DIRECTLY RESOLVING PARTICLES IN AN ELECTRIC FIELD AND APPLICATIONS TO HETEROGENEOUS DIELECTRIC MATERIALS AND BIOMEDICAL ENGINEERING

Qianlong Liu[a)] & Kenneth L. Reifsnider
DOE Energy Frontier Research Center, Department of Mechanical Engineering, University of South Carolina, Columbia, SC, 29208, U.S.A.

Summary We extend Prosperetti's seminal Physalis method for finite-sized particles in fluid flow to directly resolve dielectric particles in an electric field. The method can be used to accurately predict, for the first time, the local charge distribution, force and torque on particles and to accurately account for the mutual fluid-particle, particle-particle, and particle-boundary interactions. The method is very accurate and able to satisfy exactly the discontinuous interface conditions, efficient to simulate up to one million particles using a PC, and unique in the computational world. These features make the method especially important to applications to heterogeneous dielectric materials and biomedical engineering.

Prosperetti seminally developed the Physalis method [1] to directly resolve finite-sized particles in fluid flow [2, 3, 4]. Recently, we extended the method to directly resolve dielectric particles in an electric field [5, 6, 7]. The method can be used to accurately predict, for the first time, the local charge distribution, force and torque on particles and to accurately account for the mutual fluid-particle, particle-particle, and particle-boundary interactions. The method has been shown to be remarkably efficient and convenient to investigate heterogeneous mixtures of dielectrics and conductors consisting of up to one million circular or one hundred thousand 3D spherical particles. The discontinuous interface conditions between two different media are satisfied exactly in the method. The features make the method to have important applications to heterogeneous dielectric materials and biomedical engineering.

Understanding force and moments associated with local morphology is essential in porous heterogeneous functional materials (now called HeteroFoaMs [8] in the literature). HeteroFoaMs are the physical foundation for many natural and man-made material systems such as the lungs and vascular systems in animals, the electrodes of batteries and fuel cells, and functional membranes used in medical devices and fuel processing. The multi-physics of the functionality of these material systems across multi-scales in time and space is typically averaged or represented by "effective properties" of a fictitious continuum that is thought to have the same global response as the mixture of discrete phases. Unfortunately this approximate approach teaches us little (if anything) about the local physics, and neglects the subtleties of the local geometries and morphology. The effective property approach also fails to tell us how to construct and synthesize such a material system, using the physics as a guide at the local level. In a battery, for example, what local geometry is best to capture the functionality of the transport, oxidation/reduction, diffusion, electrochemistry, and conduction at the local level that is the heart of that system? Such questions must be answered with a viable local representation that can recover the physics and the morphology as a foundation for understanding and synthesis. The complex local morphologies could be simulated by proper assemblies of such particles if they can be deployed in close proximity to each other. In heterogeneous materials, distinct phases can have the same or different material state. The phases are separated by phase boundaries, e.g. solid/solid, solid/liquid, solid/gas, etc. boundaries. If the phases interact and act together to create properties and behavior that is peculiar to their specific combination, they are said to be a "material system." The classical literature concentrates on estimating the global "average" or "effective" properties of such materials, but does not provide methods or approaches that capture the local details of the interfaces between the phases, which control many of the system properties and performance. Our approach directly resolves the local geometry, tackles the mutual interactions, and calculates the local surface charge distribution that are essential in the heterogeneous dielectric material system.

The accurate calculation of force and torque on dielectric particles is also essential in many applications in biomedical engineering, particularly when the strong mutual interactions among field, particles, and walls are accurately and efficiently considered for dense particles. Owing to their dielectric properties, all dielectric particles experience dielectrophoretic (DEP) forces and torques, when subjected to electric fields, and interact with the field. These particles include some with important applications, e.g. cells, microparticles, nanoparticles, virus, DNA, and proteins. The DEP, electrorotation, orientational, and anisotropy phenomena have significant applications in many areas such as biomedical research, microfluidics, nanoparticle assembly, stem cell research, and optical traps to manipulate, separate, sort, and characterize the particles. Our numerical method accurately accounts for the mutual interactions, the frequency-dependent properties, orientation and anisotropy effects, the forces and torques on finite-sized particles (for the first time), close particles, multilayered shells, and particles up to one million. The approach opens new frontiers in biomedical engineering research.

The Physalis method is an iterative Immersed Boundary/spectral method designed to efficiently and accurately tackle complex geometries. The underlying idea of the Physalis method is to create a cage and to apply a spectral general analytical solution around a discontinuity in a surrounding field to enable the accommodation of physical and geometric discontinuities. An example of the cage is shown in Fig. 1(a). It avoids complex geometric singularities and satisfies

[a)] Corresponding author. E-mail: liu246@mailbox.sc.edu.

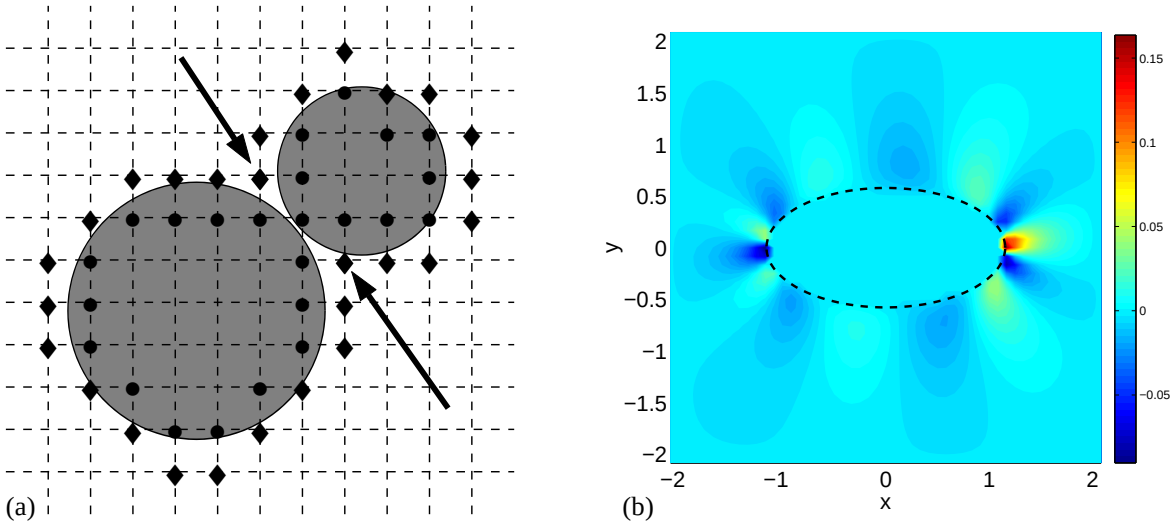

Figure 1. (a) Cage mesh points for complex geometries and the discontinuous interface conditions; (b) Numerical errors.

exactly the discontinuous interface conditions. The fundamental difference between the Physalis method and other methods is that a spectral general analytical solution is used to satisfied exactly the interface conditions in the former, while penalty methods, Lagrange multipliers, interpolation, or extrapolation are used to enforce the interface conditions in the weak sense or approximately in the latter. For example, the general solution for 2D dielectric particles can be written as

$$V = b + \sum_{n=1}^{\infty} \left[1 + \frac{\epsilon^o - \epsilon^i}{\epsilon^o + \epsilon^i} \left(\frac{r_p}{r} \right)^{2n} \right] r^n (a_n \cos n\theta + b_n \sin n\theta),$$

where b, a_n, and b_n are coefficients to be determined for the convergent solutions. Fig. 1(b) shows the numerical errors, indicating that the numerical solutions inside the particle are much more accurate than those outside of the particles. The difference implies that the closed form of the general analytical solutions is nearly recovered with very accurate solutions for these coefficients.

It is this fundamental difference that results in much more important features regarding derivative quantities, which are typically related to the gradient of the field variable but are much more important for many applications than the field variable. For other methods, the accuracy of the gradient is typically degraded during postprocessing. In contrast, in the Physalis method, the coefficients in the spectral general analytical solution are even more accurate than the solved field. Since the derivative quantities of interest can be expressed simply as algebraic functions of these coefficients, their accuracy does not degrade but rather are more accurate than the solved field. These derivative quantities include local charge distribution, force and torque on the particle, central to many engineering applications.

The convergent results yield accurate coefficients and thus the spectral analytical solutions at the interface. The derivative of the analytical field gives the accurate local surface charge distributions which show the charge and energy storage of the heterogeneous dielectric material system. The surface integrations give the force and torque on particles. In contrast to the DEP approximation which keeps only the interactions of the lowest modes, our approach gives the exact results, including all of the interactions between modes, and shows that the interactions between higher order modes may dominate as the particles are close. For non-spherical particles, we also show more complex features of the orientation and anisotropy effects. These are crucial to applications of heterogeneous biomedical systems, for example the formation of pearl chains of biological particles. For more details, we refer to our recent papers [5, 6, 7]. The present research was supported by the Department of Energy under funding for an EFRC (the HeteroFoaM Center), grant no. DE-SC0001061.

References

[1] Zhang Z., Prosperetti A.,: A second-order method for three-dimensional particle simulation. *J. Comput. Phys.* **210**:292–324, 2005.
[2] Zhang Q., Prosperetti A.,: Pressure-driven flow in a two-dimensional channel with porous walls. *J. Fluid Mech.* **631**:1–21, 2009.
[3] Liu Q., Prosperetti A.,: Wall effects on a rotating sphere. *J. Fluid Mech.* **657**:1–21, 2010.
[4] Liu Q., Prosperetti A.,: Pressure-driven flow in a channel with porous walls. *J. Fluid Mech.* **679**:77–100 2011.
[5] Liu Q.: Physalis Method for Heterogeneous Mixtures of Dielectrics and Conductors: Accurately Simulating One Million Particles Using a PC. *J. Comput. Phys.* **230**:8256–8274 2011.
[6] Liu Q.: Directly resolving particles in an electric field: local charge, force, torque, and applications. *Int. J. Numer. Meth. Engng* **In press**:DOI:10.1002/nme.3330 2011.
[7] Liu Q., Reifsnider K. L.: Heterogeneous mixtures of elliptical particles: directly resolving local and global properties and responses. *Comp. Meth. Appl. Mech. Eng.* **Submitted for publication**: 2012.
[8] Chiu, W. K. S., Virkar, A. V., Zhao, F., Reifsnider, K. L., Nelson, G. L., Rabbi, F., Liu, Q.: HeteroFoaMs: Electrode Modeling in Nano-Structured Heterogeneous Materials for Energy Systems. *J. Fuel Cell Sci. Technol.* **9**:011019 2012.