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Laminar and Turbulent Behavior Captured by A 3-D Kinetic-Based Discrete Dynamic System

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Abstract: We have derived a 3-D kinetic-based discrete dynamic system (DDS) from the lattice Boltzmann equation (LBE) for incompressible flows through a Galerkin procedure. Expressed by a poor-man lattice Boltzmann equation (PMLBE), it involves five bifurcation parameters including relaxation time from the LBE, splitting factor of large and sub-grid motion scales, and wavevector components from the Fourier space. Numerical experiments have shown that the DDS can capture laminar behaviors of periodic, subharmonic, n-period, and quasi-periodic and turbulent behaviors of noisy periodic with harmonic, noisy subharmonic, noisy quasi-periodic, and broadband power spectra. In this work, we investigated the effects of bifurcation parameters on the capturing of the laminar and turbulent flows in terms of the convergence of time series and the pattern of power spectra. We have found that the 2nd order and 3rd order PMLBEs are both able to capture laminar and turbulent flow behaviors but the 2nd order DDS performs better with lower computation cost and more flow behaviors captured. With the specified ranges of the bifurcation parameters, we have identified two optimal bifurcation parameter sets for laminar and turbulent behaviors. Beyond this work, we are exploring the regime maps for a deeper understanding of the contributions of the bifurcation parameters to the capturing of laminar and turbulent behaviors. Surrogate models (to replace the PMLBE) are being developed using deep learning techniques to overcome the overwhelming computation cost for the regime maps. Meanwhile, the DDS is being employed in the large eddy simulation of turbulent pulsatile flows to provide dynamic sub-grid scale information.

Keywords: Discrete Dynamical System, Computational Fluid Dynamics, Lattice Boltzmann Method, Surrogate Model, Turbulence Modeling.

1 Introduction

Discrete dynamical systems (DDSs) have long been of interest since the seminal paper by May[1]. Being very simple from a mathematical standpoint, a DDS can capture complicated turbulent-like behaviors in different dynamic systems[2, 3]. With a deterministic mathematical "rule" describing the time evolution of a state variable y in a discrete-time dynamical system, a logistic map, e.g. $y^{n+1} = \beta y^n (1-y^n)$, determines the time evolution of a dynamic variable (y^n) at discrete time (t^n) with the choices of the initial state (y^0) and the bifurcation parameter (β), leading to the generation of a time series[4]. Such DDSs are easily computed algebraic formulas not requiring supercomputers for their evaluation but capable of capturing the dynamic properties in different natural systems including weather forecasting[5], the motion of billiard balls[6], climate modeling[7-10], fluid dynamics[11-15], MHD turbulence[16, 17], and many others[18-20].

The "poor man's Navier-Stokes (PMNS) equation"[21], is an established DDS derived from the incompressible Navier-Stokes (N-S) equations. With very inexpensive evaluation, the PMNS equation provides deterministic maps that are chaotic and unpredictable in their detailed properties, but whose statistical properties are reproducible, just as what a turbulent flow behaves. The PMNS equation is capable of producing local time series at least in qualitative agreement with laboratory measurements and/or direct numerical simulation (DNS)[22, 23]. Hence, it has contributed to high-fidelity sub-grid scale (SGS) models for large-eddy simulation (LES), leading to an ability to simulate interactions of turbulence with other physical phenomena in the inertial subrange scales. The PMNS-based DDSs[14, 15] have often been employed for turbulence modeling[24-28]. However, there are deficiencies in the DDS derived from N-S equations that are limited to small Knudsen numbers. Deficiencies in turbulence simulation using N-S solvers have been associated with rather complicated modeling and highly expensive computation.

Kinetic-based lattice Boltzmann method (LBM)[29, 30] has been an alternative to computational fluid dynamic (CFD). It is derived from the Boltzmann equation[31, 32] and microscopic fluid physics is simplified to retain only the key elements (the local conservation laws and related symmetries) needed to guarantee accurate macroscopic behavior. Thus, the LBM is sometimes termed mesoscale CFD. The most attractive advantages of the LBM for the current research are (1) the simplicity of modeling and implementation for complex flows including turbulence [33-36] and (2) the suitability of employing the newly emerged GPU (Graphics Processing Unit) technology[37-39]—massively parallel architectures consisting of thousands of small and efficient cores designed for handling multiple tasks simultaneously. Recently, we have derived a first-ever 3-D kinetic-based DDS [40], i.e., "poor man's lattice Boltzmann equation (PMLBE)", and performed numerical experiments to demonstrate its capability to capture both laminar and turbulent flow behaviors. In this work, we further investigated the PMLBE in terms of the effects of the power terms and the bifurcation parameters on the capturing of the laminar and turbulent flows from the convergence of time series and the pattern of power spectra.

2 Problem Statement

The detailed derivation of the 3-D kinetic-based DDS, i.e., the PMLBE, and its numerical experiments are found in our previous work[40]. For the purpose of completion and comprehension of this paper, here we briefly express the major equations. Then, we state the problem of this work.

Formulation of LBM In the LBM, fluid particles are sitting at discrete grid nodes. During a time evolution, fluid particles collide at the nodes and then stream to the prescribed finite neighboring nodes along with their velocity directions. We use D3Q19 lattice model ($i = 0, \ldots, 18$). The lattice Boltzmann equation (LBE) reads

$$f_i(\vec{x} + \vec{e}_i \delta t) - f_i(\vec{x}, t) = -\frac{1}{\tau}\left[f_i(\vec{x}, t) - f_i^{eq}(\vec{x}, t)\right], \quad (1)$$

where $f_i(\vec{x}, t)$ and $f_i^{eq}(\vec{x}, t)$ are the particle distribution function and equilibrium particle distribution function, respectively, with molecular velocity $\vec{e}_i$ along the i^{th} direction at the location $\vec{x}$ and time t, δx and δt are the lattice width and time interval, respectively, and τ is the relaxation time due to particle collisions. The equilibrium particle distribution function is expressed as

$$f_i^{eq}(\vec{x}, t) = \omega_i \left\{\rho + \frac{3\vec{e}_i \cdot \vec{M}}{c^2} + \frac{9(\vec{e}_i \cdot \vec{M})^2}{2\rho c^4} - \frac{3\vec{M} \cdot \vec{M}}{2\rho c^2}\right\}, \quad (2)$$

where ω_i is the weighting factor with $\omega_0 = 1/3$, $\omega_{1,\dots,6} = 1/18$, and $\omega_{7,\dots,18} = 1/36$ for D3Q19 lattice model, $c = \delta x/\delta t$ with δx and δt the lattice width and time interval, respectively. The density ρ and density moment $\vec{M}(= \rho\vec{u})$ are obtained from the following formulas:

$$\rho \equiv \sum_{i=0}^{18} f_i \equiv \sum_{i=0}^{18} f_i^{eq} , \tag{3}$$

$$\vec{M} \equiv \sum_{i=0}^{18} \vec{e}_i f_i \equiv \sum_{i=0}^{18} \vec{e}_i f_i^{eq} . \tag{4}$$

Equation (1), together with Eqs. (2)–(4), are the governing equations that we use to derive the PMLE for the 3-D kinetic-based DDS.

Decomposition of large scale and SGS To decompose the motion scales, we first separate the f_i into large scale and SGS denoted by ~ and *, respectively,

$$f_i(\vec{x},t) = \tilde{f}_i(\vec{x},t) + f_i^*(\vec{x},t). \tag{5}$$

When substituting the decomposed f_i into the governing equation, the only term that has not been decomposed is the equilibrium particle distribution function $f_i^{eq}(\vec{x},t)$. To accomplish the decomposition of $f_i^{eq}(\vec{x},t)$ in Eq. (2), we first separate density and momentum in the same way as for f_i:

$$\rho = \tilde{\rho} + \rho^* = \sum_{i=0}^{18} \tilde{f}_i + \sum_{i=0}^{18} f_i^*, \tag{6}$$

$$\vec{M} = \tilde{\vec{M}} + \vec{M}^* = \sum_{i=0}^{18} \vec{e}_i \tilde{f}_i + \sum_{i=0}^{18} \vec{e}_i f_i^*. \tag{7}$$

Substituting Eq. (6) and (7) into Eqs. (1) and (2) results in:

$$\tilde{f}_i(\vec{x} + \vec{e}_i\delta t, t + \delta t) + f_i^*(\vec{x} + \vec{e}_i\delta t, t + \delta t) = \left(1 - \frac{1}{\tau}\right)\left[\tilde{f}_i(\vec{x},t) + f_i^*(\vec{x},t)\right] + \frac{\omega_i}{\tau}\left\{\tilde{\rho} + \rho^* + \frac{3\vec{e}_i\cdot\left(\tilde{\vec{M}}+\vec{M}^*\right)}{c^2} + \frac{9\left[\vec{e}_i\cdot\left(\tilde{\vec{M}}+\vec{M}^*\right)\right]^2}{2\tilde{\rho}c^4}\left(1 - \frac{\rho^*}{\tilde{\rho}}\right) - \frac{3\left(\tilde{\vec{M}}+\vec{M}^*\right)\cdot\left(\tilde{\vec{M}}+\vec{M}^*\right)}{2\tilde{\rho}c^2}\left(1 - \frac{\rho^*}{\tilde{\rho}}\right)\right\}. \tag{8}$$

Noticing $\left|\frac{\rho^*}{\tilde{\rho}}\right| < 1$, we have introduced $\frac{1}{1+\tilde{\rho}/\rho^*} \approx 1 - \frac{\rho^*}{\tilde{\rho}}$.

Equation (8) contains three types of terms: pure large scale with ~, pure SGS scale with *, and the mixture of both. For the mixed-scale terms, we introduce a splitting factor β, and assign a β portion of the mixed terms to the large scale, and the remaining $(1-\beta)$ portion to SGS. Equation (8) can then be split into the two scales as follows:

$$\tilde{f}_i(\vec{x} + \vec{e}_i\delta t, t + \delta t) - \tilde{f}_i(\vec{x},t) = -\frac{1}{\tau}\tilde{f}_i(\vec{x},t) + \frac{\omega_i}{\tau}\left\{\tilde{\rho} + \frac{3\vec{e}_i\cdot\tilde{\vec{M}}}{c^2} + \frac{9}{2\tilde{\rho}c^4}\left(\vec{e}_i\cdot\tilde{\vec{M}}\right)^2 - \frac{3}{2\tilde{\rho}c^2}\tilde{\vec{M}}\cdot\tilde{\vec{M}}\right\} + \frac{\beta\omega_i}{\tau}\left\{\frac{9}{2\tilde{\rho}c^4}\left[2\left(\vec{e}_i\cdot\tilde{\vec{M}}\right)\left(\vec{e}_i\cdot\vec{M}^*\right) + \left(\vec{e}_i\cdot\rho^*\right)^2\right] - \frac{9\rho^*}{2\tilde{\rho}^2c^4}\left[\left(\vec{e}_i\cdot\tilde{\vec{M}}\right)^2 + 2\left(\vec{e}_i\cdot\tilde{\vec{M}}\right)\left(\vec{e}_i\cdot\vec{M}^*\right) + \left(\vec{e}_i\cdot\vec{M}^*\right)^2\right] - \frac{3}{2\tilde{\rho}c^2}\left(\tilde{\vec{M}}\cdot\vec{M}^* + \vec{M}^*\cdot\vec{M}^*\right) + \frac{3\rho^*}{2\tilde{\rho}^2c^2}\left(\tilde{\vec{M}}\cdot\tilde{\vec{M}} + \tilde{\vec{M}}\cdot\vec{M}^* + \vec{M}^*\cdot\vec{M}^*\right)\right\}, \tag{9}$$

and

$$f_i^*(\vec{x} + \vec{e}_i\delta t, t + \delta t) - f_i^*(\vec{x},t) = -\frac{1}{\tau}f_i^*(\vec{x},t) + \frac{\omega_i}{\tau}\left\{\rho^* + \frac{3\vec{e}_i\cdot\vec{M}^*}{c^2}\right\} + \frac{(1-\beta)\omega_i}{\tau}\left\{\frac{9}{2\tilde{\rho}c^4}\left[2\left(\vec{e}_i\cdot\tilde{\vec{M}}\right)\left(\vec{e}_i\cdot\vec{M}^*\right) + \left(\vec{e}_i\cdot\vec{M}^*\right)^2\right] - \frac{9\rho^*}{2\tilde{\rho}^2c^4}\left[\left(\vec{e}_i\cdot\tilde{\vec{M}}\right)^2 + 2\left(\vec{e}_i\cdot\tilde{\vec{M}}\right)\left(\vec{e}_i\cdot\vec{M}^*\right) + \left(\vec{e}_i\cdot\vec{M}^*\right)^2\right] - \frac{3}{2\tilde{\rho}c^2}\left(\tilde{\vec{M}}\cdot\vec{M}^* + \vec{M}^*\cdot\vec{M}^*\right) + \frac{3\rho^*}{2\tilde{\rho}^2c^2}\left(\tilde{\vec{M}}\cdot\tilde{\vec{M}} + \tilde{\vec{M}}\cdot\vec{M}^* + \vec{M}^*\cdot\vec{M}^*\right)\right\}. \tag{10}$$

Now we differentiate Eq. (10) with respect to time and obtain:

$$\frac{df_i^*(\vec{x},t)}{dt}\delta t = -\frac{1}{\tau}f_i^*(\vec{x},t) + \frac{\omega_i}{\tau}\left\{\rho^* + \frac{3\vec{e}_i\cdot\vec{M}^*}{c^2}\right\} + \frac{(1-\beta)\omega_i}{\tau}\left\{\frac{9}{2\tilde{\rho}c^4}\left[2\left(\vec{e}_i\cdot\tilde{\vec{M}}\right)\left(\vec{e}_i\cdot\vec{M}^*\right) + \left(\vec{e}_i\cdot\vec{M}^*\right)^2\right] - \frac{9\rho^*}{2\tilde{\rho}^2c^4}\left[\left(\vec{e}_i\cdot\tilde{\vec{M}}\right)^2 + 2\left(\vec{e}_i\cdot\tilde{\vec{M}}\right)\left(\vec{e}_i\cdot\vec{M}^*\right) + \left(\vec{e}_i\cdot\vec{M}^*\right)^2\right] - \frac{3}{2\tilde{\rho}c^2}\left(\tilde{\vec{M}}\cdot\vec{M}^* + \vec{M}^*\cdot\vec{M}^*\right) + \frac{3\rho^*}{2\tilde{\rho}^2c^2}\left(\tilde{\vec{M}}\cdot\tilde{\vec{M}} + \tilde{\vec{M}}\cdot\vec{M}^* + \vec{M}^*\cdot\vec{M}^*\right)\right\}, \qquad (11)$$

where $d/dt \equiv \partial/\partial t + \vec{e}_i\cdot\nabla$ is the material time derivative along the characteristic line $\vec{e}_i$.

Construction of PMLBE we construct the Fourier expansion of the distribution function separated into large scale and SGS scale as follows:

$$f_i(\vec{x},t) = \sum_{\vec{k}=\vec{0}}^{\infty} a_{i,\vec{k}}(t)\varphi_{i,\vec{k}}(\vec{x}) = \underbrace{\sum_{\vec{k}=\vec{0}}^{\vec{N}} a_{i,\vec{k}}(t)\varphi_{i,\vec{k}}(\vec{x})}_{\tilde{f}_i(\vec{x},t)} + \underbrace{\sum_{\vec{k}=\vec{N}+\vec{I}}^{\infty} a_{i,\vec{k}}(t)\varphi_{i,\vec{k}}(\vec{x})}_{f_i^*(\vec{x},t)}, \qquad (12)$$

where $\vec{k}$ is the wavevector, $a_{\vec{k}}$ and $\varphi_{\vec{k}}$ are the Fourier coefficients and tensor product basis of $\vec{k}$, respectively $\vec{I}$ is a unit vector in wave space, and $\vec{N}$ represents the wavevector that separates large-scale and SGS distribution functions. When the functions $\varphi_{\vec{k}}$ of our chosen subset is from $\vec{0}$ to $\vec{N}$, the linear combination of the vectors is defined as the large-scale distribution function $\tilde{f}_i$. In other words, the SGS distribution function is simply the remainder of the complete Fourier expansion, where the functions $\varphi_{\vec{k}}$ of our chosen subset is from $\vec{N}$ to ∞. We assume that the tensor product basis set $\{\varphi_{\vec{k}}\}$ is complete in the function space L^2, orthonormal, and divergence-free, exhibiting properties analogous to the complex exponential with respect to differentiation.

Substituting $f_i^*(\vec{x},t) = \sum_{\vec{k}=\vec{N}+\vec{I}}^{\infty} a_{i,\vec{k}}(t)\varphi_{i,\vec{k}}(\vec{x})$ into Eq. (11), recalling Eqs. (6) and (7), rearranging the terms, and constructing Galerkin inner products with given basis functions for each term result in

$$a_{i,\vec{k}}(t+\delta t) = \left(1 - \delta t\vec{e}_i\cdot\vec{k} - \frac{1}{\tau}\right)a_{i,\vec{k}}(t) + \frac{\omega_i}{\tau}\left[\sum a_{j,\vec{k}}(t) + \frac{3\vec{e}_i\cdot\sum\vec{e}_j a_{j,\vec{k}}(t)}{c^2}\right] + \frac{9(1-\beta)\omega_i}{2\tau\left(\sum\tilde{f}_j\right)^2c^4}\left\{\sum\tilde{f}_j\left[2\left(\vec{e}_i\cdot\sum\vec{e}_j\tilde{f}_j\right)\left(\vec{e}_i\cdot\sum\vec{e}_j a_{j,\vec{k}}(t)\right) + \left(\vec{e}_i\cdot\sum\vec{e}_j a_{j,\vec{k}}(t)\right)^2\right] - \left[\sum a_{j,\vec{k}}(t)\left(\vec{e}_i\cdot\sum\vec{e}_j\tilde{f}_j\right)^2 + 2\sum a_{j,\vec{k}}(t)\left(\vec{e}_i\cdot\sum\vec{e}_j\tilde{f}_j\right)\left(\vec{e}_i\cdot\sum\vec{e}_j a_{j,\vec{k}}(t)\right) + \sum a_{j,\vec{k}}(t)\left(\vec{e}_i\cdot\sum\vec{e}_j a_{j,\vec{k}}(t)\right)^2\right] - \frac{\sum\tilde{f}_j c^2}{3}\left(\sum\vec{e}_j\tilde{f}_j\cdot\sum\vec{e}_j a_{j,\vec{k}}(t) + \sum\vec{e}_j a_{j,\vec{k}}(t)\cdot\sum\vec{e}_j a_{j,\vec{k}}(t)\right) + \frac{c^2}{3}\left(\sum a_{j,\vec{k}}(t)\sum\vec{e}_j\tilde{f}_j\cdot\sum\vec{e}_j\tilde{f}_j + \sum a_{j,\vec{k}}(t)\sum\vec{e}_j\tilde{f}_j\cdot\sum\vec{e}_j a_{j,\vec{k}}(t) + \sum a_{j,\vec{k}}(t)\sum\vec{e}_j a_{j,\vec{k}}(t)\cdot\sum\vec{e}_j a_{j,\vec{k}}(t)\right)\right\}, \qquad (13)$$

where $\sum(\ldots)$ means $\sum_{j=0}^{18}(\ldots)$. Equation (13) is the so-called PMLBE for the 3-D kinetic-based DDS. The PMLBE contains 5 bifurcation parameters, which are relaxation time (τ) from the LBE, splitting factor (β) for separating large and sub-grid motion scales, and wavevector components (k_1, k_2, k_3) from the Fourier space. It contains three power orders of $a_{j,\vec{k}}(t)$ after we neglect the terms higher than the 3rd order.

Identification of laminar and turbulent behavior We search for laminar and turbulent flow behavior through the time series and the pattern of power spectral density (PSD). With the specified bifurcation parameters and initial conditions, the time series for the Fourier coefficients $a_{j,\vec{k}}$ are generated by performing time evolution via Eq. (13). Then the PSD can be calculated from the time series. The software package 'pwelch' in MATLAB is used to estimate PSDs. In 'pwelch', we select the Hanning window; the number of input data points is 2^{13}, and the number of overlapped samples is 2^{12}. The DDS is classified as divergence if its time series does not converge. When a time series is convergent, we calculate PSD from the time series. In our previous work [40], we have demonstrated that the PMLBE can capture laminar behaviors of periodic, subharmonic, n-period, and quasi-periodic, and turbulent behaviors of noisy periodic with harmonic, noisy subharmonic, noisy quasi-periodic, and broadband power spectra. The laminar and turbulent power spectra were determined by the number and pattern of peaks in a PSD. We predefined the splitting factor β $(= 0.7)$ from experience. By varying the bifurcation parameters over the ranges of $0.5 < \tau < 1$ and $0.01 < k_a < 1$ with $a = 1,2,3$, we have studied more than 30 thousand combinations of bifurcation parameters to get results for that work.

In this work, we further study how the PMLBE and the selection of the bifurcation parameters affect the DDS to capture laminar and turbulent behavior. Understanding the PMLBE and the selection of bifurcation parameters is important to successfully apply the DDS into an LES of pulsatile turbulence. Based on the experience from the previous work [40], we only use the number of peaks, N=1000, on the PSD to distinguish the two behaviors.

3 Results

In this section, we present our numerical experiments on how power orders in the PMLBE and the five bifurcation parameters affect the capturing of the laminar and turbulent behavior. To set up the computation of this 3-D kinetic DDS, we select the range of τ as $0.6 \leq \tau \leq 1.2$, the range of k_a $(a = 1,2,3)$ as $0 \leq k_a \leq 1$, and the range of splitting factor as $0.5 \leq \beta \leq 0.8$. For each bifurcation parameter, we uniformly divide the range into 10 points. Thus, we have a total of 100,000 combination sets of the five bifurcation parameters. In the LBM, we often select $\delta x = \delta t = 1$, meaning the particles stream one lattice unit per time step, thus, c=1 in Eq. (2). The initial value of the SGS information $a_{j,\vec{k}}$ and large-scale information $\tilde{f}_i$ are given as follows. By assigning velocity components and density, the initial condition of $\tilde{f}_i$ $(i = 0, \dots, 18)$ can be calculated from the equilibrium Eq. (2), under the assumption that the DDS is in equilibrium initially. For the SGS, the initial conditions used in the following numerical experiments are $\vec{u}^* = (0.1445, 0.1014, 0.1758)$ and r^*=0.1. For the large scale, the initial conditions are $\tilde{\vec{u}} = (1.758, 1.445, 1.014)$ and $\tilde{r}$=1.0. Basically, the number of particles and the velocity for large scale are set to be 10 times larger than the SGS variables.

The PMLBE contains three power orders of the dynamic variable: $a_{j,\vec{k}}(t)$, $a^2_{j,\vec{k}}(t)$, and $a^3_{j,\vec{k}}(t)$. As the LBM is no more than the 2nd order accuracy in space and 1st order accuracy in time, we want to explore up to what order of power is needed in PMLBE. In terms of the computation cost, the fewer terms, the faster computation. If we neglect only the 3rd order terms and both the 2nd and 3rd order terms, Eq. (13) becomes

$$a_{i,\vec{k}}(t+\delta t) = \left(1 - \delta t \vec{e}_i \cdot \vec{k} - \frac{1}{\tau}\right) a_{i,\vec{k}}(t) + \frac{\omega_i}{\tau}\left[\sum a_{j,\vec{k}}(t) + \frac{3\vec{e}_i \cdot \sum \vec{e}_j a_{j,\vec{k}}(t)}{c^2}\right] + \frac{9(1-\beta)\omega_i}{2\tau\left(\sum \tilde{f}_j\right)^2 c^4}\Big\{\sum \tilde{f}_j \left[2\left(\vec{e}_i \cdot \sum \vec{e}_j \tilde{f}_j\right)\left(\vec{e}_i \cdot \sum \vec{e}_j a_{j,\vec{k}}(t)\right) + \left(\vec{e}_i \cdot \sum \vec{e}_j a_{j,\vec{k}}(t)\right)^2\right] - \Big[\sum a_{j,\vec{k}}(t)\left(\vec{e}_i \cdot \sum \vec{e}_j \tilde{f}_j\right)^2 + 2\sum a_{j,\vec{k}}(t)\left(\vec{e}_i \cdot \sum \vec{e}_j \tilde{f}_j\right)\left(\vec{e}_i \cdot \sum \vec{e}_j a_{j,\vec{k}}(t)\right)\Big] - \frac{\sum \tilde{f}_j c^2}{3}\left(\sum \vec{e}_j \tilde{f}_j \cdot \sum \vec{e}_j a_{j,\vec{k}}(t) + \sum \vec{e}_j a_{j,\vec{k}}(t) \cdot \sum \vec{e}_j a_{j,\vec{k}}(t)\right) + \frac{c^2}{3}\left(\sum a_{j,\vec{k}}(t) \sum \vec{e}_j \tilde{f}_j \cdot \sum \vec{e}_j \tilde{f}_j + \sum a_{j,\vec{k}}(t) \sum \vec{e}_j \tilde{f}_j \cdot \sum \vec{e}_j a_{j,\vec{k}}(t)\right)\Big\}, \quad (14)$$

and

$$a_{i,\vec{k}}(t+\delta t) = \left(1 - \delta t \vec{e}_i \cdot \vec{k} - \frac{1}{\tau}\right) a_{i,\vec{k}}(t) + \frac{\omega_i}{\tau}\left[\sum a_{j,\vec{k}}(t) + \frac{3\vec{e}_i \cdot \sum \vec{e}_j a_{j,\vec{k}}(t)}{c^2}\right] + \frac{9(1-\beta)\omega_i}{2\tau\left(\sum \tilde{f}_j\right)^2 c^4}\Big[2\sum \tilde{f}_j \left(\vec{e}_i \cdot \sum \vec{e}_j \tilde{f}_j\right)\left(\vec{e}_i \cdot \sum \vec{e}_j a_{j,\vec{k}}(t)\right) - \sum a_{j,\vec{k}}(t)\left(\vec{e}_i \cdot \sum \vec{e}_j \tilde{f}_j\right)^2 - \frac{\sum \tilde{f}_j c^2}{3} \sum \vec{e}_j \tilde{f}_j \cdot \sum \vec{e}_j a_{j,\vec{k}}(t) + \frac{c^2}{3} \sum a_{j,\vec{k}}(t) \sum \vec{e}_j \tilde{f}_j \cdot \sum \vec{e}_j \tilde{f}_j\Big], \quad (15)$$

respectively.

Behavior / DDS	Laminar	Turbulent
Eq. (13)	4.37%	0.13%
Eq. (14)	7.47%	0.37%

Table 1 Comparison of the capability to capture laminar and turbulent behavior between the 3rd order DDS (Eq. 13) and 2nd order DDS (Eq. 14)

Within the specified ranges of the bifurcation parameters, Eq. (15) captures neither laminar nor turbulent behavior as no time series is convergent. This is because the DDS only contains the 1st order $a_{i,\vec{k}}(t)$, which is too simple to capture flow dynamics. Whereas both Eqs. (13) and (14) can capture laminar and turbulent behaviors. Among the total 100,000 bifurcation parameter points, Eqs. (13) and (14) capture 4373 and 7472 laminar behaviors and 127 and 365 turbulent behaviors, respectively. The corresponding percentages are listed in Table 1. Considering Eq. (14) is more computationally efficient than Eq. (13) as it has fewer terms, we will focus on Eq. (14) for the remaining study. We now sort the laminar and turbulent behaviors in terms of β, τ, and k_a $(a = 1,2,3)$ and calculate the percentage out of the corresponding number of laminar or turbulent behaviors one by one. The percentage distributions are shown in Table 2. For each bifurcation parameter, there exists a maximum percentage. For laminar behavior, β=0.73, τ=1.0, $k_1 = 0.33$, $k_2 = 0.22$,and $k_3 = 0.22$ forms the optimal combination of bifurcation parameters. Whereas the optimal combination for turbulent behavior is β=0.6, τ=1.0, $k_1 = 0.11$, $k_2 = 0.22$,and $k_3 = 0.11$. In general, the wavevector components should correspond to the same value as they are isotropic. The differences, 0.33 vs. 0.22 in laminar behavior and 0.11 vs. 0.22 in turbulent behavior might be due to the sparse point distribution in the range.

Laminar behavior	β	0.50	0.53	0.57	0.60	0.63	0.67	0.70	**0.73**	0.77	0.80
	%	0.28	1.32	3.80	7.57	11.18	14.01	15.85	**16.51**	15.71	13.76
	τ	0.6	0.67	0.73	0.80	0.87	0.93	**1.00**	1.07	1.13	1.20
	%	0.21	0.94	2.68	6.88	12.43	15.46	**16.13**	15.91	14.82	14.55
	k_1	0	0.11	0.22	**0.33**	0.44	0.56	0.67	0.78	0.89	1.0
	%	6.71	13.72	18.48	**19.61**	18.00	13.61	7.68	2.15	0.04	0.00
	k_2	0	0.11	**0.22**	0.33	0.44	0.56	0.67	0.78	0.89	1.0
	%	11.75	16.07	**20.21**	20.16	16.37	10.80	4.35	0.29	0.00	0.00
	k_3	0	0.11	**0.22**	0.33	0.44	0.56	0.67	0.78	0.89	1.0
	%	17.12	21.77	**23.61**	19.49	12.55	4.87	0.59	0.00	0.00	0.00
Turbulent Behavior	β	0.50	0.53	0.57	**0.60**	0.63	0.67	0.70	0.73	0.77	0.80
	%	0.82	9.32	17.53	**20.00**	19.45	12.33	9.32	4.11	5.75	1.37
	τ	0.6	0.67	0.73	0.80	0.87	0.93	**1.00**	1.07	1.13	1.20
	%	0.27	2.19	3.84	5.21	8.49	15.34	**16.16**	13.42	20.55	14.52
	k_1	0	**0.11**	0.22	0.33	0.44	0.56	0.67	0.78	0.89	1.0
	%	8.77	**22.19**	21.37	21.10	13.15	9.59	3.56	0.27	0.00	0.00
	k_2	0.00	0.11	**0.22**	0.33	0.44	0.56	0.67	0.78	0.89	1.0
	%	11.51	22.47	**23.56**	16.16	13.70	9.04	2.74	0.82	0.00	0.00
	k_3	0.00	**0.11**	0.22	0.33	0.44	0.56	0.67	0.78	0.89	1.0
	%	19.45	**27.67**	24.38	15.34	9.59	3.56	0.00	0.00	0.00	0.00

Table 2 Effects of bifurcation parameters on the capturing of laminar and turbulent behavior from Eq. (14).

3 Conclusions and Future Work

We have investigated how the power order terms and the bifurcation parameters in the PMLBE affect the capturing of laminar and turbulent behaviors. It is found that the 1st order PMLBE is divergent and thus not capable to capture either laminar or turbulent behaviors as it is too simple (linear). The 2nd order and 3rd order PMLBEs are both able to capture flow behaviors but the 2nd order DDS performs better with lower computation cost and more flow behaviors captured. Form the sorting of flow behavior capturing for each bifurcation parameter, we have identified two optimal bifurcation parameter sets: β=0.73, τ=1.0, $k_1 = 0.33$, $k_2 = 0.22$,and

$k_3 = 0.22$ for laminar behavior and β=0.6, τ=1.0, $k_1 = 0.11$, $k_2 = 0.22$,and $k_3 = 0.11$ for turbulent behavior, which will be useful for the specification of the bifurcation parameters when we introduce the DDS into our LES modeling of pulsatile flows. The immediate future work is to produce regime maps to further explore the effects of the PMLBE and the bifurcation parameters on the capturing of the specific patterns of laminar behaviors including periodic, subharmonic, n-period, and quasi-periodic, and turbulent behaviors of noisy periodic with harmonic, noisy subharmonic, noisy quasi-periodic, and broadband power spectra. It requires much finer points (close to continuous) in the range of each bifurcation thus the computation will be extremely high. To overcome this bottleneck, we are developing surrogate models using deep learning techniques. Trained by finite quality points from PMLBE, the surrogate models will capture the same laminar and turbulent behaviors with significantly reduced computation time. Meanwhile, the 3-D kinetic–based DDS will be applied in our LES modeling of pulsatile flows in near future.

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