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Computing Residual Diffusivity by Adaptive Basis Learning via Spectral Method

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Dedicated to Professor Zhenhuan Teng on the occasion of his 80th birthday

Abstract. We study the residual diffusion phenomenon in chaotic advection computationally via adaptive orthogonal basis. The chaotic advection is generated by a class of time periodic cellular flows arising in modeling transition to turbulence in Rayleigh-Bénard experiments. The residual diffusion refers to the non-zero effective (homogenized) diffusion in the limit of zero molecular diffusion as a result of chaotic mixing of the streamlines. In this limit, the solutions of the advection-diffusion equation develop sharp gradients, and demand a large number of Fourier modes to resolve, rendering computation expensive. We construct adaptive orthogonal basis (training) with built-in sharp gradient structures from fully resolved spectral solutions at few sampled molecular diffusivities. This is done by taking snapshots of solutions in time, and performing singular value decomposition of the matrix consisting of these snapshots as column vectors. The singular values decay rapidly and allow us to extract a small percentage of left singular vectors corresponding to the top singular values as adaptive basis vectors. The trained orthogonal adaptive basis makes possible low cost computation of the effective diffusivities at smaller molecular diffusivities (testing). The testing errors decrease as the training occurs at smaller molecular diffusivities. We make use of the Poincaré map of the advection-diffusion equation to bypass long time simulation and gain accuracy in computing effective diffusivity and learning adaptive basis. We observe a non-monotone relationship between residual diffusivity and the amount of chaos in the advection, though the overall trend is that sufficient chaos leads to higher residual diffusivity.

AMS subject classifications: 76R99, 35B27, 65T40, 65M70

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1. Introduction

Diffusion enhancement in fluid advection has been studied for nearly a century, dating back to the pioneering work of Taylor [13] in 1921. It is a fundamental problem to characterize and quantify the large scale effective diffusion (denoted by D^E) in fluid flows containing complex and turbulent streamlines. Much progress has been made based on the passive scalar model [9]:

$$T_t + (\boldsymbol{v} \cdot D)\, T = D_0 \Delta T, \tag{1.1}$$

where T is a scalar function (e.g., temperature or concentration), $D_0 > 0$ is a constant (the so called molecular diffusion), $\boldsymbol{v}\,(\boldsymbol{x}, t)$ is a prescribed incompressible velocity field, D and Δ are the spatial gradient and Laplacian operators.

When the flow is steady, periodic and two dimensional, precise asymptotics of D^E are known. A prototypical example is the steady cellular flow [4,5], $\boldsymbol{v} = (-H_y, H_x)$, $H = \sin x \sin y$, see also [11,14,15] for its application in effective speeds of front propagation. The asymptotics of the effective diffusion along any unit direction in the cellular flow obeys the square root law in the advection dominated regime: $D^E = O(\sqrt{D_0}) \gg D_0$ as $D_0 \downarrow 0$, [5,6]. This is intuitively due to the ordered streamlines of the steady cellular flows where enhanced transport occurs along saddle to saddle connections and a diffusing particle escapes closed streamlines by hopping from cell to cell. However, if the streamlines are fully chaotic (well-mixed), the enhancement can follow a very different law. The simplest such example is the time periodic cellular flow:

$$\boldsymbol{v} = (\cos(y), \cos(x)) + \theta \cos(t)(\sin(y), \sin(x)), \quad \theta \in (0,1]. \tag{1.2}$$

The first term of (1.2) is a steady cellular flow with a $\pi/4$ rotation, and the second term is a time periodic perturbation that introduces an increasing amount of disorder in the flow trajectories as θ becomes larger. At $\theta = 1$, it is fully mixing, and empirically sub-diffusive [17]. The flow (1.2) has served as a model of chaotic advection for Rayleigh-Bénard experiment [3]. Numerical simulations [2,10] suggest that at $\theta = 1$, the effective diffusion along the x-axis, $D^E_{11} = O(1)$ as $D_0 \downarrow 0$, the so called *residual diffusion* arises. As $D_0 \downarrow 0$, the solutions develop sharp gradients, and render accurate computation costly, especially if one is interested in D^E parametrized by θ.

Let us recall the formula for effective diffusivity tensor [2]:

$$D^E_{ij} = D_0 \left(\delta_{ij} + \langle Dw_i \cdot Dw_j \rangle \right), \tag{1.3}$$

where w is a mean zero space-time periodic vector solution of:

$$w_t + (\boldsymbol{v} \cdot Dw) - D_0 \Delta w = -\boldsymbol{v}, \tag{1.4}$$

and the bracket denotes space-time average over the periods. The solution of (1.4) is unique by the Fredholm alternative. The correction to D_0 is positive definite in (1.3).

In this paper, we shall construct adaptive basis functions to handle the singular solutions of (1.4) at small D_0. First, we compute w by the spectral method, because