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An hp-Adaptive Minimum Action Method Based on a Posteriori Error Estimate

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Abstract. In this work, we develop an hp-adaptivity strategy for the minimum action method (MAM) using a posteriori error estimate. MAM plays an important role in minimizing the Freidlin-Wentzell action functional, which is the central object of the Freidlin-Wentzell theory of large deviations for noise-induced transitions in stochastic dynamical systems. Because of the demanding computation cost, especially in spatially extended systems, numerical efficiency is a critical issue for MAM. Difficulties come from both temporal and spatial discretizations. One severe hurdle for the application of MAM to large scale systems is the global reparametrization in time direction, which is needed in most versions of MAM to achieve accuracy. We recently introduced a new version of MAM in [22], called tMAM, where we used some simple heuristic criteria to demonstrate that tMAM can be effectively coupled with h-adaptivity, i.e., the global reparametrization can be removed. The target of this paper is to integrate hp-adaptivity into tMAM using a posteriori error estimation techniques, which provides a general adaptive MAM more suitable for parallel computing. More specifically, we use the zero-Hamiltonian constraint to define an indicator to measure the error induced by linear time scaling, and the derivative recovery technique to construct an error indicator and a regularity indicator for the transition paths approximated by finite elements. Strategies for hp-adaptivity have been developed. Numerical results are presented.

AMS subject classifications: 60H35, 65C20, 65N20, 65N30

Key words: Large deviation principle, small random perturbations, minimum action method, rare events, uncertainty quantification.

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1 Introduction

Small random perturbations of dynamical systems can introduce rare but important events, e.g., the transitions between different stable equilibrium states of a deterministic dynamical system. Such noise-induced transitions have been observed on both small and large scales, and are critical in many physical, biological and chemical systems. Examples include nucleation events of phase transitions, chemical reactions, regime change in climate, conformation changes of biomolecules, hydrodynamic instability, etc.

The Freidlin-Wentzell (F-W) theory of large deviations provides a rigorous mathematical framework to understand the transitions induced by small noise in general dynamical systems. The key object of the F-W theory of large deviations is the F-W action functional, and the critical quantities are the minimizer of the F-W action functional and the associated minimum value. Starting from [8], the large deviation principle given by the F-W theory has been approximated numerically, and the numerical methods are, in general, called minimum action method (MAM).

Consider an ordinary differential equations perturbed by small white noise

$$d\boldsymbol{X}_t = \boldsymbol{b}(\boldsymbol{X}_t)dt + \sqrt{\varepsilon}d\boldsymbol{W}_t, \tag{1.1}$$

where ε is a small positive parameter. We are interested in two types of problems:

$$\text{Problem I:} \quad \inf_{\substack{\boldsymbol{\phi}(0)=\boldsymbol{x}_1,\\ \boldsymbol{\phi}(T)=\boldsymbol{x}_2}} \left[S_T(\boldsymbol{\phi}) = \frac{1}{2}\int_0^T |\dot{\boldsymbol{\phi}} - \boldsymbol{b}(\boldsymbol{\phi})|^2 dt \right] \tag{1.2}$$

and

$$\text{Problem II:} \quad V(\boldsymbol{x}_1,\boldsymbol{x}_2) = \inf_{T>0} \inf_{\substack{\boldsymbol{\phi}(0)=\boldsymbol{x}_1,\\ \boldsymbol{\phi}(T)=\boldsymbol{x}_2}} S_T(\boldsymbol{\phi}), \tag{1.3}$$

where $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$ are two points in the phase space, $S_T(\boldsymbol{\phi})$ is called the action functional, and $V(\boldsymbol{x}_1,\boldsymbol{x}_2)$ the quasi-potential from point $\boldsymbol{x}_1$ to $\boldsymbol{x}_2$. Here $\boldsymbol{\phi}(t)$ is a transition path connecting $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$ on the time interval $[0,T]$. The minimizers of Problem I and II characterize the difficulty of the noise-induced transition from $\boldsymbol{x}_1$ to the vicinity of $\boldsymbol{x}_2$, see Eqs. (2.4) and (2.5). In Problem I, the transition is restricted to a certain time scale T, which is relaxed in Problem II. Let $\boldsymbol{\phi}^*(t)$ be the minimizer of either Problem I or Problem II, which is also called the minimal action path (MAP), or the instanton in physical literature related to path integral. From the application point of view, solving Problem I and II is important. For example, the minimizer of F-W action functional can be used to construct an asymptotically efficient estimator in important sampling, where optimization problems like Problem I and II need to be solved effectively [5, 17]. The MAM can help to explore a high-dimensional phase space [18, 27]. Another example is the nonlinear instability of wall-bounded shear flows, which can be modelled as a rare event of Navier-Stokes equations perturbed by small noise [20,23]. The most probable transition path provides useful information that is difficult or impossible to obtain in a deterministic way.