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A novel coupling of noise reduction algorithms for particle flow simulations

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ABSTRACT

Proper orthogonal decomposition (POD) and its extension based on time-windows have been shown to greatly improve the effectiveness of recovering smooth ensemble solutions from noisy particle data. However, to successfully de-noise any molecular system, a large number of measurements still need to be provided. In order to achieve a better efficiency in processing time-dependent fields, we have combined POD with a well-established signal processing technique, wavelet-based thresholding. In this novel hybrid procedure, the wavelet filtering is applied within the POD domain and referred to as WAVinPOD. The algorithm exhibits promising results when applied to both synthetically generated signals and particle data. In this work, the simulations compare the performance of our new approach with standard POD or wavelet analysis in extracting smooth profiles from noisy velocity and density fields. Numerical examples include molecular dynamics and dissipative particle dynamics simulations of unsteady force- and shear-driven liquid flows, as well as phase separation phenomenon. Simulation results confirm that WAVinPOD preserves the dimensionality reduction obtained using POD, while improving its filtering properties through the sparse representation of data in wavelet basis. This paper shows that WAVinPOD outperforms the other estimators for both synthetically generated signals and particle-based measurements, achieving a higher signal-to-noise ratio from a smaller number of samples. The new filtering methodology offers significant computational savings, particularly for multi-scale applications seeking to couple continuum informations with atomistic models. It is the first time that a rigorous analysis has compared de-noising techniques for particle-based fluid simulations.

1. Introduction

Particle-based simulations, e.g. molecular dynamics, are well suited to investigate the effects of fluid–solid interactions and are widely used to study a broad range of complex physical phenomena [1]. For example, molecular dynamics (MD) can be performed to solve classical many-body problems from various fields, including rheology, tribology, and biological systems at the molecular scale. Dissipative particle dynamics (DPD) is another particle-based method that is gaining popularity and

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can be viewed as a coarse-graining of molecular dynamics (a DPD particle is a collection of MD molecules), allowing for mesoscale modelling of complex fluids, e.g. surfactant solutions.

In particle simulations, the system evolves from some initial condition to a final state, preserving constraints of motion. The output of the calculation is a system variable, X, as a function of time. According to the quasi-ergodic hypothesis, the mean value of a sampled quantity, $X(t)$, for an equilibrium system is equal to its ensemble average, $\langle X \rangle$. In general, the mean of a property is often subject to fluctuations making any statistical interpretation of the data challenging. Uncertainty in the measurements is increased through thermal fluctuations introduced by thermostats and sampling with a finite number of particles. These effects are generally referred to as *noise*, and a major challenge in particle simulations is to filter, or *de-noise*, the fluctuations to obtain an accurate ensemble prediction. To produce a *good* approximation, cumulative averaging over large time intervals can be performed, but the computational intensity of the simulations is then substantially increased. Additionally, in unsteady flow simulations, it is difficult to establish the number of time-steps over which the averaging should performed. The development of an efficient filtering technique that provides clean particle distribution functions and smooth gradients, particularly when coupling across different length and time-scales (multi-scale modelling), is highly desirable.

Proper orthogonal decomposition (POD) is a statistical method that identifies a low-dimensional space by separating independent variations from linearly dependent aspects of data. In other words, it extracts correlations from the measurements through a low-rank approximation. The use of POD in interpreting coherent structures in turbulence is now well established [2] and the technique has recently been applied as a noise reduction tool for MD and DPD simulations [3]. Wavelet thresholding, on the other hand, is a non-linear procedure pioneered by Donoho and Johnstone [4] that was proposed from several optimality criteria, such as asymptotic minimax. It allows the analysis of signals at different resolutions and smooths out unwanted variations at a chosen level of detail. Both techniques have had some success but retain certain weaknesses. Classical orthogonal methods require large matrices to extract de-noised information, whereas wavelet-based thresholding is sensitive to the choice of filters used for the wavelet transform (WT). Wavelet thresholding can also over-smooth analysed signals or introduce *Gibbs*-like oscillations [5], and does not reduce the dimensionality as well as POD.

The aim of this work is to develop a method with the capability to improve the efficiency of estimating the unknown structures from particle-based simulation by solving the statistical inverse problem. We will briefly outline the theoretical basis of POD and wavelet transforms, along with their application to noise filtering. For particle-based simulations, we discuss an extension to POD based on *time windows* (WPOD) [3]. By considering their strengths and weaknesses, we propose a new approach, WAVinPOD, which shows good potential for improving the analysis of simulation data. Our method allows for a more efficient noise reduction, obtaining higher average signal-to-noise ratios and smaller errors in L_2 and Frobenius norm than either POD or wavelet thresholding alone. Our paper is organised as follows: the basic theory for the methods is briefly described in Sec. 2, followed by the results of applying WAVinPOD, POD, and wavelet thresholding to synthetic signals. A comparison of the performance of each technique in de-noising particle-based simulations is presented in Sec. 4, followed by some concluding remarks on the new approach.

2. Theoretical background

This section provides a brief mathematical description of POD and wavelet thresholding. Our novel procedure, WAVinPOD, is also introduced. A more extensive discussion on proper orthogonal decomposition can be found in Refs. [2,6,7], and a more detailed review of wavelet theory is given in Refs. [8–10].

2.1. Proper orthogonal decomposition

Proper orthogonal decomposition is often used for finding a low-dimensional approximate description of high-dimensional data that contains a large number of interrelated variables. In addition to order reduction, POD is also applied for feature extraction by revealing coherent structures within the data. The method was introduced to the turbulence community by Lumley [11]. However, the same procedure was developed independently by several groups and is known under different names, including *Principal Component Analysis* and the *Karhunen–Loéve Decomposition*, depending on the area of application.

The basis of POD is to describe a function, $f(t,x)$, as a finite sum of its variables:

$$f(t,x) \approx \sum_{n=1}^{r} \alpha_n(t)\phi_n(x), \tag{1}$$

where t and x represent the temporal and spatial components of the data, respectively. When r (a total number of elements) approaches infinity, the estimate becomes exact. Applying POD establishes a set of orthonormal basis functions (modes), $\phi_n(x)$, such that the first $k < r$ terms provide the best approximation of the function $f(t,x)$. Define an element $A(\tau^s, x)$ of the real $N \times M$ matrix as a measurement from the x-th probe taken at the τ^s-th time instant. An orthogonal decomposition