithm.

In order to obtain \( \Gamma_k(x, \varepsilon) \), we need to approximate \( \nabla_x \Gamma_{k-1}(x, \varepsilon) f(x, \Gamma_{k-1}(x, \varepsilon)) \). Actually, this term is the directional derivative of \( \Gamma_{k-1}(x, \varepsilon) \) along \( f(x, \Gamma_{k-1}(x, \varepsilon)) \). Similar to what we did previously in Subsection 4.3.1, we notice that

\[
\nabla_x \Gamma_{k-1}(x, \varepsilon) f(x, \Gamma_{k-1}(x, \varepsilon))
\]

\[
= \lim_{\tau \to 0} \frac{\Gamma_{k-1}(x + f(x, \Gamma_{k-1}(x, \varepsilon))\tau, \varepsilon) - \Gamma_{k-1}(x, \varepsilon)}{\tau}.
\]
Therefore, one may use numerical derivative to approximate this term, that is,
\[
\nabla_x \Gamma_{k-1}(x, \varepsilon) f(x, \Gamma_{k-1}(x, \varepsilon)) \approx \frac{\Delta y + \gamma}{\tau},
\]
where \(\Delta y = \Gamma_{k-1}(x + f(x, \Gamma_{k-1}(x, \varepsilon))\tau, \varepsilon) - \Gamma_{k-1}(x, \varepsilon)\) with \(\tau\) suitably chosen. Then we need to solve an equation in the form of (4.1), whose solution can be approximated by the microscopic solver.

**Remark 4.2.** Using the iterative formula, we can obtain high-order \(\Gamma_{k}(x, \varepsilon)\) by recursion. Actually, one can use the algorithm introduced in Subsection 4.3.1 to obtain \(\Gamma_{k}(x, \varepsilon)\) where \(k \geq 3\) by recursion in a similar way.

### 4.3.3. Summary and several remarks
We summarize the algorithms introduced in Subsections 4.3.1 and 4.3.2 in Algorithms 4.1 and 4.2, respectively.

**Algorithm 4.1** Approximating \(\Gamma_{k}(x, \varepsilon)\) using the methods in Subsection 4.3.1.

```plaintext
function HMMtype1(x, \varepsilon, k)
    if k equals to 0 then
        \(\hat{\gamma}_0(x, \varepsilon) \leftarrow y_M(x, 0)\);
        return \(\hat{\gamma}_0(x, \varepsilon)\);
    else if k equals to 1 then
        \(\hat{\gamma}(x) \leftarrow y_M(x, 0)\);
        \(\hat{\gamma}_1(x)\) according to (4.4);
        \(\hat{\Gamma}_1(x, \varepsilon) \leftarrow \hat{\gamma}(x) + \varepsilon \hat{\gamma}_1(x)\);
        return \(\hat{\Gamma}_1(x, \varepsilon)\);
    else if k equals to 2 then
        \(\hat{\gamma}(x) \leftarrow y_M(x, 0)\) and \(\hat{\mathcal{G}}(x) \leftarrow \frac{\partial g}{\partial y}(x, \hat{\gamma}(x))\);
        \(\hat{\gamma}_1(x)\) according to (4.4);
        \(\hat{\Gamma}_1(x, \varepsilon) \leftarrow \hat{\gamma}(x) + \varepsilon \hat{\gamma}_1(x)\);
        \(\hat{F}_1(x) \leftarrow f(x, \hat{\Gamma}_1(x, \varepsilon))\);
        \(\hat{\Gamma}_2(x, \varepsilon) \leftarrow \hat{\Gamma}_1(x, \varepsilon) + \hat{\mathcal{G}}(x)^{-1} \left( \varepsilon \hat{F}_1(x, \hat{\Gamma}_2(x, \varepsilon)) - g(x, \hat{\Gamma}_1(x, \varepsilon)) \right)\);
        return \(\hat{\Gamma}_2(x, \varepsilon)\);
    else
        \(\hat{\Gamma}_{k-1}(x, \varepsilon) \leftarrow \text{HMMtype1}(x, \varepsilon, k - 1)\);
        \(\hat{F}_{k-1}(x) \leftarrow f(x, \hat{\Gamma}_{k-1}(x, \varepsilon))\);
        \(\hat{\Gamma}_{k-1}(x + \hat{F}_{k-1}(x)\tau, \varepsilon) \leftarrow \text{HMMtype1}(x + \hat{F}_{k-1}(x)\tau, \varepsilon, k - 1)\);
        \(\hat{\Gamma}_k(x, \varepsilon) \leftarrow y_M(x, \hat{\Gamma}_{k-1}(x + \hat{F}_{k-1}(x)\tau, \varepsilon) - \hat{\Gamma}_{k-1}(x, \varepsilon))\);
    end if
end function
```

**Remark 4.3.** These two algorithms are recursive algorithms. In order to evaluate \(\hat{\Gamma}_k(x, \varepsilon)\) for one time, Algorithm 4.2 needs to call the microscopic solver for \((2^{k+1} - 1)\) times, while Algorithm 4.1 needs one time if \(k \leq 1\), and \((3 \times 2^{k-2} - 1)\) times otherwise. One can notice that Algorithm 4.1 calls the microscopic solver for fewer times than Algorithm 4.2, at the expense of computing the Jacobian matrix of \(g(x, y)\). The computation cost increases exponentially as \(k\) increases. In addition, a larger \(k\) may lead to more accumulations of numerical error (See Remark 5.5).

**Remark 4.4.** Another advantage of high-order HMM is that it can give a better estimation of the fast variable \(y\) at the next time step, as the initial value of the microscopic solver. In both algorithms, when calculating \(\hat{\Gamma}_k(x, \varepsilon)\), we need to approximate the directional derivative of \(\Gamma_{k-1}(x, \varepsilon)\) along...
We have the following result. The proof of Theorem 5.1 can be found in Appendix C.

Algorithm 4.2 Approximating $\Gamma_k(x, \varepsilon)$ using the methods in Subsection 4.3.2.

function HMMType2$(x, \varepsilon, k)$
if $k$ equals to 0 then
  $\hat{\Gamma}_0(x, \varepsilon) \leftarrow \hat{y}_M(x, 0)$;
  return $\hat{\Gamma}_0(x, \varepsilon)$;
else
  $\hat{\Gamma}_{k-1}(x, \varepsilon) \leftarrow$ HMMType2$(x, \varepsilon, k - 1)$;
  $\hat{F}_{k-1}(x) \leftarrow f(x, \hat{\Gamma}_{k-1}(x, \varepsilon))$;
  $\hat{\Gamma}_{k}(x, \varepsilon) \leftarrow \hat{y}_M \left(x, \frac{\Gamma_{k-1}(x + \hat{F}_{k-1}(x), \varepsilon) - \Gamma_{k-1}(x, \varepsilon)}{\tau} \right)$;
  return $\hat{\Gamma}_k(x, \varepsilon)$;
end if
end function

$f(x, \Gamma_{k-1}(x, \varepsilon))$. For example, in Algorithm 4.2 at a microscopic time step $t = t_n$, we need $\frac{\Delta y}{\varepsilon}$ to approximate $\nabla_x \Gamma_{k-1}(x_n, \varepsilon) f(x_n, \Gamma_{k-1}(x_n, \varepsilon))$. At the next time step $t = t_{n+1}$, one can use $\hat{\Gamma}_k(x_n, \varepsilon) + \frac{\Delta y}{\varepsilon} \Delta t$ as $y_{n+1}$, which may reduce sampling error. Similar strategies can be used in a Runge-Kutta type macroscopic solver.

Remark 4.5. In both algorithms, we use the forward difference formula to approximate the directional derivatives. We may use higher-order difference formulas for higher accuracy, for example, the central difference formula. See Remark 5.3.

5. Numerical Analysis. Now we present some results of numerical analysis on our algorithms. We focus on Algorithm 4.2. Some results here are also applicable to Algorithm 4.1.

As mentioned before, there are three main sources of errors of HMM, including modeling error, sampling error and truncation error of the macroscopic solver. We have proven that the modeling error can be reduced to $O(\varepsilon^{k+1})$. The truncation error of the macroscopic solver depends on what the macroscopic solver is. In classical HMM, sampling error mainly comes from the microscopic solver. Numerical analysis of sampling error in classical HMM can be found in [9]. In our algorithms, another source of sampling error is numerical derivatives. In addition, numerical error may accumulate in our recursive algorithms.

5.1. Numerical derivatives. Now we analyze the sampling error generated by the numerical derivatives directly. In this part, the round-off error and error from the microscopic solver is disregarded. In other words, we would like to analyze the error between $\Gamma_k(x, \varepsilon)$ and $\Gamma_k^{\text{df}}(x, \varepsilon)$, where $\Gamma_k(x, \varepsilon)$ and $\Gamma_k^{\text{df}}(x, \varepsilon)$ are defined as follows:

$$
\Gamma_0(x, \varepsilon) = \Gamma_0^{\text{df}}(x, \varepsilon) = \gamma(x).
$$

$$
g(x, \Gamma_{k+1}(x, \varepsilon)) = \varepsilon \nabla_x \Gamma_k(x, \varepsilon) f(x, \Gamma_k(x, \varepsilon)), \quad k \in \mathbb{N},
$$

$$
g(x, \Gamma_{k+1}^{\text{df}}(x, \varepsilon)) = \varepsilon \left( \frac{\Gamma_k^{\text{df}}(x + f(x, \Gamma_k^{\text{df}}(x, \varepsilon)))}{\tau} - \frac{\Gamma_k^{\text{df}}(x, \varepsilon)}{\tau} \right), \quad k \in \mathbb{N}.
$$

The last equality of (5.1) can also be written as

$$
\hat{\Gamma}_{k+1}^{\text{df}}(x, \varepsilon) = \hat{g}_x^{-1} \left( \varepsilon \left( \frac{\Gamma_k^{\text{df}}(x + f(x, \Gamma_k^{\text{df}}(x, \varepsilon)))}{\tau} - \frac{\Gamma_k^{\text{df}}(x, \varepsilon)}{\tau} \right) \right).
$$

We have the following result. The proof of Theorem 5.1 can be found in Appendix C.

**Theorem 5.1.** For any $k = 0, 1, \ldots, \left\lfloor \frac{L}{2} \right\rfloor$,

$$
\left\| \Gamma_k(\cdot, \varepsilon) - \Gamma_k^{\text{df}}(\cdot, \varepsilon) \right\|_{K - 2k, \infty} = O(\varepsilon \tau).
$$
Therefore, $\varepsilon k+1 = O(\frac{\varepsilon k}{\tau} + \varepsilon \tau)$. In this way, one can calculate that

$$e_0^d = 0, e_1^d = O(\varepsilon \tau), e_2^d = O(\varepsilon^2 + \varepsilon \tau), e_3^d = O(\frac{\varepsilon^3}{\tau} + \varepsilon^2 + \varepsilon \tau), \ldots.$$  

However, this is not a good estimate. For example, when $k = 2$, the modeling error turns out to be $O(\varepsilon^3)$, while the bound for the sampling error is $O(\varepsilon^2 + \varepsilon \tau)$. Actually, if we have some additional assumptions on the regularity of $f$ and $g$, then we can improve the bound for this type of error to $O(\varepsilon \tau)$.

**Remark 5.3.** In the spirit of Remark 4.5, we can use central difference formula rather than forward difference formula. Notice Item 2 in Lemma C.1, we can prove that for any $k = 0, 1, \ldots, \lfloor \frac{K}{2} \rfloor$,

$$\left\| \Gamma_k(\cdot, \varepsilon) - \hat{\Gamma}_k^d(\cdot, \varepsilon) \right\|_{K-3k, \infty} = O(\varepsilon \tau^2),$$

where $\hat{\Gamma}_k^d$ is replaced by central difference formula. The proof is exactly like that of Theorem 5.1.

### 5.2. Accumulation of numerical error

Due to the round-off error and error from the microscopic solver, one cannot obtain $\hat{\Gamma}_k^d(x, \varepsilon)$ exactly as in (5.1). This may lead to accumulation of numerical error. In this part, we aim to analyze the error between $\hat{\Gamma}_k^d$ and $\hat{\Gamma}_k^r$, where $\hat{\Gamma}_k^d$ is defined in (5.1), and $\hat{\Gamma}_k^r$ satisfies that

$$\left\| \hat{\Gamma}_k^d(\cdot, \varepsilon) - \hat{\Gamma}_k^r(\cdot, \varepsilon) \right\| = \eta_k, \quad k \in \mathbb{N}.$$  

**Theorem 5.4.** For any $k = 0, 1, \ldots, \lfloor \frac{K}{2} \rfloor$,

$$\left\| \hat{\Gamma}_k^r(\cdot, \varepsilon) - \hat{\Gamma}_k^d(\cdot, \varepsilon) \right\|_{0, \infty} = \mathcal{O} \left( \sum_{j=0}^{k} \frac{\varepsilon j}{\tau^{j-k}} \eta_k \right).$$

**Proof.** Let $e_k^d = \left\| \hat{\Gamma}_k^d(\cdot, \varepsilon) - \hat{\Gamma}_k^r(\cdot, \varepsilon) \right\|$. Notice that when $k = 0, 1, \ldots, \lfloor \frac{K}{2} \rfloor$, $\nabla \hat{\Gamma}_k^d(x, \varepsilon)$ is bounded
by Theorem 5.1. One can obtain by Remark 2.3 that
\[
\left| \hat{\Gamma}_{k+1}^t(x, \varepsilon) - \hat{\Gamma}_{k+1}^d(x, \varepsilon) \right| \\
\leq \left| \hat{\Gamma}_{k+1}^t(x, \varepsilon) - \hat{\Gamma}_{k+1}^d(x, \varepsilon) \right| \\
+ \left| \hat{\Gamma}_{k+1}^d(x, \varepsilon) - \hat{\Gamma}_{k+1}^t(x, \varepsilon) \right| \\
\leq O \left( \eta_{k+1} + \frac{\varepsilon}{\tau} \right).
\]
Therefore, \( e_{k+1}^t = O \left( \eta_{k+1} + \frac{\varepsilon}{\tau} c_k^t \right) \), and then the proof is completed by induction.

Remark 5.5. For fixed \( k \), let \( \eta = \max_{j=0,1,\ldots,k} \eta_j \). By Theorem 5.4, if \( \varepsilon = O(\tau) \), then
\[
\left\| \hat{\Gamma}_k^t(\cdot, \varepsilon) - \hat{\Gamma}_k^d(\cdot, \varepsilon) \right\|_{0, \infty} = O(\eta);
\]
if \( \tau = o(\varepsilon) \), then
\[
\left\| \hat{\Gamma}_k^t(\cdot, \varepsilon) - \hat{\Gamma}_k^d(\cdot, \varepsilon) \right\|_{0, \infty} = O \left( \frac{\varepsilon^k}{\eta} \right).
\]

5.3. Global error. In Subsections 5.1 and 5.2, we have analyzed the numerical error when calculating \( \Gamma_k(x, \varepsilon) \). Now we would like to figure out how it influences the global error. Let
\[
\kappa = \left\| \Gamma(x, \varepsilon) - \hat{\Gamma}(x, \varepsilon) \right\|_{0, \infty} < +\infty.
\]
We would like to compare the solutions of the following two ODEs:
\[
\frac{dX_k}{dt} = f(X_k, \Gamma_k(X_k, \varepsilon)),
\]
and
\[
\frac{d\hat{X}_k}{dt} = f(\hat{X}_k, \hat{\Gamma}_k(X_k, \varepsilon)).
\]
By Gronwall’s inequality and the boundedness of \( \nabla_x \Gamma_k(x, \varepsilon) \) when \( k = 0, 1, \ldots, K \) (See Corollary C.6), one can deduce the following proposition. By Proposition 5.6, one obtains that the order of global error between \( X_k(t) \) and \( \hat{X}_k(t) \) in a finite time horizon is the same as order of \( L^\infty \)-error between \( \Gamma_k(\cdot, \varepsilon) \) and \( \hat{\Gamma}_k(\cdot, \varepsilon) \), if \( X_k(0) = \hat{X}_k(0) \).

Proposition 5.6. For \( k = 0, 1, \ldots, K \), there exists a constant \( C > 0 \) such that
\[
|X_k(t) - \hat{X}_k(t)|^2 \leq e^{Ct} \left( |X_k(0) - \hat{X}_k(0)|^2 + \kappa^2 \right).
\]
6. Numerical Experiments. In this section, we perform numerical simulations on several examples to demonstrate numerical efficiency of our models and algorithms developed in the previous sections.

The numerical experiments are set up as follows. We conduct the simulations in the time interval $[0, T]$. We use the coupled solver in the interval $[0, T_c]$, where $T_c$ is determined by the criteria in Remark 4.1. The coupled solver utilizes the common 4th-order explicit Runge-Kutta scheme (RK4) with time step $\Delta t_c$. The HMM-type algorithms are used in the interval $[T_c, T]$. The macroscopic solver utilizes RK4 with time step size $\Delta t$. The microscopic solver utilizes the Forward Euler scheme (FE) with number of steps $M$ and the time step size $\delta t = \alpha \varepsilon$, where $\alpha$ is a given constant dependent on the problem. We compare the $L_2$-norm error of slow variable, that is, $|x(T) - x_N|$. In all numerical experiments, the initial values $(x_0, y_0)$ and the terminal time $T$ are specified to ensure the dissipativity of the system on $[0, T]$.

6.1. A naive example. In this part, we use a naive example to test the accuracy and efficiency of our algorithms.

Example 6.1. Let us consider the following example:

\[
\begin{aligned}
\frac{dx}{dt} &= y, \\
\frac{dy}{dt} &= \varepsilon (x - y), \\
x|_{t=0} &= x_0, \quad y|_{t=0} = y_0,
\end{aligned}
\]

with $x_0 = 1$, $y_0 = 2$, $T = 4$. The exact solution of this example is

\[
x(t) = \frac{-\lambda_2 x_0 + y_0}{\lambda_1 - \lambda_2} e^{\lambda_1 t} + \frac{\lambda_1 x_0 - y_0}{\lambda_1 - \lambda_2} e^{\lambda_2 t},
\]

where $\lambda_1 = -1 + \sqrt{1 + 4\varepsilon^2}$ and $\lambda_2 = -1 - \sqrt{1 + 4\varepsilon^2}$.

Parameters: $\varepsilon = 1.0 \times 10^{-5}$, $\tau = 1.0 \times 10^{-5}$, $M = 1$, $\alpha = 1.0$, $\Delta t_c = 1.0 \times 10^{-5}$, $\Delta t = 5.0 \times 10^{-3}$, $\hat{\beta} = 1$.

Algorithm 4.1 and the forward difference formula are adopted. We compare our HMM$k$ solvers with the coupled solver, with respect to the numerical error and the total computing time. To ensure fairness when comparing the accuracy of different HMM-type algorithms, we use the same $T_c$. In other words, we take $k = 2$ in Remark 4.1 for all the HMM-type algorithms. The numerical results are reported in Table 1.

| solver   | error      | time (s) | $T_c$     |
|----------|------------|----------|-----------|
| coupled  | 2.1832e-09 | 5.44     | 4.0e+00   |
| HMM0     | 2.1836e-03 | 0.02     | 4.0e-04   |
| HMM1     | 4.6017e-08 | 0.04     | 4.0e-04   |
| HMM2     | 2.3441e-09 | 0.09     | 4.0e-04   |

For one thing, our high order numerical homogenization method reduces the numerical error, compared with the classical HMM0 solver. For another thing, the HMM2 solver uses far less time than the coupled solver to reach roughly the same error. In this numerical example, the time cost of HMM-type algorithms is mainly due to the macroscopic solver, since here it is easy to compute $\gamma(x)$ by the microscopic solver. By this numerical experiment, we exhibit the accuracy and efficiency of our method.

6.2. Model validation. In the previous section, we have already proven that the modeling error of HMM$k$ method turns out to be $O(\varepsilon^{k+1})$. In this part, we would like to test and verify this modeling error estimate by numerical experiments. Let us consider the following three numerical examples. For each numerical example, we compare numerical error between numerical solutions and the reference solution.
Example 6.2. Enzyme reaction equation [5, 18]:

$$\begin{align*}
\frac{dx}{dt} &= -x + (x + c)y, \\
\frac{dy}{dt} &= \frac{1}{\varepsilon} (x - (x + 1)y), \\
x|_{t=0} &= x_0, \ y|_{t=0} = y_0,
\end{align*}$$

with $x_0 = 1$, $y_0 = 0$, $c = 0.5$, $T = 1$.

Parameters: $\tau = 1.0 \times 10^{-6}$, $M = 10$, $\alpha = 0.5$, $\Delta t_{\varepsilon} = 1.0 \times 10^{-5}$, $\hat{\beta} = 1.5$.

Algorithm 4.1 and the central difference formula are adopted. The reference solution is given by the coupled solver with time step size $\Delta t$. See Figure 1(b) for fixed $\varepsilon = 1.0 \times 10^{-2}$ and different $\varepsilon$. See Figure 1(b) for fixed $\varepsilon = 1.0 \times 10^{-2}$ and different $\Delta t$.

Example 6.3. Forced Van der Pol equation [16]:

$$\begin{align*}
\frac{dx^{(1)}}{dt} &= -y + a \sin(2\pi x^{(2)}), \\
\frac{dx^{(2)}}{dt} &= b, \\
\frac{dy}{dt} &= \frac{1}{\varepsilon} \left( y + x^{(1)} - \frac{1}{3} y^3 \right), \\
x|_{t=0} &= (x^{(1)}, x^{(2)})|_{t=0} = x_0, \ y|_{t=0} = y_0,
\end{align*}$$

with $x_0 = (3, 1)$, $y_0 = 1$, $a = 2$, $b = 1$, $T = 1$.

Parameters: $\tau = 1.0 \times 10^{-6}$, $M = 25$, $\alpha = 0.1$, $\Delta t_{\varepsilon} = 1.0 \times 10^{-5}$, $\hat{\beta} = 0.01$.

Algorithm 4.2 and the forward difference formula are adopted. The reference solution is given by the coupled solver with time step size $\Delta t_{\varepsilon}$. See Figure 2(b) for fixed $\Delta t = 1.0 \times 10^{-2}$ and different $\varepsilon$. See Figure 2(b) for fixed $\varepsilon = 1.0 \times 10^{-4}$ and different $\Delta t$.

Example 6.4. Cubic Chua’s model [7]:

$$\begin{align*}
\frac{dx^{(1)}}{dt} &= -dx^{(2)}, \\
\frac{dx^{(2)}}{dt} &= -ay + x^{(1)} + bx^{(2)}, \\
\frac{dy}{dt} &= \frac{1}{\varepsilon} (x^{(2)} - c_1 y^3 - c_2 y^2 - c_1 y), \\
x|_{t=0} &= (x^{(1)}, x^{(2)})|_{t=0} = x_0, \ y|_{t=0} = y_0,
\end{align*}$$

with $x_0 = (1, 1)$, $y_0 = 1$, $a = 0.7$, $b = 0.25$, $c_1 = 7$, $c_2 = 15$, $c_3 = 20$, $d = 1$, $T = 1$.

Parameters: $\tau = 1.0 \times 10^{-6}$, $M = 10$, $\alpha = 0.1$, $\Delta t_{\varepsilon} = 1.0 \times 10^{-5}$, $\hat{\beta} = 10$.

Algorithm 4.2 and the central difference formula are adopted. The reference solution is given by the coupled solver with time step size $\Delta t_{\varepsilon}$. See Figure 3(a) for fixed $\Delta t = 1.0 \times 10^{-2}$ and different $\varepsilon$. See Figure 3(b) for fixed $\varepsilon = 1.0 \times 10^{-2}$ and different $\Delta t$.

The results in Figures 1(a), 2(a), and 3(a) show the order of numerical error. By numerical investigation, the theoretical result that the modeling error of HMMk is of order $O(\varepsilon^{k+1})$ is verified. The results in Figures 1(b), 2(b), and 3(b) indicate whether the modeling error or the truncation error of macroscopic solver takes a dominant position in the numerical error.

6.3. Numerical derivative. It has been proven that the sampling error generated by numerical derivatives is $O(\varepsilon \tau)$, if the forward difference formula is adopted. As seen in Remark 5.3, when the central difference formula is adopted, this part of error turns out to be $O(\varepsilon^2)$. Let us consider the following numerical example.
(a) Different $\varepsilon$ and fixed $\Delta t$

(b) Different $\Delta t$ and fixed $\varepsilon$

Fig. 1. Numerical results for Example 6.2.

(a) Different $\varepsilon$ and fixed $\Delta t$

(b) Different $\Delta t$ and fixed $\varepsilon$

Fig. 2. Numerical results for Example 6.3.
Example 6.5. Van der Pol equation [30, 12]:
\[
\begin{align*}
\frac{dx}{dt} &= y, \\
\frac{dy}{dt} &= -\frac{1}{\varepsilon}((x^2 - 1)y + x), \\
x|_{t=0} &= x_0, \quad y|_{t=0} = y_0,
\end{align*}
\]
with \(x_0 = 4, y_0 = 2, T = 5\).

Parameters: \(M = 20, \alpha = 0.1, \Delta t_c = 1.0 \times 10^{-5}, \Delta t = 2.0 \times 10^{-2}, \beta = 3\).

Algorithm 4.2 is adopted. The reference solution is given by the coupled solver with time step size \(\Delta t_c\). We test the numerical error for different \(\tau\) and different \(\varepsilon\). See Figure 4(a) for the forward difference formula. See Figure 4(b) for the central difference formula.

From the numerical results, one can see that, when \(\tau\) is relatively large, the numerical error is approximately \(O(\varepsilon \tau)\) for the forward difference formula, and \(O(\varepsilon \tau^2)\) for the central difference formula. Therefore, the theoretical analysis in Subsection 5.1 is verified.

7. Conclusions. We proposed a high-order numerical homogenization method for the dissipative ordinary differential equations. We developed the correction models based on the asymptotic approximations and a novel iterative formula. The corresponding numerical algorithms are designed in the framework of the heterogeneous multiscale methods. We provide some theoretical analysis on our algorithms. By numerical investigation, not only the error estimates are verified, but also the efficiency of our methods is exhibited.

Acknowledgements. Zeyu Jin is supported by the Elite Undergraduate Training Program of School of Mathematical Sciences in Peking University. Ruo Li is partially supported by the National Key R&D Program of China (No. 2020YFA0712000) and the National Science Foundation in China (No. 11971041).

Appendix A. Well-posedness of (3.5) for Small \(\varepsilon\).

Theorem A.1. Under the assumptions in Example 3.2, for each \(M > \|A_{22}^{-1}A_{21}\|\), there exists \(\delta \in (0, \varepsilon_0]\), such that for each \(\varepsilon \in (0, \delta]\), there exists a unique solution \((C^*, d^*)\) to (3.5) such that \(\|C^*\| \leq M\). Furthermore, \(C^* + A_{22}^{-1}A_{21} = O(\varepsilon)\) and \(d^* + A_{22}^{-1}b_2 = O(\varepsilon)\).

Proof. First, we consider the equation (3.5a). It is easy to see that the solution of (3.5a) is the fixed point of the mapping
\[
\mathcal{T}: C \mapsto -A_{22}^{-1}A_{21} + \varepsilon A_{22}^{-1}CA_{11} + \varepsilon A_{22}^{-1}CA_{12}C.
\]
We define a set \(\mathcal{E} = \{C \in \mathbb{R}^{n_x \times n_x} : \|C\| \leq M\}\), where \(M > \|A_{22}^{-1}A_{21}\|\) is arbitrary. Let \(M_1 = \|A_{22}^{-1}\| (\|A_{11}\| + \|A_{12}\|)\). When \(C \in \mathcal{E}\), we have that
\[
\|TC\| \leq \|A_{22}^{-1}A_{21}\| + \varepsilon M_1 \|C\| + \varepsilon M_1 \|C\|^2 \leq \|A_{22}^{-1}A_{21}\| + \varepsilon M_1 \|M + M^2\|.
\]
We take \(\delta_1 = \min\left\{\varepsilon_0, \frac{M - \|A_{22}^{-1}A_{21}\|}{\varepsilon M_1 (M + M^2)}\right\} > 0\). For each \(\varepsilon \in (0, \delta_1]\), we have that \(\mathcal{T}: \mathcal{E} \to \mathcal{E}\). For each \(C, \tilde{C} \in \mathcal{E}\),
\[
\|TC - T\tilde{C}\| = \|A_{22}^{-1}(C - \tilde{C})A_{11} + \varepsilon A_{22}^{-1}(C - \tilde{C})A_{12}C + \varepsilon A_{22}^{-1}\tilde{C}A_{12}(C - \tilde{C})\|
\leq \varepsilon M_1 (1 + 2M) \|C - \tilde{C}\|.
\]
We take \(\delta_2 = \min\{\delta_1, \frac{1}{2M_1 (1 + 2M)}\} > 0\). Then for each \(\varepsilon \in (0, \delta_2]\), \(\mathcal{T}\) is a contraction mapping on \(\mathcal{E}\). Therefore, there exists a unique solution \(C^*\) to (3.5a) in \(\mathcal{E}\). We take \(\delta = \min\{\delta_2, \frac{1}{2M_1 M}\}\). For each \(\varepsilon \in (0, \delta]\),
\[
\|A_{22}^{-1}C^*A_{12}\| \leq \varepsilon M_1 M \leq \frac{\varepsilon}{\delta} < 1.
\]
Thus, \(A_{22} - \varepsilon C^*A_{12}\) is invertible. With \(C^*\) fixed, there exists a unique solution \(d^*\) to (3.5b) in \(\mathbb{R}^{n_y}\), and \(d^*\) is uniformly bounded in \(\varepsilon \in (0, \delta]\). Furthermore, we notice that
\[
C^* + A_{22}^{-1}A_{21} = \varepsilon (A_{22}^{-1}C^*A_{11} + A_{22}^{-1}C^*A_{12}C^*) = O(\varepsilon),
\]
\[
d^* + A_{22}^{-1}b_2 = \varepsilon (A_{22}^{-1}C^*A_{12}d^* + A_{22}^{-1}C^*b_1) = O(\varepsilon).
\]
Then the proof is completed. \(\square\)
(a) Different $\varepsilon$ and fixed $\Delta t$

(b) Different $\Delta t$ and fixed $\varepsilon$

Fig. 3. Numerical results for Example 6.4.

(a) Forward difference formula

(b) Central difference formula

Fig. 4. Numerical results for Example 6.5.
Appendix B. Proof of Theorem 3.8.

Proof of Theorem 3.8. By Remark 2.3, one can obtain that
\[
|\Gamma_1(x, \varepsilon) - \gamma(x) - \varepsilon \gamma_1(x)| \leq \frac{1}{\beta} |g(x, \Gamma_1(x, \varepsilon)) - g(x, \gamma(x) + \varepsilon \gamma_1(x))| \\
= \frac{1}{\beta} |\varepsilon \nabla \gamma(x) f(x, \gamma(x)) - g(x, \gamma(x) + \varepsilon \gamma_1(x))|.
\]

By (3.9b) and Taylor’s expansion of \(g(x, y)\) at \((x, \gamma(x))\),
\[
\varepsilon \nabla \gamma(x) f(x, \gamma(x)) - g(x, \gamma(x) + \varepsilon \gamma_1(x)) \\
= \varepsilon G_y(x) \gamma_1(x) - \left( g(x, \gamma(x)) + \varepsilon G_y(x) \gamma_1(x) + \mathcal{O}(\varepsilon^2) \right) \\
= \mathcal{O}(\varepsilon^2),
\]
where \(\mathcal{O}(\varepsilon^2)\) can be controlled uniformly thanks to Assumption 2.1. In other words, there exists a constant \(C_1 > 0\) such that \(|\varepsilon \nabla \gamma(x) f(x, \gamma(x)) - g(x, \gamma(x) + \varepsilon \gamma_1(x))| \leq C_1 \varepsilon^2\). Therefore,
\[
|\Gamma_1(x, \varepsilon) - \gamma(x) - \varepsilon \gamma_1(x)| \leq \frac{C_1}{\beta} \varepsilon^2,
\]
which completes the proof of (3.14a).

By the expression of \(\gamma_1(x)\) in (3.9b), one gets that
\[
(\text{B.1}) \\
g(x, \Gamma_1(x, \varepsilon)) = \varepsilon G_y(x) \gamma_1(x).
\]

For the sake of clarity, we consider the \(i\)-th component of (B.1), that is,
\[
(\text{B.2}) \\
g^i(x, \Gamma_1(x, \varepsilon)) = \varepsilon \sum_{k=1}^{n_y} \frac{\partial g^i}{\partial y^k}(x, \gamma(x)) \gamma_1^k(x).
\]

Taking the derivative of (B.2) with respect to \(x^j\), we obtain that
\[
\frac{\partial g^i}{\partial x^j}(x, \Gamma_1(x, \varepsilon)) + \sum_{k=1}^{n_y} \frac{\partial g^i}{\partial y^k}(x, \Gamma_1(x, \varepsilon)) \frac{\partial \Gamma_1^k}{\partial x^j}(x, \varepsilon) \\
= \varepsilon \sum_{k=1}^{n_y} \left( \frac{\partial^2 g^i}{\partial y^k \partial x^j}(x, \gamma(x)) + \sum_{\ell=1}^{n_y} \frac{\partial^2 g^i}{\partial y^k \partial y^{\ell}}(x, \gamma(x)) \frac{\partial \gamma_1^\ell}{\partial x^j}(x) \right) \gamma_1^k(x) \\
+ \varepsilon \sum_{k=1}^{n_y} \frac{\partial g^i}{\partial y^k}(x, \gamma(x)) \frac{\partial \gamma_1^k}{\partial x^j}(x).
\]

Actually (B.3) yields that \(\nabla_x \Gamma_1(x, \varepsilon)\) is uniformly bounded in \(\varepsilon \in (0, \varepsilon_0]\), since
\[
\nabla_x \Gamma_1(x, \varepsilon) = G_y(x)^{-1} A,
\]
where \(A = A(x, \varepsilon) = [A^{i,j}]_{i,j=1}^{n_y,n_y}, A^{i,j}\) is defined as
\[
A^{i,j} = \varepsilon \sum_{k=1}^{n_y} \left( \frac{\partial^2 g^i}{\partial y^k \partial x^j}(x, \gamma(x)) + \sum_{\ell=1}^{n_y} \frac{\partial^2 g^i}{\partial y^k \partial y^{\ell}}(x, \gamma(x)) \frac{\partial \gamma_1^\ell}{\partial x^j}(x) \right) \gamma_1^k(x) \\
+ \varepsilon \sum_{k=1}^{n_y} \frac{\partial g^i}{\partial y^k}(x, \gamma(x)) \frac{\partial \gamma_1^k}{\partial x^j}(x) - \frac{\partial g^i}{\partial x^j}(x, \Gamma_1(x, \varepsilon)).
\]
and it is obvious that $A(x, \varepsilon)$ is uniformly bounded in $\varepsilon \in (0, \varepsilon_0]$ due to Assumption 2.1. By (3.14a) and Taylor’s expansion of $\frac{\partial g \cdot}{\partial x}$ and $\frac{\partial g \cdot}{\partial \gamma}$ at $(x, \gamma(x))$, one obtains that

$$
(B.4) \quad \frac{\partial g^i}{\partial x^j}(x, \Gamma_1(x, \varepsilon)) = \frac{\partial g^i}{\partial x^j}(x, \gamma(x)) + \varepsilon \sum_{k=1}^{n_y} \frac{\partial^2 g^i}{\partial x^j \partial y^k}(x, \gamma(x)) \gamma^k_i(x) + O(\varepsilon^2),
$$

and

$$
(B.5) \quad \frac{\partial g^i}{\partial y^k}(x, \Gamma_1(x, \varepsilon)) = \frac{\partial g^i}{\partial y^k}(x, \gamma(x)) + \varepsilon \sum_{l=1}^{n_y} \frac{\partial^2 g^i}{\partial y^k \partial y^l}(x, \gamma(x)) \gamma^l_i(x) + O(\varepsilon^2),
$$

where both $O(\varepsilon^2)$ can be controlled uniformly due to Assumption 2.1. In addition, the $(i,j)$-component of (3.10) can be written as

$$
(B.6) \quad \frac{\partial g^i}{\partial y^j}(x, \gamma(x)) = - \sum_{k=1}^{n_y} \frac{\partial g^i}{\partial y^k}(x, \gamma(x)) \frac{\partial \gamma^k_i}{\partial x^j}(x).
$$

By (B.3), (B.4), (B.5), (B.6) and the uniform boundedness of $\nabla_x \Gamma_1(x, \varepsilon)$, one can obtain that

$$
(B.7) \quad \sum_{k=1}^{n_y} \left( \frac{\partial g^i}{\partial y^k}(x, \gamma(x)) + \varepsilon B^{i,k} \right) \cdot \left( \frac{\partial \gamma^k_i}{\partial x^j}(x) - \frac{\partial g^i}{\partial x^j}(x) - \varepsilon \frac{\partial \gamma^k_i}{\partial x^j}(x) \right) = O(\varepsilon^2),
$$

where $O(\varepsilon^2)$ can be controlled uniformly, $B = B(x) = [B^{i,k}]_{i,k=1}^{n_y}$ defined as

$$
B^{i,k} = \sum_{l=1}^{n_y} \frac{\partial^2 g^i}{\partial y^k \partial y^l}(x, \gamma(x)) \gamma^l_i(x).
$$

(B.7) can be rewritten as

$$
(B.8) \quad (G_y(x) + \varepsilon B)(\nabla_x \Gamma_1(x, \varepsilon) - \nabla \gamma(x) - \varepsilon \nabla \gamma_1(x)) = O(\varepsilon^2).
$$

Notice that $B(x)$ is uniformly bounded thanks to Assumption 2.1. Therefore, as long as $\varepsilon$ is sufficiently small, $G_y(x) + \varepsilon B$ is invertible and $(G_y(x) + \varepsilon B)^{-1}$ is uniformly bounded. Therefore, the proof of (3.14b) is completed by (B.8).

By Remark 2.3, one obtains that

$$
|\Gamma_2(x, \varepsilon) - \gamma(x) - \varepsilon \gamma_1(x) - \varepsilon^2 \gamma_2(x)|
\leq \frac{1}{\beta} |g(x, \Gamma_2(x, \varepsilon)) - g(x, \gamma(x) + \varepsilon \gamma_1(x) + \varepsilon^2 \gamma_2(x))|
\leq \frac{1}{\beta} |\nabla_x \Gamma_1(x, \varepsilon) f(x, \gamma(x)) - g(x, \gamma_1(x) + \gamma_1(x) + \varepsilon^2 \gamma_2(x))|.
$$

By (3.14a), (3.14b) and Taylor’s expansion of $f(x, y)$ at $(x, \gamma(x))$, one gets that

$$
(B.9) \quad \varepsilon \nabla_x \Gamma_1(x, \varepsilon) f(x, \gamma(x)) = \varepsilon \nabla \gamma(x) f(x) + \varepsilon^2 \nabla \gamma(x) f_y(x) \gamma_1(x) + \nabla \gamma_1(x) F(x) + O(\varepsilon^3).
$$

By Taylor’s expansion of $g(x, y)$ at $(x, \gamma(x))$, one gets that

$$
(B.10) \quad g(x, \gamma(x) + \gamma_1(x) + \varepsilon^2 \gamma_2(x)) = \varepsilon G_y(x) \gamma_1(x) + \varepsilon^2 \left( G_y(x) \gamma_2(x) + \frac{1}{2} \sum_{j,k=1}^{n_y} G_y^{j,k} \gamma^j_i(x) \gamma^k_i(x) \right) + O(\varepsilon^3).
$$
By comparing (B.9) and (B.10), one obtains that
\[ |\varepsilon \nabla \Gamma_1(x, \varepsilon) f(x, \Gamma_1(x, \varepsilon)) - g(x, \gamma(x) + \varepsilon \gamma_1(x) + \varepsilon^2 \gamma_2(x))| = O(\varepsilon^3), \]
where \(O(\varepsilon^3)\) can be controlled uniformly thanks to Assumption 2.1. In other words, there exists a constant \(C_2 > 0\) such that
\[ |\Gamma_2(x, \varepsilon) - \gamma(x) - \varepsilon \gamma_1(x) - \varepsilon^2 \gamma_2(x)| \leq \frac{C_2}{\beta} \varepsilon^3. \]
Thus, the proof for (3.14c) is completed.

Appendix C. Proofs of Theorems 3.9, 3.10, and 5.1.

C.1. Several lemmas. In the proofs of these three theorems, we have to calculate high-order gradients of vector-valued functions. Here we present several facts about high-order derivatives.

Lemma C.1. Suppose that the functions \(A, \xi, \eta\) in this lemma are sufficiently smooth. We have the following conclusions.

1. Assume that \(k \geq 0\) and \(\xi, \eta \in W^{k, \infty}(\mathbb{R}^n, \mathbb{R})\), then
\[ |\xi \eta|_{k, \infty} \lesssim \sum_{j=0}^{k} |\xi|_{j, \infty} |\eta|_{k-j, \infty}, \]
where the bound is dependent on \(k\), and independent of \(\xi\) and \(\eta\).

2. Assume that \(k \geq 0\). Let \(\xi : \mathbb{R}^n \to \mathbb{R}\) and \(\eta : \mathbb{R}^m \to \mathbb{R}^n\) be sufficiently smooth functions. If \(\nabla \xi \in W^{k, \infty}\) and \(\nabla \eta \in W^{k, \infty}\), then
\[ |\xi \circ \eta|_{k+1, \infty} \lesssim \sum_{j=1}^{k+1} |\xi|_{j, \infty} \|\nabla \eta\|_{k+1-j, \infty}^2, \]
where the bound is dependent on \(k\), and independent of \(\xi\) and \(\eta\). In particular, if \(\xi \in W^{k+1, \infty}\) and \(\nabla \eta \in W^{k, \infty}\), then \(\xi \circ \eta \in W^{k+1, \infty}\).

3. Assume that \(k \geq 0\). Let \(A : \mathbb{R}^m \to \mathbb{R}^{n \times n}\) is a matrix-valued function. If \(\nabla A \in W^{k, \infty}\) and \(A(\cdot)^{-1} \in L^\infty\), then
\[ |A(\cdot)^{-1}|_{k+1, \infty} \lesssim \sum_{j=1}^{k+1} \|A(\cdot)^{-1}\|_{0, \infty}^{j+1} \|\nabla A\|_{k+1-j, \infty}^j, \]
where the bound is dependent on \(k\), and independent of \(A\).

Proof. Item 1 is a direct corollary of Leibniz rule.

As for Item 2, first we notice that
\[ \nabla_\cdot ((\xi \circ \eta)(x)) = ((\nabla \xi) \circ \eta)(x) \cdot \nabla \eta(x), \]
which yields directly that the conclusion holds for \(k = 0\). Now we assume that the conclusion holds for all non-negative integers that are less than \(k\), and then one can obtain by Item 1 and the induction hypothesis...
that
\[ |\xi \circ \eta|_{k+2, \infty} = \left| \left( (\nabla \xi) \circ \eta \right) \cdot \nabla \eta \right|_{k+1, \infty} \]
\[ \lesssim \sum_{i=0}^{k+1} |(\nabla \xi) \circ \eta|_{i, \infty} |\nabla \eta|_{k+1-i, \infty} \]
\[ \lesssim |\xi|_{1, \infty} |\nabla \eta|_{k+1, \infty} + \sum_{i=1}^{k+1} \sum_{j=1}^{k+1} |\xi|_{j+1, \infty} \|\nabla \eta\|_{i-j, \infty}^{j} |\nabla \eta|_{k+1-i, \infty} \]
\[ \leq |\xi|_{1, \infty} |\nabla \eta|_{k+1, \infty} + \sum_{j=1}^{k+1} \sum_{i=j}^{k+1} |\xi|_{j+1, \infty} \|\nabla \eta\|_{k+1-j, \infty}^{j+1} \]
\[ \lesssim \sum_{j=1}^{k+2} |\xi|_{j, \infty} \|\nabla \eta\|_{k+2-j, \infty}^{j}, \]
which completes the proof.

As for Item 3, one can notice first that
\[ \frac{\partial A(x)^{-1}}{\partial x^i} = -A(x)^{-1} \frac{\partial A(x)}{\partial x^i} A(x)^{-1}, \forall i = 1, 2, \ldots, m. \]
Then the conclusion can be proved similarly to Item 2.

**Lemma C.2.** Suppose that \( \Phi : \mathbb{R}^n \times [-\delta, \delta] \to \mathbb{R} \) is sufficiently smooth. If there exists \( k, \ell \in \mathbb{N} \) such that the function \( \Phi(x, s) \) satisfies
\[ \frac{\partial^{i} \Phi}{\partial s^i}(x, 0) = 0, \forall i = 0, 1, \ldots, \ell, \]
and
\[ \sup_{s \in [-\delta, \delta]} \left\| \frac{\partial^{\ell+1} \Phi}{\partial s^{\ell+1}}(\cdot, s) \right\|_{k, \infty} < +\infty, \]
then
\[ \|\Phi(\cdot, h)\|_{k, \infty} = \mathcal{O}(|h|^{\ell+1}), \text{ as } h \to 0. \]

**Proof.** By Taylor’s expansion, for each \( j = 0, 1, \ldots, k \), there exists \( \theta \in [0, 1] \) such that
\[ |\nabla_j^{2} \Phi(x, h)| = \frac{1}{(\ell + 1)!} \left| \nabla_j^{2} \frac{\partial^{\ell+1} \Phi}{\partial s^{\ell+1}}(x, \theta h) h^{\ell+1} \right| \lesssim \sup_{s \in [-\delta, \delta]} \left\| \frac{\partial^{\ell+1} \Phi}{\partial s^{\ell+1}}(\cdot, s) \right\|_{k, \infty} \left| h \right|^{\ell+1}, \]
which completes the proof.

**Corollary C.3.** Suppose that \( \xi : \mathbb{R}^n \to \mathbb{R} \) and \( \eta : \mathbb{R}^n \to \mathbb{R}^n \) are sufficiently smooth, and \( \eta \in W^{k, \infty} \).

We have the following conclusions.
1. If \( \nabla^2 \xi \in W^{k, \infty} \), then
\[ \| \xi(\cdot + \eta(\cdot) h) - \xi(\cdot) - h \nabla \xi(\cdot) \eta(\cdot) \|_{k, \infty} = \mathcal{O}(|h|^2), \text{ as } h \to 0. \]
2. If \( \nabla^{3} \xi \in W^{k, \infty} \), then
\[ \| \xi(\cdot + \eta(\cdot) h) - \xi(\cdot) - h \nabla \xi(\cdot) \eta(\cdot) - 2 h \nabla^2 \xi(\cdot) \eta(\cdot) \|_{k, \infty} = \mathcal{O}(|h|^3), \text{ as } h \to 0. \]

**Proof.** Let \( \Phi(x, s) = \xi(x + \eta(x)s) - \xi(x) - s \nabla \xi(x) \eta(x) \). By direct calculation, one can obtain that
\[ \frac{\partial \Phi}{\partial x}(x, s) = \nabla \xi(x + \eta(x)s) \eta(x) - \nabla \xi(x) \eta(x), \]
\[ \frac{\partial^2 \Phi}{\partial s^2}(x, s) = \sum_{i_1, i_2 = 1}^{n} \frac{\partial^2 \xi}{\partial x^{i_1} \partial x^{i_2}}(x + \eta(x)s) \eta^{i_1}(x) \eta^{i_2}(x), \]
\[ \frac{\partial^3 \Phi}{\partial s^3}(x, s) = \sum_{i_1, i_2, i_3 = 1}^{n} \frac{\partial^3 \xi}{\partial x^{i_1} \partial x^{i_2} \partial x^{i_3}}(x + \eta(x)s) \eta^{i_1}(x) \eta^{i_2}(x) \eta^{i_3}(x). \]
Notice that $\Phi(x,0) = \frac{\partial \Phi}{\partial s}(x,0) = 0$. By Lemma C.1, $\Phi(x,s)$ satisfies the conditions of Lemma C.2 when $\ell = 1$, which yields Item 1. Similarly, $\Phi(x,s) - \Phi(x,-s)$ satisfies Lemma C.2 when $\ell = 2$, which completes the proof.

**Lemma C.4.** If $z_0, z_1 \in C^k(\mathbb{R}^n, \mathbb{R}^n)$ for some $k = 1, 2, \ldots, K$, then there exist unique $y_0, y_1 \in C^k(\mathbb{R}^n, \mathbb{R}^n)$ satisfying that $g(x,y_i(x)) = z_i(x)$ for $i = 0, 1$. In addition, if $z_i \in W^{k,\infty}$ for $i = 0, 1$, then
\[
\|y_1 - y_0\|_{k,\infty} \lesssim z_1 - z_0\|_{k,\infty},
\]
where the bound is dependent on $\beta$, $k$ and $\|z_i\|_{k,\infty}$ where $i = 0, 1$.

**Proof.** By Remark 2.3 and implicit function theorem for $g(x,y) - sz_1(x) - (1-s)z_0(x) = 0$ with respect to $y$, there exists a unique function $y = y(x,s) \in C^k(\mathbb{R}^n \times [0,1], \mathbb{R}^n)$ such that
\[
g(x,y(x,s)) = sz_1(x) + (1-s)z_0(x).
\]

Now we assume that $z_i \in W^{k,\infty}$ for $i = 0, 1$. Let $y_i(x) = y(x,i)$ for $i = 0, 1$. For each $j = 0, 1, \ldots, k$, there exists $\theta \in [0,1]$ such that
\[
\|\nabla^j y_1(x) - \nabla^j y_0(x)\| \leq \left| \frac{\partial}{\partial \theta} \nabla^j y(x,\theta) \right|.
\]
By (C.1), one obtains that
\[
\frac{\partial y}{\partial s}(x,s) = \left( \frac{\partial y}{\partial y}(x,y(x,s)) \right)^{-1} (z_1(x) - z_0(x))
\]
and
\[
\nabla_x y(x,s) = \left( \frac{\partial y}{\partial y}(x,y(x,s)) \right)^{-1} \left(s \nabla z_1(x) + (1-s)\nabla z_0(x) - \frac{\partial y}{\partial x}(x,y(x,s)) \right).
\]
We assert that $\sup_{s \in [0,1]} \|\nabla_x y(\cdot,s)\|_{k-1,\infty}$ is bounded, where the bound is dependent on $\beta$, $k$ and $\|z_i\|_{k,\infty}$.

By (C.4), $\sup_{s \in [0,1]} \|\nabla_x y(\cdot,s)\|_{0,\infty}$ is bounded. Now assume that $\sup_{s \in [0,1]} \|\nabla_x y(\cdot,s)\|_{j,\infty}$ is bounded for some $j = 0, 1, \ldots, k - 2$. Lemma C.1 yields that $\sup_{s \in [0,1]} \left\| \frac{\partial y}{\partial \theta}(\cdot,y(\cdot,s)) \right\|_{j+1,\infty}$ and then $\sup_{s \in [0,1]} \|\nabla y(\cdot,s)\|_{j+1,\infty}$ are bounded, which yields the assertion.

By the above assertion and Lemma C.1, $\left( \frac{\partial y}{\partial y}(x,y(x,s)) \right)^{-1}$ is bounded in $W^{k,\infty}$, where the bound depends on $\beta$, $k$ and $\|z_i\|_{k,\infty}$. Therefore, by (C.3), one obtains that
\[
\sup_{s \in [0,1]} \left\| \frac{\partial y}{\partial \theta}(\cdot,s) \right\|_{k,\infty} \lesssim \|z_1 - z_0\|_{k,\infty}.
\]
Together with (C.2), the proof is completed.

**Lemma C.5.** Assume that $y_i : \mathbb{R}^n \to \mathbb{R}^n$ satisfies that $y_i \in C^{k+1}$ and $\nabla y_i \in W^{k,\infty}$ for each $i = 0, 1$ and some $k = 0, 1, \ldots, K - 1$. If $y_1 - y_0 \in C^\infty$, then
\[
\|\nabla y_1(\cdot)f(\cdot,y_1(\cdot)) - \nabla y_0(\cdot)f(\cdot,y_0(\cdot))\|_{k,\infty} \lesssim \|y_1 - y_0\|_{k+1,\infty},
\]
where the bound depends on $f$, $k$ and $\|\nabla y_i\|_{k,\infty}$ with $i = 0, 1$.

**Proof.** Let $\Phi(x,s) = sy_1(x) + (1-s)y_0(x)$ and $\Psi(x,s) = \nabla_x \Phi(x,s)f(x,\Phi(x,s))$. For each $j = 0, 1, \ldots, k$, there exists $\theta \in [0,1]$ such that
\[
\|\nabla_x^j \Psi(x,1) - \nabla_x^j \Psi(x,0)\| \leq \left| \frac{\partial}{\partial \theta} \nabla_x^j \Psi(x,\theta) \right|.
\]
Actually,
\[
\frac{\partial \Psi}{\partial s}(x, s) = \nabla_x \left( \frac{\partial \Phi}{\partial s}(x, s) \right) f(x, \Phi(x, s)) + \nabla_x \Phi(x, s) \frac{\partial f}{\partial y}(x, \Phi(x, s)) \frac{\partial \Phi}{\partial s}(x, s)
\]
(C.5)
\[
= (\nabla y_1(x) - \nabla y_0(x)) f(x, \Phi(x, s)) + \nabla_x \Phi(x, s) \frac{\partial f}{\partial y}(x, \Phi(x, s))(y_1(x) - y_0(x)).
\]
By Lemma C.1, one obtains that \( \sup_{s \in [0,1]} \| f(\cdot, \Phi(\cdot, s)) \|_{k, \infty} \) and \( \sup_{s \in [0,1]} \left\| \nabla_x \Phi(\cdot, s) \frac{\partial f}{\partial y}(\cdot, \Phi(\cdot, s)) \right\|_{k, \infty} \) are bounded, and the bound depends on \( f \), \( k \) and \( \| \nabla y_i \|_{k, \infty} \) with \( i = 0, 1 \). Therefore,
\[
\sup_{s \in [0,1]} \left\| \frac{\partial \Psi}{\partial s}(\cdot, s) \right\|_{k, \infty} \lesssim \| y_1 - y_0 \|_{k+1, \infty},
\]
which completes the proof. □

**Corollary C.6.** For \( k = 0, 1, \ldots, K \),
\[
\| \Gamma_{k+1}(\cdot, \cdot) - \Gamma_k(\cdot, \cdot) \|_{K-k, \infty} = O(\varepsilon^{k+1}).
\]

**Proof.** By (3.10) and Lemma C.1, one can prove by induction that \( \| \nabla_x \Gamma_0(\cdot, \cdot) \|_{K, \infty} \) is bounded. Therefore, \( \| \varepsilon \nabla_x \Gamma_0(\cdot, \cdot) f(\cdot, \Gamma_0(\cdot, \cdot)) \|_{K, \infty} = O(\varepsilon) \). By Lemma C.4, \( \| \Gamma_1(\cdot, \cdot) - \Gamma_0(\cdot, \cdot) \|_{K, \infty} = O(\varepsilon) \). Now assume that (C.6) holds for \( 0, 1, \ldots, k \), where \( k \leq K - 1 \). By the induction hypothesis, \( \| \nabla_x \Gamma_{j}(\cdot, \cdot) \|_{K-k-1, \infty} \) are bounded for \( j = 0, 1, \ldots, k+1 \). By Lemma C.5, one obtains that
\[
\| \nabla_x \Gamma_{k+1}(\cdot, \cdot) f(\cdot, \Gamma_k(\cdot, \cdot)) - \nabla_x \Gamma_k(\cdot, \cdot) f(\cdot, \Gamma_k(\cdot, \cdot)) \|_{K-k-1, \infty} = O(\varepsilon^{k+1}).
\]
By Lemma C.4, the proof is completed. □

**C.2. Proof of Theorem 3.9.**
**Proof of Theorem 3.9.** We prove this theorem by induction.
When \( k = 0 \), there exists a constant \( C > 0 \) dependent on \( k \) such that
\[
\frac{d|z_0|^2}{dt} = \frac{2}{\varepsilon} \langle z_0, g(x, y) - g(x, \gamma(x)) \rangle - 2 \langle z_0, \nabla \gamma(x) f(x, y) \rangle \\
\leq -\frac{2\beta}{\varepsilon} |z_0|^2 + C |z_0| \leq \frac{A}{\varepsilon} |z_0|^2 + \frac{C^2}{4(2\beta - A)} \varepsilon.
\]
Here the last inequality is due to Cauchy inequality. By Gronwall inequality,
\[
|z_0(t)|^2 \leq \frac{C^2}{A(2\beta - A)} \varepsilon^2 (1 - e^{-\frac{\varepsilon}{A}}) \leq \frac{C^2}{A(2\beta - A)} \varepsilon^2 + e^{-\frac{\varepsilon}{A}} |z_0(0)|^2.
\]
Assuming that the theorem holds for \( k - 1 \), where \( k = 1, 2, \ldots, K \). One obtains that
\[
\frac{d|z_k|^2}{dt} = \frac{2}{\varepsilon} \langle z_k, g(x, y) - g(x, \Gamma_k(\cdot, \cdot)) \rangle \\
+ 2 \langle z_k, \nabla_x \Gamma_{k-1}(x, \cdot) f(x, \Gamma_{k-1}(x, \cdot)) - \nabla_x \Gamma_k(x, \cdot) f(x, y) \rangle \\
\leq -\frac{2\beta}{\varepsilon} |z_k|^2 + 2 |z_k| \cdot |\nabla_x \Gamma_{k-1}(x, \cdot) f(x, \Gamma_{k-1}(x, \cdot)) - \nabla_x \Gamma_k(x, \cdot) f(x, y)|.
\]
**Corollary C.6** and **Assumption 2.1** yield that there exists a constant \( C > 0 \) such that
\[
2|\nabla_x \Gamma_{k-1}(x, \cdot) f(x, \Gamma_{k-1}(x, \cdot)) - \nabla_x \Gamma_k(x, \cdot) f(x, y)| \\
\leq 2|\nabla_x \Gamma_k(x, \cdot) f(x, \Gamma_{k-1}(x, \cdot)) - \nabla_x \Gamma_k(x, \cdot) f(x, \Gamma_{k-1}(x, \cdot))| \\
+ 2 |\nabla_x \Gamma_k(x, \cdot) f(x, \Gamma_{k-1}(x, \cdot)) - \nabla_x \Gamma_k(x, \cdot) f(x, y)| \\
\leq C \varepsilon^k + C |z_{k-1}|.
\]
Take $\tilde{A} \in (A, 2\beta)$. Combing (C.7) and (C.8), one gets by Cauchy inequality that
\[
\frac{d|z_k|^2}{dt} \leq -\frac{2\varepsilon}{C} |z_k|^2 + C\varepsilon^2 |z_k| + C|z_{k-1}| \cdot |z_k|
\]
(C.9)
\[
\leq -\frac{\tilde{A}}{\varepsilon} |z_k|^2 + \frac{C^2}{2(2\beta - A)} \varepsilon^{2k+1} + \frac{C^2}{2(2\beta - A)} \varepsilon |z_{k-1}|^2.
\]

The induction hypothesis says that there exists $C_{k-1} > 0$ such that
(C.10) \[ |z_{k-1}(t)|^2 \leq C_{k-1}(e^{2k} + e^{-\frac{\tilde{A}}{\varepsilon}}|z_{k-1}(0)|^2). \]

By (C.9), (C.10) and Gronwall’s inequality, one gets that
\[
|z_k(t)|^2 \leq \frac{C^2(1 + C_{k-1})}{2A(2\beta - A)} (1 - e^{-\frac{2\varepsilon}{C}}) e^{2k+2} + e^{-\frac{\tilde{A}}{\varepsilon}} |z_k(0)|^2 + \frac{C^2 C_{k-1} e^{-1}}{2A(2\beta - A)} e^{-\frac{\tilde{A}}{\varepsilon}} |z_{k-1}(0)|^2.
\]
(C.11)
\[
\leq \frac{C^2(1 + C_{k-1})}{2A(2\beta - A)} e^{2k+2} + e^{-\frac{\tilde{A}}{\varepsilon}} |z_k(0)|^2 + \frac{C^2 C_{k-1} e^{-1}}{2A(2\beta - A)} e^{-\frac{\tilde{A}}{\varepsilon}} |z_{k-1}(0)|^2.
\]
By Corollary C.6, one gets that
(C.12) \[ |z_{k-1}(0)|^2 \leq 2|z_k(0)|^2 + 2|z_k(0) - z_{k-1}(0)|^2 \leq 2|z_k(0)|^2 + C e^{2k}. \]

By (C.11) and (C.12), the theorem holds for $k$. Then the theorem is thus proved. □

C.3. Proof of Theorem 3.10.

Proof of Theorem 3.10. Since $\nabla_x f(x, y), \nabla_y f(x, y)$ and $\nabla_x \Gamma_k(x, \varepsilon)$ are all bounded, then there exists a constant $C > 0$ such that
\[
\left| \frac{d(x - X_k)}{dt} \right| = |f(x, y) - f(X_k, \Gamma_k(x, \varepsilon))| 
\leq |f(x, z_k + \Gamma_k(x, \varepsilon)) - f(x, \Gamma_k(x, \varepsilon))| + |f(x, \Gamma_k(x, \varepsilon)) - f(X_k, \Gamma_k(x, \varepsilon))| 
\leq C|z_k| + C|x - X_k|.
\]

Then one obtains that
\[
\frac{1}{2} \frac{d|x - X_k|^2}{dt} = \left< x - X_k, \frac{d(x - X_k)}{dt} \right> \leq |x - X_k| \cdot \left| \frac{d(x - X_k)}{dt} \right| \leq C|z_k| \cdot |x - X_k| + C|x - X_k|^2.
\]

Therefore, by Theorem 3.9 and Cauchy-Schwarz inequality, there exists a constant $C_k > 0$ such that
\[
\frac{d|x - X_k|^2}{dt} \leq C_k(|x - X_k|^2 + \varepsilon^{2k+2} + e^{-\frac{\tilde{A}}{\varepsilon}} |z_k(0)|^2).
\]

By Gronwall inequality,
\[
|x(t) - X_k(t)|^2 \leq e^{C_k t} |x(0) - X_k(0)|^2 + \varepsilon^{2k+2}(e^{C_k t} - 1) + C_k \frac{e^{C_k t} - e^{-\frac{\tilde{A}}{\varepsilon}}}{t} |z_k(0)|^2,
\]
which completes the proof. □

C.4. Proof of Theorem 5.1.

Proof of Theorem 5.1. When $k = 0$, (5.2) is straightforward since $\Gamma_0(x, \varepsilon) = \Gamma_0^d(x, \varepsilon)$. Assume that (5.2) holds for $0, 1, \ldots, k$ where $k = 0, 1, \ldots, \frac{N}{2} - 1$. By Lemma C.4, it suffices to show that
\[
\left\| \Gamma_k^d(\cdot + f(\cdot, \Gamma_k^d(\cdot, \varepsilon))\tau, \varepsilon) - \Gamma_k^d(\cdot, \varepsilon) - \tau \nabla_x \Gamma_k^d(\cdot, \varepsilon) f(\cdot, \Gamma_k^d(\cdot, \varepsilon)) \right\|_{K_{-2k-2, \infty}} = O(\tau^2).
\]
(C.13)
By the induction hypothesis, \( \left\| \nabla x \hat{\Gamma}^d_k(\cdot, \varepsilon) \right\|_{K - 2k - 1, \infty} \) is bounded. By Lemma C.5,

\[
(C.14) \quad \left\| \tau \nabla x \hat{\Gamma}^d_k(\cdot, \varepsilon)f(\cdot, \hat{\Gamma}^d_k(\cdot, \varepsilon)) - \tau \nabla x \Gamma_k(\cdot, \varepsilon)f(\cdot, \Gamma_k(x, \varepsilon)) \right\|_{K - 2k - 1, \infty} = O(\tau^2).
\]

Since \( \left\| \nabla x \hat{\Gamma}^d_k(\cdot, \varepsilon) \right\|_{K - 2k - 2, \infty} \) is bounded, one obtains by Corollary C.3 that

\[
(C.15) \quad \left\| \hat{\Gamma}^d_k(\cdot + f(\cdot, \hat{\Gamma}^d_k(\cdot, \varepsilon))\tau, \varepsilon) - \hat{\Gamma}^d_k(\cdot, \varepsilon) - \tau \nabla x \hat{\Gamma}^d_k(\cdot, \varepsilon)f(\cdot, \hat{\Gamma}^d_k(\cdot, \varepsilon)) \right\|_{K - 2k - 2, \infty} = O(\tau^2).
\]

By \( (C.14) \) and \( (C.15) \), one can obtain \( (C.13) \). Then the proof is completed. 

\[ \Box \]

REFERENCES

[1] A. Abdulle, W. E, B. Engquist, and E. Vanden-Eijnden, The heterogeneous multiscale method, Acta Numerica, 21 (2012), pp. 1–87.
[2] R. K. Brayton, F. G. Gustavsson, and G. D. Hachtel, A new efficient algorithm for solving differential-algebraic systems using implicit backward differentiation formulas, Proceedings of the IEEE, 60 (1972), pp. 98–108.
[3] H. Brezis, Functional analysis, Sobolev spaces and partial differential equations, Springer Science & Business Media, 2010.
[4] R. Car and M. Parrinello, Unified approach for molecular dynamics and density-functional theory, Physical Review Letters, 55 (1985), p. 2471.
[5] J. Carr, Applications of centre manifold theory, vol. 35, Springer Science & Business Media, 2012.
[6] P. Chartier, A. Murua, and J. M. Sanz-Serna, Higher-order averaging, formal series and numerical integration I: B-series, Foundations of Computational Mathematics, 10 (2010), pp. 695–727.
[7] L. Chua, M. Komuro, and T. Matsumoto, The double scroll family, IEEE Transactions on Circuits and Systems, 33 (1986), pp. 1072–1118.
[8] S. M. Cox and A. J. Roberts, Initial conditions for models of dynamical systems, Physica D: Nonlinear Phenomena, 85 (1995), pp. 126–141.
[9] W. E, Analysis of the heterogeneous multiscale method for ordinary differential equations, Communications in Mathematical Sciences, 1 (2003), pp. 423–436.
[10] W. E, The heterogeneous multiscale method: A ten-year review, in American Physical Society, 2012.
[11] B. Engquist and Y.-H. Tsai, Heterogeneous multiscale methods for stiff ordinary differential equations, Mathematics of Computation, 74 (2005), pp. 1707–1742.
[12] K. Eriksson, C. Johnson, and A. Logg, Explicit time-stepping for stiff ODEs, SIAM Journal on Scientific Computing, 25 (2004), pp. 1142–1157.
[13] G. Freiling, A survey of nonsymmetric Riccati equations, Linear Algebra and its Applications, 351 (2002), pp. 243–270.
[14] C. W. Gear and I. G. Kevrekides, Projective methods for stiff differential equations: problems with gaps in their eigenvalue spectrum, SIAM Journal on Scientific Computing, 24 (2003), pp. 1091–1106.
[15] D. Givon, R. Kupferman, and A. Stuart, Extracting macroscopic dynamics: model problems and algorithms, Nonlinearity, 17 (2004), pp. R55–R127.
[16] J. Guckenheimer, K. Hoffman, and W. Weckesser, The forced van der Pol equation I: The slow flow and its bifurcations, SIAM Journal on Applied Dynamical Systems, 2 (2003), pp. 1–35.
[17] S. He and Q.-L. Dong, An existence-uniqueness theorem and alternating contraction projection methods for inverse variational inequalities, Journal of Inequalities and Applications, (2018), pp. 1–19.
[18] F. G. Hennec, H. M. Tsuchiya, and R. Aris, On the mathematical status of the pseudo-steady state hypothesis of biochemical kinetics, Mathematical Biosciences, 1 (1967), pp. 95–113.
[19] Y. Jiang, R. Li, and S. Wu, A second order time homogenized model for sediment transport, Multiscale Modeling & Simulation, 14 (2016), pp. 963–996.
[20] P. Kaps, S. W. H. Poon, and T. D. Bui, Rosenbrock methods for stiff ODEs: A comparison of Richardson extrapolation and embedding technique, Computing, 34 (1985), pp. 17–40.
[21] J. Laskar, Large-scale chaos in the solar system, Astronomy and Astrophysics, 287 (1994), pp. L9–L12.
[22] F. Legoll, T. Lelievre, and G. Samaey, A micro-macro parareal algorithm: application to singularly perturbed ordinary differential equations, SIAM Journal on Scientific Computing, 35 (2013), pp. A1951–A1986.
[23] S. Macnamara, K. Burrage, and R. B. Sidje, Multiscale modeling of chemical kinetics via the master equation, Multiscale Modeling & Simulation, 6 (2008), pp. 1146–1168.
[24] G. C. Papanicolaou, Some probabilistic problems and methods in singular perturbations, The Rocky Mountain Journal of Mathematics, (1976), pp. 653–674.
[25] G. Pavliotis and A. Stuart, Multiscale methods: averaging and homogenization, Springer Science & Business Media, 2008.
[26] A. J. Roberts, Appropriate initial conditions for asymptotic descriptions of the long term evolution of dynamical systems, Journal of the Australian Mathematical Society, 31 (1989), pp. 48–75.
[27] E. K. Ryu and S. Boyd, Primer on monotone operator methods, Applied & Computational Mathematics, 15 (2016), pp. 3–43.
[28] W. C. Su, Z. Gajic, and X. M. Shen, *The exact slow-fast decomposition of the algebraic Ricatti equation of singularly perturbed systems*, IEEE Transactions on Automatic Control, 37 (1992), pp. 1456–1459.

[29] F. Verhulst, *Methods and applications of singular perturbations: boundary layers and multiple timescale dynamics*, vol. 50, Springer Science & Business Media, 2005.

[30] G. Wanner and E. Hairer, *Solving ordinary differential equations II*, vol. 375, Springer Berlin Heidelberg, 1996.

[31] S. Wu, *Multiscale modelling and simulation for the channel morphodynamic problems in large timescale*, PhD thesis, Peking University, 2015.

[32] Y. Zhang, T.-S. Lee, and W. Yang, *A pseudobond approach to combining quantum mechanical and molecular mechanical methods*, The Journal of Chemical Physics, 110 (1999), pp. 46–54.