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# An Improved Adaptive Minimum Action Method for the Calculation of Transition Path in Non-Gradient Systems

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**Abstract.** The minimum action method (MAM) is to calculate the most probable transition path in randomly perturbed stochastic dynamics, based on the idea of action minimization in the path space. The accuracy of the numerical path between different metastable states usually suffers from the "clustering problem" near fixed points. The adaptive minimum action method (aMAM) solves this problem by relocating image points equally along arc-length with the help of moving mesh strategy. However, when the time interval is large, the images on the path may still be locally trapped around the transition state in a tangle, due to the singularity of the relationship between arc-length and time at the transition state. Additionally, in most non-gradient dynamics, the tangent direction of the path is not continuous at the transition state so that a geometric corner forms, which brings extra challenges for the aMAM. In this note, we improve the aMAM by proposing a better monitor function that does not contain the numerical approximation of derivatives, and taking use of a generalized scheme of the Euler-Lagrange equation to solve the minimization problem, so that both the path-tangling problem and the non-smoothness in parametrizing the curve do not exist. To further improve the accuracy, we apply the Weighted Essentially non-oscillatory (WENO) method for the interpolation to achieve better performance. Numerical examples are presented to demonstrate the advantages of our new method.

**AMS subject classifications**: 82C26, 60H30, 34F05

**Key words**: Rare event, transition path, minimum action method, moving mesh, WENO.

## 1 Introduction

The calculation of quasi-potential and the most probably transition path between stable equilibria in metastable systems is of interest to researchers in the study of dynamics of

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complex and stochastic systems in long time scales [1]. The minimum action method (MAM) [2] was introduced to find such optimal paths by directly minimizing the action functional, which is the rate function in the large deviation theory [1]. The action minimizer within a certain rare-event subset in the path space, i.e., the minimum action path, carries the dominant contribution to the probability for the corresponding rare events. So, conditioned on the occurrence of rare events, the minimum action path is the most probable path under the influence of small noise in the long run. In many applications, the path represents the progressive physical process of important rare events such as phase transformation, chemical reaction, etc. Therefore, the numerical study of how to calculate the path efficiently is of great importance.

There have been quite many developments of numerical methods for the minimum action path. Firstly, when the system is of gradient type, *i.e.*, the dynamics is gradient flow driven by a potential energy, the variational problem for the minimum action path gets simplified and it turns out that essentially the optimal transition path is simply the time-reversed trajectory of the gradient flow. The joint location of the "uphill" path from one well and the "downhill" path toward the other well in the phase space is an index-1 saddle point which serves as transition state. The min-mode eigen-direction of the saddle point collapses with the tangential direction of the path from the *both* sides. This result reveals a second important feature for the gradient system: the tangential direction of the path is always continuous (belonging to $C^1$ curve), even when it crosses the separatrix via the saddle point. In practice, the path-finding algorithms, such as the string method [3] never searches the "uphill" and "downhill" paths separately since the saddle point is unknown *a priori*, but these methods search the whole path once for all between local minima and then locate the saddle point from the numerical path and split the path into "uphill" and "downhill" segments for interpretations.

But in the non-gradient systems, the above features of the path no longer holds, due to the lack of detailed balance for the stationary probability distribution. The "uphill" path and the "downhill" path are distinctively different in nature. More importantly, they meet at the saddle point from different directions in two sides of the separatrix: a sharp corner is usually formed where the path crosses the separatrix. The "uphill" path escapes the characteristic boundary by choosing a direction different from the eigen-direction of the saddle point. The path then exhibits non-smoothness, meaning that if the path $\varphi$ is written in terms of arc length parameter $s\in[0,1]$, then the tangent vector $\varphi'(s)$ is not continuous at $s_*$, even though $|\varphi'(s)|\equiv const$, where $\varphi(s_*)$ is the location of the saddle point. This is a generic phenomenon for transition path in non-gradient system and it is the origin of the non-Gaussian skewed distribution of the exist point on boundary. It also affects the prefactor estimation of mean exist time for non-gradient systems [4,5]. Refer to the work of [6,7,9] for theoretical analysis of the connection to effect of focusing and caustics. To visualize this non-smooth feature of the paths, we shall present two examples including the Maier-Stein model in [8] in the figures shown later.

To locate the saddle points, on the other hand, the direct search of saddle point, such as the dimer method [10] or the gentlest ascent dynamics [11, 12], sounds an alterna-