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A reduced-order model for heat transfer in multiphase flow and practical aspects of the proper orthogonal decomposition

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ABSTRACT

This paper discusses two practical aspects of reduced-order models (ROMs) based on proper orthogonal decomposition (POD) and presents the derivation and implementation of a ROM for non-isothermal multiphase flow. The POD method calculates basis functions for a reduced-order representation of two-phase flow by calculating the eigenvectors of an autocorrelation matrix composed of snapshots of the flow. The flow is divided into transient and quasi-steady regions and two methods are shown for clustering snapshots in the transient region. Both methods reduce error as compared to the constant sampling case. The ROM for non-isothermal flow was developed using numerical results from a full-order computational fluid dynamics model for a two-dimensional non-isothermal fluidized bed. Excellent agreement is shown between the reduced- and full-order models. The composition of the autocorrelation matrix is also considered for an isothermal case. An approach treating field variables separately is shown to produce less error than a coupled approach.

1. Introduction

Recent advances in computer hardware have led to a wide range of new possibilities in the computational simulation of fluid flow. Despite these advances, some flows contain sufficient complexity to make numerical simulation a challenge. Multiphase flow in fluidized beds is one example. These flows contain dominant spatial features that are difficult to identify and process variables whose interactions are difficult to assess. High-fidelity, low cost models for these flows are a necessity for both design and control. One promising approach for this problem is reduced-order modeling.

Reduced-order models (ROMs) have come into wide use in the simulation of fluid flows and seek to identify the dominant spatial characteristics of the flow and then solve for the weighting coefficients for these "modes" instead of solving the governing equations at many grid points (Dowell et al., 1999). This allows a reduction in the degrees of freedom of the governing systems of equations from tens of thousands or more to hundreds or less.

Early attempts to model fluid flows with ROMs focused on solving for small perturbations around a steady nonlinear flow field (Florea & Hall, 1994; Florea, Hall, & Cizmas, 1997, 1998; Hall, 1994; Hall, Florea, & Lanzkron, 1995). More recently, the validity of these methods has been extended through the application of proper orthogonal decomposition (POD) (Cizmas & Palacios, 2003; Park & Lee, 1998; Utturkar, Zhang, & Shyy, 2005). The POD method has been used to identify the dominant spatial features of multiphase flow (Cizmas, Palacios, O'Brien, & Syamlal, 2003) and a reduced-order model based on POD has been implemented to reduce the computational time needed to simulate a two-dimensional isothermal multiphase flow at minimum fluidization (Yuan, Cizmas, & O'Brien, 2005).

Interpolation methods have been used to calculate the temporal weighting functions (Ding, Wu, He, & Tao, 2008) and to enhance the robustness of the ROM for parameter changes (Farhat & Amsallem, 2008). Error estimation in POD-based ROMs has been assessed to determine the regions of validity for POD (Homescu, Petzold, & Serban, 2005). Specific error estimates have been given for POD-based ROMs for the Navier–Stokes equations (Wang & Ma, 2009) and random fuzzy variables have been used to quantify error propagation through POD-based ROMs (Chen & Hoo, 2010).

The effect of projecting partial differential equations (PDEs) with stable numerical solution methods onto truncated bases has been carefully considered (Rempfer, 2000). The stability requirements of the Runge–Kutta integration of the ODEs resulting from the Galerkin projection of the Navier–Stokes equations onto a suitable basis has been established (Giles, 1997). Further, the stability of the POD-based ROM for the linearized Euler equations, including the effect of the boundary conditions, has been analyzed (Barone, Kalashnikova, Segalman, & Thornquist, 2009). Stabilization schemes have been developed to improve the accuracy of

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POD-based ROMs (Gloerfelt, 2008; Iollo, Lanteri, & Desideri, 2000; Kalb & Deane, 2007). Spectral viscosity methods have been used to correct long-term errors due to dissipative PDEs (Sirisup & Karniadakis, 2004). The addition of shift-modes has been used to improve the accuracy of models in transient flow regimes (Noack, Afanasiev, Morzynski, Tadmor, & Thiele, 2003).

Reviews of POD-based ROMs have been presented (Dowell & Tang, 2003; Lucia, Beran, & Silva, 2004). Specifically, POD based ROMs have been used to model rocket nozzles for flow control (Lucia, Pachter, & Beran, 2002) and for modeling airfoil cascades in the frequency domain (Epureanu, Dowell, & Hall, 2000). Models have been presented for deforming grids both with (Anttonen, King, & Beran, 2003) and without multi-POD (Anttonen, King, & Beran, 2005) as well as for flow over heaving (Lewin & Haj-Hariri, 2005) and deforming airfoils (Bourguet, Braza, & Dervieux, 2011).

POD-based ROMs have been implemented for modeling aero-icing (Nakakita, Nadarajah, & Habashi, 2010) as well as to study flow-fields for use in particle modeling (O'Donnell & Helenbrook, 2007). Steady supersonic flow has been predictively modeled (Qamar & Sanghi, 2009). A finite element approach for solving Burgers' equation has also been reduced using POD (Luo, Zhou, & Yang, 2009). Recently, adaptive POD has been developed and applied to the reaction/diffusion equations to model chemical reactions (Singer & Green, 2009) and the transition to turbulence around a NACA 0012 airfoil has been modeled and analyzed using a POD-based ROM (Bourguet, Braza, Sevrain, & Bouhadji, 2009).

POD has been used extensively to analyze the low-dimensional characteristics of experimental data (Tinney, Glauser, Eaton, & Taylor, 2006; Tinney, Glauser, & Ukeiley, 2008) and computational simulations (Caraballo, Samimy, Scott, Narayanan, & DeBonis, 2003; Noack, Papas, & Monkewitz, 2005). The effect of spatial grid (Tinney, 2009) and time step (Brenner, Cizmas, O'Brien, & Breault, 2009) refinement has been assessed. The challenges inherent to applying POD to problems with moving discontinuities have been considered (Lucia, King, & Beran, 2003). Non-POD ROMs for moving discontinuities have been developed (Maple, King, Wolff, & Orkwis, 2003). Very recently, methods for augmenting the POD basis (Brenner, Fontenot, Cizmas, O'Brien, & Breault, 2010) and adding artificial viscosity to POD-based ROMs have been proposed for modeling moving discontinuities (Borggaard, Iliescu, & Wang, 2011).

POD-based ROMs have also been used to model non-isothermal flows (Gunes, 2002) and methods have been devised to properly couple the energy variable (Rowley, Colonius, & Murray, 2004). They have been put to practical use in modeling the temperature field in glass furnaces (Op den Camp, Verheijen, Huisman, & Backx, 2008) and, when used as part of a multi-scale model, heat transfer in computer data centers (Samadiani & Joshi, 2010). Recently, a genetic algorithm has been used to replace the Galerkin projection in the POD-based ROM to improve robustness and more easily incorporate boundary conditions (Alonso, Velazquez, & Vega, 2009).

The objective of this paper is to present the derivation, implementation and verification of a reduced-order model for non-isothermal multiphase flow and to describe some practical aspects that arise in the modeling of flow using ROMs based on POD. These aspects include: (i) the effect of time sampling on approximation error, and (ii) the influence of the form of the autocorrelation matrix from which the basis functions are computed on the approximation error. In the next section we present the hydrodynamic model used to represent the fluidized bed. This is followed by a brief discussion of the algorithm used to solve the governing equations specified by this model. Next, the POD method is described and the reduced-order model for two-dimensional isothermal flow is summarized. The non-isothermal reduced-order model is derived and two model problems are described. Next, methods for sampling the data and creating the autocorrelation matrix are presented, including the results of the study. Verification of the non-isothermal model is completed and the results are discussed. Conclusions are subsequently presented.

2. Hydrodynamic model

The fluidized bed was modeled using a two-phase hydrodynamic model (Syamlal, Rogers, & O'Brien, 1994). The governing equations were based on the laws of mass, momentum and energy conservation. In this model, the gas- and solids-phase mass balance equations are given by

$$\frac{\partial}{\partial t}(\epsilon_m \rho_m) + \nabla \cdot (\epsilon_m \rho_m \vec{v}_m) = 0 \tag{1}$$

where m denotes the phase, ρ is the density, ϵ is the volume fraction, and $\vec{v}$ is the velocity vector.

The gas- and solids-phase momentum balance equations are given by

$$\frac{\partial}{\partial t}(\epsilon_m \rho_m \vec{v}_m) + \nabla \cdot (\epsilon_m \rho_m \vec{v}_m \vec{v}_m) = -\epsilon_m \nabla p_g + \nabla \cdot \bar{\bar{S}}_m + F_{gs}(\vec{v}_s - \vec{v}_g) + \epsilon_m \rho_m \vec{g}. \tag{2}$$

Here the first two terms of the right hand side represent the normal and shear surface forces, respectively. The third term is the contribution of the drag force on the solids and the fourth term is the body force due to gravity.

The gas-phase energy balance equation is

$$\epsilon_g \rho_g C_{pg}\left(\frac{\partial T_g}{\partial t} + \vec{v}_g \cdot \nabla T_g\right) = -\nabla \cdot \vec{q}_g + \gamma_g (T_s - T_g) - \Delta H_g + \gamma_{Rg}(T_{Rg}^4 - T_g^4) \tag{3}$$

and the solids-phase energy balance equation is given by

$$\epsilon_s \rho_s C_{ps}\left(\frac{\partial T_s}{\partial t} + \vec{v}_s \cdot \nabla T_s\right) = -\nabla \cdot \vec{q}_s + \gamma_s (T_s - T_g) - \Delta H_s + \gamma_{Rs}(T_{Rs}^4 - T_s^4), \tag{4}$$

where $\vec{q}_m$ is the conductive heat flux, ΔH_m is the heat of reaction and γ_{Rm} is the heat transfer coefficient. Here m denotes the phase, either gas or solids. The constant pressure specific heat coefficients for the gas- and solids-phases are C_{pg} and C_{ps}, respectively.

3. Full-order model

The term "full-order model" (FOM) refers to the numerical model used to solve these governing equations and generate the database of snapshots used by the POD method. The FOM was developed at the Department of Energy's National Energy Technology Laboratory and the implementation is the Multiphase Flow with Interface eXchanges (MFIX) code (Syamlal et al., 1994). For isothermal cases, this code solves a discretized version of Eq. (2) and uses correction algorithms that satisfy Eq. (1) to calculate the gas pressure and solids volume fraction. For non-isothermal cases, discretized versions of Eqs. (3) and (4) are also solved.

The solutions of these equations were collected throughout the time domain to form a database of snapshots for both the isothermal and non-isothermal cases. For the isothermal case, snapshots of six field variables were captured: x- and y-direction gas and solids velocities, gas pressure, and void fraction ($\epsilon = \epsilon_g = 1 - \epsilon_s$). For the non-isothermal case, the gas and solids temperature fields were also collected.