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Particle transport modeling in pulmonary airways with high-order elements

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ABSTRACT

Inhaled particles can be either harmful (e.g., smoke, exhaust, viruses) or beneficial (e.g., a therapeutic drug). The accurate and computationally efficient simulation of particle transport and deposition remains a challenge because it requires the simultaneous solution of the Navier–Stokes equations and multiple advection–diffusion mass transport equations when the particles are modeled as multiple mono-dispersed populations. The solution of these equations requires that multiple length scales be resolved since the ratio of advection to diffusion varies among the different equations. Here, the spectral element method is examined because the high-order approximation provides greater flexibility in resolving multiple length scales. The problem geometry is based on the Weibel model A of the human airway for convergence tests and the first three generations of a typical rat airway for experimental validation. Particles in the size range 1 to 100 nm are simulated for deposition results. The particle concentration and flux were determined using meshes of varying coarseness to represent the geometry along with basis polynomials of order 5 to 11. The higher-order elements accurately propagate the short wavelengths contained in the advection–diffusion solution without sacrificing efficiency for the more computationally expensive Navier–Stokes solution. As the diffusion coefficient in the advection–diffusion equation decreases (i.e., particle size increases) the advantages of the spectral elements become apparent for the coupled system.

1. Introduction

The simulation of nano-particle transport (i.e., 1–100 nm particles) in the airways requires the solution of both the Navier–Stokes equations, which are based on an Eulerian reference frame, and multiple advection–diffusion equations, which are also based on an Eulerian reference frame. This coupled system of equations is often referred to as the Eulerian–Eulerian particle tracking problem, and applications range from pollution concentrations in the atmosphere to particle deposition in complex airways. Even though the Navier–Stokes equations and the advection–diffusion equations have a similar mathematical structure (i.e., both equations have diffusive and advective terms), the differences between them for specific problems can make this a computationally challenging, multi-physics problem. Accurate and efficient particle tracking through a complex geometry, such as the human airways, requires capturing the physical properties of both the fluid and particle fields. The focus here is on the development of an approximation strategy that is highly accurate, scalable, and computationally efficient.

Many previous models of nano-particle transport in the airways have been based on 1st- or 2nd-order finite volume or finite difference methods to resolve the fluid field represented by the Navier–Stokes equations, and then generating a particle solution as a post-processing step using a similar method after each time step [1–6]. As we will demonstrate, when the fluid velocity field is turbulent or the particle concentration transport is advection dominated, low-order methods are less efficient than high-order methods for fully resolving all the scales of motions. Most previous studies have also approximated the turbulent, high-order modes using turbulence models with Reynolds averaged Navier–Stokes equations (RANS) or subgrid scale models with large eddy simulations (LES). For weakly turbulent and transition flows, these models may not adequately represent the fluid solution and lead to an inaccurate particle solution since the flows lack the inertial subrange needed for subgrid scale models [7].

Direct numerical simulation (DNS) resolves all the scales of motion but is computationally expensive and scales with the Reynolds number ($\sim Re^{9/4}$) [8]. Low-order methods quickly become computationally infeasible for even moderate values of the Reynolds number. By using higher-order methods of approximation, the higher modes of the flow and physical dissipation can be directly resolved and accurately accounted for with fewer grid points due to minimal numerical dispersion and diffusion error [9]. Therefore, for flows of moderate Reynolds numbers (<4000), all scales of motion can be resolved with modest computational effort. It has been shown that bifurcating biological flows with Reynolds numbers

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less than 3000 can be fully resolved with high-order spectral element simulations using one to four million grid points [7,10].

Since the particle solution in the problem of interest is sufficiently dilute (< 100 $\mu g/m^3$, [11]) and the motion of the particles does not affect the fluid motion, it is possible to completely decouple the particle solution from the fluid field. For particles larger than 1 M, particle motion can be tracked by integrating the equation of motion to ascertain the position. The Lagrangian method depends on determining the trajectories of many particles to statistically study the concentration changes over time. This method has been shown to be useful for tracking larger, more advection dominated particles. However, the trajectories can become very complex within even simple flow fields, and it may require integrating millions of particle trajectories to converge to a solution [12,13]. By treating the particle concentration as a field, rather than individual particles, the solution can be obtained similarly to the fluid field [14]. The transport of the particle concentration field is computed using the advection–diffusion equation, which shares many mathematical properties with the Navier–Stokes equations. However, the advection–diffusion equation contains relevant modes that are much sharper than the Navier–Stokes counterpart when the diffusion coefficient is significantly less than the inverse Reynolds number, and the need to properly resolve and propagate the high-order modes becomes even more important. Spectral elements, which can capture the higher-order modes with a modest number of discretization nodes, can be far more effective than low-order approaches at propagating a particle solution without overburdening the fluid counterpart by requiring a highly refined mesh. Spectral elements have been demonstrated to accurately and efficiently propagate the solution to the advection–diffusion equation [15,16]. They have also been demonstrated in a coupled system. However, previous studies either used buoyant particles or utilized the analogous heat convection–diffusion equation; both of which have diffusion parameters on the same order as the inverse Reynolds number[14,17–20].

This study demonstrates the Eulerian–Eulerian method for particle tracking using high-order spectral elements. The simulations present the unique issues associated with a coupled system with diffusion coefficients at least an order of magnitude less than the inverse Reynolds number. Prior work on the coupled system has been relatively neglected except for a few cases where the inverse Reynolds number of the fluid is always equal to the diffusion coefficient or analogous parameter. The problem parameters were chosen to reflect particle deposition in an idealized human central airway. This problem has been studied by several different groups using low-order methods and contains weakly turbulent pulsing flow if the larynx is not included and a turbulent laryngeal jet if the larynx is included [1,2,12,21]. In some cases, highly accurate fluid and particle fields are necessary to properly analyze particle deposition and develop targeted drug delivery systems, and high-order methods are well suited to these situations. If a highly accurate numerical solution is not needed or if other sources of error are significant, high-order methods may not be appropriate. This investigation explores the importance of the mesh, approximation order, and time-step size in simulating advective particles in an incompressible fluid field. As validation of the simulation results, the particle deposition predictions are compared with experimental results on a rodent's central airway.

2. Methods

2.1. Spectral element method and discretization

The spectral element method (SEM) contains several key attributes that can be both beneficial and detrimental to the simulation depending on application. A single mesh can be generated to model a given domain, and with SEM, the order of approximation can be changed from one simulation to next without modifying the original mesh. SEM adds secondary nodes between element vertices based on the Gauss–Lobatto–Legendre (GLL) points to create a far more dense mesh. The number of degrees of freedom for one-dimension can be defined as $n \approx EN$, where E is the number of elements and N is the order of approximation. For three-dimensions, $n \approx EN^3$, and the mesh is isometrically refined with increasing N. Typical values of N range from 4 – 16, and the nodes are increasingly clustered towards the element boundaries as the polynomial order is increased [7]. The high-order approximations lead to significantly lower diffusion and dispersion error than their low-order counterparts, even with fewer degrees of freedom. Also, due to the natural matrix-free operator evaluation and tensor-product meshes, the computation costs scale optimally [22]. These are valuable assets when assessing a problem with a large range of scales of motion, such as particle tracking in turbulent flows.

The SEM method for $\mathbf{P}_N$–$\mathbf{P}_{N-2}$ discretization of the Navier–Stokes equations, where $\mathbf{P}$ represents a polynomial of degree N, is based on the work of Fischer et al. [15,22–24] and Deville et al. [9] and combined with similar discretization for the advection–diffusion equation. The Navier–Stokes equation in the domain Ω is

$$\frac{\partial u}{\partial t} + \mathbf{u}\cdot\Delta\mathbf{u} = -\nabla_p + \frac{1}{Re}\nabla^2\mathbf{u} \quad \nabla\cdot\mathbf{u} = 0, \tag{1}$$

where $\mathbf{u}$ is a vector representing the velocity field, t is the time, and p is a pressure that is normalized with density. Eq. 1 requires appropriate initial and boundary conditions. The values of velocity, time, and pressure are all properly scaled and in non-dimensional form using a characteristic velocity U, length scale L, and the kinematic viscosity, ν. For this work, the characteristic velocity is set to the average inlet velocity at the peak flow rate, and the characteristic length scale is set to the inlet diameter of the target geometry. The kinematic viscosity is taken to be that of air at 20°C. The Reynolds number, $\mathrm{Re} = UL/\nu$, is a non-dimensional quantity relating the fluid's inertial effects to its viscous effects.

Once the velocity field is solved at a given time step, it can be used in the advection–diffusion equation to determine the particle concentration. The unsteady advection–diffusion equation,

$$\frac{dC_j}{dt} + \mathbf{u}\cdot\nabla C_j = \mathcal{D}_j\Delta C_j \tag{2}$$

is also subject to appropriate initial and boundary conditions. Here the $\mathbf{u}$ is the divergence free velocity field computed previously with the Navier–Stokes equations (Eq. 1). The concentration of monodispersed particles is the scalar, C, and D is the diffusion coefficient, which is dependent upon the physical characteristics of the particle (e.g., particle size and shape). In this case, the diffusion coefficient is a dimensionless quantity representing the ratio of particle diffusion to advection. Multiple unsteady advection–diffusion equations are required to model a poly-dispersed particle flow.

The advection–diffusion equation is mathematically similar to the Navier–Stokes equations except that it is propagating a scalar species rather than a vector quantity, and it lacks the pressure term and continuity constraint. The discretization is similar to that described previously for the Navier–Stokes equations. Since the advection–diffusion calculation is passive and does not affect the fluid velocity field, it can be solved multiple times for various values of the diffusion coefficient at each time step without recomputing the velocity solution. Thus, a wide range of particle size concentrations can be determined without the repeated computational burden that is associated with the Navier–Stokes equations.