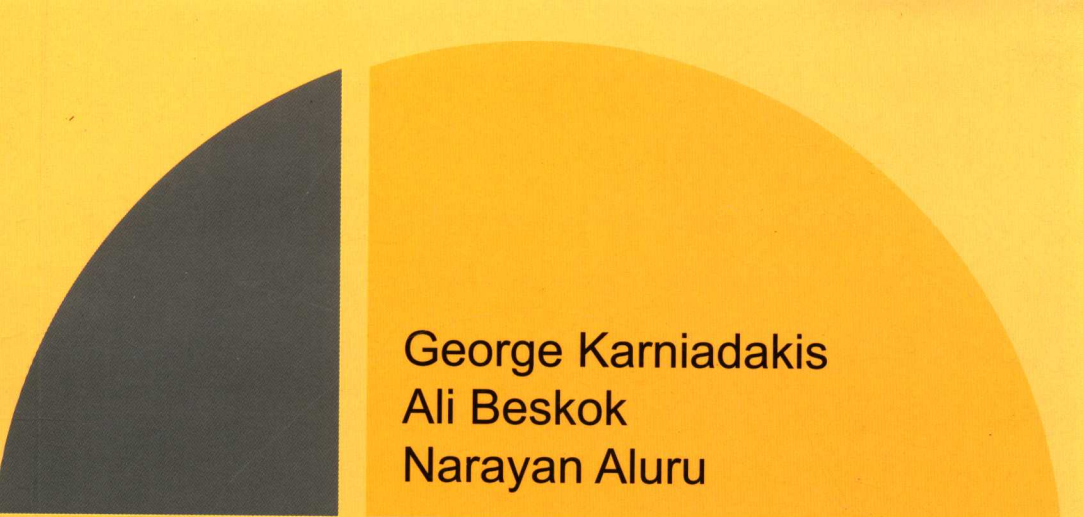




George Karniadakis
Ali Beskok
Narayan Aluru

Interdisciplinary Applied Mathematics

Microflows and Nanoflows

Fundamentals and Simulation

微流和纳米流的原理与模拟

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Foreword by Chih-Ming Ho

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著 者: George Karniadakis, Ali Beskok and Narayan Aluru

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George Karniadakis
Center for Fluid Mechanics
Brown University
Providence, RI 02912
USA

Ali Beskok
Department of Mechanical Engineering
Texas A & M University
College Station, TX 77843
USA

Narayan Aluru
Beckmann Institute for the Advancement
of Science and Technology
University of Illinois at Urbana-Champaign
Urbana, IL 61801
USA

Editors

S.S. Antman
Department of Mathematics and
Institute for Physical Science and Technology
University of Maryland
College Park, MD 20742
USA
ssa@math.umd.edu

J.E. Marsden
Control and Dynamical Systems
Mail Code 107-81
California Institute of Technology
Pasadena, CA 91125
USA
marsden@cds.caltech.edu

L. Sirovich
Division of Applied Mathematics
Brown University
Providence, RI 02912
USA
chico@camelot.mssm.edu

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by George Karniadakis, Ali Beskok and Narayan Aluru

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Volume 29

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Imaging, Vision, and Graphics

Mathematical Biology

L. Glass, J.D. Murray

Mechanics and Materials

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The purpose of this series is to meet the current and future needs for the interaction between various science and technology areas on the one hand and mathematics on the other. This is done, firstly, by encouraging the ways that mathematics may be applied in traditional areas, as well as point towards new and innovative areas of applications; and, secondly, by encouraging other scientific disciplines to engage in a dialog with mathematicians outlining their problems to both access new methods and suggest innovative developments within mathematics itself.

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Foreword by Chih-Ming Ho

Fluid flow through small channels has become a popular research topic due to the emergence of biochemical lab-on-the-chip systems and micro electromechanical system fabrication technologies, which began in the late 1980s. This book provides a comprehensive summary of using computational tools (Chapters 14–18) to describe fluid flow in micro and nano configurations. Although many fundamental issues that are not observed in macro flows are prominent in microscale fluid dynamics, the flow length scale is still much larger than the molecular length scale, allowing for the continuum hypothesis to still hold in most cases (Chapter 1). However, the typical Reynolds number is much less than unity, due to the small transverse length scale, which results in a high-velocity gradient. For example, a 10^5 sec^{-1} shear rate is not an uncommon operating condition, and thus high viscous forces are prevalent, resulting in hundreds or thousands of ψ hydrodynamic pressure drops across a single fluidic network. Consequently, it is not a trivial task to design micropumps that are able to deliver the required pressure head without suffering debilitating leakage. Electrokinetic and surface tension forces (Chapters 7 and 8) are used as alternatives to move the embedded particles and/or bulk fluid. The high viscous damping also removes any chance for hydrodynamic instabilities, which are essential for effective mixing. Mixing in micro devices is often critical to the overall system's viability (Chapter 9). Using electrokinetic force to reach chaotic mixing is an interesting research topic. In these cases, the electrical properties, e.g., dielectric constants, rather than the viscosity determine the efficiency of transport.

The National Nano Initiative, established first in the USA (www.nano.gov)

and subsequently in many other countries, has pushed the length scale range of interest from microns down to nanometers. Flows in these regimes start to challenge the fundamental assumptions of continuum mechanics (Chapter 1). The effects of the molecules in the bulk of the fluid versus those molecules in proximity to a solid boundary become differentiated (Chapter 10). These are extremely intriguing aspects to be investigated for flows in small configurations. The demarcation between the continuum and the noncontinuum boundary has yet to be determined and inevitably will have a tremendous influence on the understanding of small-scale fluid behavior as well as system design.

The ratio between the size of the channel and that of the molecule is not the only parameter that validates the continuum assumption. In biological applications, for example, molecules with large conformation changes, electrical charges, and polar structures are frequently encountered. These variables make it impossible to determine whether a flow can be considered a continuum based only on a ratio of sizes (Chapter 11). When a continuum flow of a Newtonian fluid is assumed, molecular effects are defined by the governing equations of traditional fluid mechanics. Interactions among fluid molecules are expressed by a physical constant, which is viscosity. The no-slip condition represents the interactions between the fluid and the solid surface molecules. Both viscosity and the no-slip condition are concepts developed under the framework of continuum. Deviations from the bulk viscosity and the no-slip condition can lead to other results due to the breakdown of the continuum assumption (Chapters 2 and 10).

In the nanoflow regime, not many molecules are situated far away from the channel wall. Therefore, the motion of the bulk fluid is significantly affected by the potential fields generated by the molecules near the solid wall. Near the surface, the fluid molecules do not flow freely. At a distance of a few fluid molecule layers above the surface, the flow has very different physical constants from the bulk flow. The surface effects are strong not only in nano configurations (Chapter 10); even in microfluidic devices, the performance, e.g., surface fouling, is dependent on the surface property. We frequently spend more time on modifying the surface properties than on designing and fabricating devices. As a result of our limited understanding of fluidic behavior within nanoscale channels (Chapters 10 through 13), many vital systematic processes of today's technology are arduously, yet imperfectly, designed. Delivering and stopping a picoliter volume of fluid to a precise location with high accuracy as well as the separation and mixing of nano/micro particles in a fluid medium of high ionic concentration remains a challenging task. By furthering the understanding of fluid interactions in the nano world, many of the interesting mysteries and challenges that have puzzled scientists will be revealed.

Preface

We are grateful to Springer, in particular to Senior Editor Michael J. Heugelen, for accepting this book for publication. The main difference between fluid mechanics at microscale and in macroscale can be possibly classified into four aspects:

- noncontinuum effects
- surface-dominated effects
- low Reynolds number effects, and
- multiscale and multiphysics effects

1. Gas Flow (Chapters 2–6)
 2. Liquid Flow (Chapters 7–13)
 3. Simulation Techniques (Chapters 14–15)
- Some of these effects can be simulated with relatively simple models. However, others require sophisticated numerical methods. In the microscale, the flow is *granular* for liquids and *rarefied* for gases, and the walls “move.” In addition, other phenomena such as thermal creep, electrokinetics, viscous heating, anomalous diffusion, and even quantum and chemical effects may become important. Most important, the material of the wall and the quality of its surface play a very important role in the momentum and energy exchange. One could argue that at least for gases the situation is similar to low-pressure high-altitude aeronautical flows, which were studied extensively more than 40 years ago. Indeed, there is a similarity in a certain regime of the Knudsen number. However, most gas microflows correspond to a low Reynolds number and low Mach number, in contrast to their aeronautical counterparts. Moreover, the typical microgeometries are of very large aspect ratio, and this poses more challenges for numerical modeling, but also creates opportunities for obtaining semianalytical results. For liquids no such analogy exists and their dynamics in confined

In the early 1990s, microchannel flow experiments at the University of Pennsylvania by the groups of H. Bau and J. Zemel revealed intriguing results for both liquids and gases that sparked excitement and new interest in the study of low Reynolds number flows in microscale. Another influential development at about the same time was the fabrication of the first microchannel with integrated pressure sensors by the groups of C.M. Ho (UCLA) and Y.C. Tai (Caltech). While the experimental results obtained at the University of Pennsylvania indicated global deviations of microflows from canonical flows, pointwise measurements for gas flows with pressure sensors, and later with temperature sensors, revealed a new flow behavior at microscale not captured by the familiar continuum theory. In microgeometries the flow is *granular* for liquids and *rarefied* for gases, and the walls “move.” In addition, other phenomena such as thermal creep, electrokinetics, viscous heating, anomalous diffusion, and even quantum and chemical effects may become important. Most important, the material of the wall and the quality of its surface play a very important role in the momentum and energy exchange. One could argue that at least for gases the situation is similar to low-pressure high-altitude aeronautical flows, which were studied extensively more than 40 years ago. Indeed, there is a similarity in a certain regime of the Knudsen number. However, most gas microflows correspond to a low Reynolds number and low Mach number, in contrast to their aeronautical counterparts. Moreover, the typical microgeometries are of very large aspect ratio, and this poses more challenges for numerical modeling, but also creates opportunities for obtaining semianalytical results. For liquids no such analogy exists and their dynamics in confined

co-authors (G.K. and A.B.) are very pleased to have a new co-author, Prof. N.R. Arora, whose unique contributions have made this new volume pos-

microgeometries, especially at the submicron range, is much more complex.

The main differences between fluid mechanics at microscales and in the macrodomain can be broadly classified into four areas:

- Noncontinuum effects,
- surface-dominated effects,
- low Reynolds number effects, and
- multiscale and multiphysics effects.

Some of these effects can be simulated with relatively simple modifications of the standard numerical procedures of computational fluid dynamics. However, others require new simulation approaches not used typically in the macrodomain, based on multiscale algorithms. For gas microflows, compressibility effects are very important because of relatively large density gradients, although the Mach number is typically low. Depending on the degree of rarefaction, corrections at the boundary or everywhere in the domain need to be incorporated. Increased rarefaction effects may make the constitutive models for the stress tensor and the heat flux vector in the Navier–Stokes equations invalid. On the other hand, working with the Boltzmann equation or with molecular dynamics implementation of Newton’s law directly is computationally prohibitive for complex microgeometries. The same is true for liquids, since atomistic simulation based on Newton’s law for individual atoms is restricted to extremely small volumes. Therefore, mesoscopic and hybrid atomistic–continuum methods need to be employed for both gas and liquid microflows to deal effectively with deviations from the continuum and to provide a link with the large domain sizes. Most important, microflows occur in devices that involve simultaneous action in the flow, electrical, mechanical, thermal, and other domains. This, in turn, implies that fast and flexible algorithms and low-dimensional modeling are required to make full-system simulation feasible, similar to the achievements of the 1980s in VLSI simulation.

There has been significant progress in the development of microfluidics and nanofluidics at the application as well as at the fundamental and simulation levels since the publication of an earlier volume of this book (2001). We have, therefore, undertaken the “nontrivial” task of updating the book in order to include these new developments. The current book covers length scales from angstroms to microns (and beyond), while the first volume covered scales from one hundred nanometers to microns (and beyond). We have maintained the emphasis on fundamental concepts with a mix of semi-analytical, experimental, and numerical results, and have outlined their relevance to modeling and analyzing functional devices. The first two co-authors (GK and AB) are very pleased to have a new co-author, Prof. N.R. Aluru, whose unique contributions have made this new volume pos-

sible. We are also grateful to Springer, and in particular to Senior Editor in Mathematics Dr. Achi Dosanjh, who gave us this opportunity.

The majority of the new developments are in Chapters 7 through 18, most of which contain totally new material. In addition, all other Chapters (1 through 6) have been modified, and in some cases new material has also been added. We have divided the material into three main categories by subject:

1. Gas Flows (Chapters 2–6).
2. Liquid Flows (Chapters 7–13)
3. Simulation Techniques (Chapters 14–18)

The last category also contains two Chapters (17 and 18) on low-dimensional modeling and simulation, in addition to chapters on multiscale modeling of gas and liquid flows. The entire material can be used in a two-semester first- or second-year graduate course. Also, selected chapters can be used for a short course or an undergraduate-level course.

In the following we present a brief overview of the material covered in each chapter.

In Chapter 1 we provide highlights of the many concepts and devices that we will discuss in detail in the subsequent chapters. For historic reasons, we start with some prototype Micro-Electro-Mechanical-Systems (MEMS) devices and discuss such fundamental concepts as breakdown of constitutive laws, new flow regimes, and modeling issues encountered in microfluidic and nanofluidic systems. We also address the question of full-system simulation of microsystems and introduce the concept of macromodeling.

In Chapter 2 we first present the basic equations of fluid dynamics for both incompressible and compressible flows, and discuss appropriate nondimensionalizations. Subsequently, we consider the compressible Navier–Stokes equations and develop a general boundary condition for velocity slip. The validity of this model is assessed in subsequent chapters.

In Chapter 3 we consider shear-driven gas flows with the objective of modeling several microsystem components. In order to circumvent the difficulty of understanding the flow physics for complex engineering geometries, we concentrate on prototype flows such as the linear and oscillatory Couette flows in the slip, transition, and free-molecular flow regimes, and flow in shear-driven microcavities and microgrooves.

In Chapter 4 we present pressure-driven gas flows in the slip, transition and free molecular flow regimes. In the slip flow regime, we first validate simulation results based on compressible Navier–Stokes solutions employing various slip models introduced in Chapter 2. In addition, we examine the accuracy of the one-dimensional Fanno theory for microchannel flows, and we study inlet flows and effects of roughness. In the transition and free-molecular regime we develop a unified model for predicting the velocity

profile and mass flowrate for pipe and duct flows.

In Chapter 5 we consider heat transfer in gas microflows. In the first section we concentrate on the thermal creep (transpiration) effects that may be important in channels with tangential temperature gradients on their surfaces. We also study other temperature-induced flows and investigate the validity of the heat conduction equation in the limit of zero Knudsen number. In the second and third sections we investigate the combined effects of thermal creep, heat conduction, and convection in pressure-, force-, and shear-driven channel flows.

In Chapter 6 we consider rarefied gas flows encountered in applications other than simple microchannels. In the first section, we present the lubrication theory and its application to the slider bearing and squeezed film problems. In the second and third sections, we consider separated flows in internal and external geometries in the *slip flow* regime in order to investigate the validity of continuum-based slip models under flow separation. In the fourth section, we present theoretical and numerical results for Stokes flow past a sphere including rarefaction effects. In the fifth section we summarize important results on gas flows through microfilters used for capturing and detecting airborne biological and chemical particles. In the last section, we consider high-speed rarefied flows in micronozzles, which are used for controlling the motion of microsatellites.

In Chapter 7 we present basic concepts and a mathematical formulation of microflow control and pumping using electrokinetic effects, which do not require any moving components. We cover electroosmotic and electrophoretic transport in detail both for steady and time-periodic flows, and we discuss simple models for the near-wall flow. We also present dielectrophoresis, which enables separation and detection of similar size particles based on their polarizability.

In Chapter 8 we consider surface tension-driven flows and capillary phenomena involving wetting and spreading of liquid thin films and droplets. For microfluidic delivery on open surfaces, electrowetting and thermocapillary along with dielectrophoresis have been employed to move continuous and discrete streams of fluid. A new method of actuation exploits optical beams and photoconductor materials in conjunction with electrowetting. Such electrically or chemically defined paths can be reconfigured dynamically using electronically addressable arrays that respond to electric potential, temperature, or laser beams and control the direction, timing, and speed of fluid droplets. In addition to the above themes, we also study bubble transport in capillaries including both classical theoretical results and more recent theoretical and experimental results for electrokinetic flows.

In Chapter 9 we consider micromixers and chaotic advection. In microchannels the flow is laminar and steady, so diffusion is controlled solely by the diffusivity coefficient of the medium, thus requiring excessive amounts of time for complete mixing. To this end, chaotic advection has been exploited in applications to accelerate mixing at very low speeds. Here, we

present the basic ideas behind chaotic advection, and discuss examples of passive and active mixers that have been used in microfluidic applications. We also provide effective quantitative measures of characterizing mixing.

In Chapter 10 we consider simple liquids in nanochannels described by standard Lennard–Jones potentials. A key difference between the simulation of the fluidic transport in confined nanochannels and at macroscopic scales is that the well-established continuum theories based on Navier–Stokes equations may not be valid in confined nanochannels. Therefore, atomistic scale simulations are required to shed fundamental insight on fluid transport. Here we discuss density distribution, diffusion transport, and validity of the Navier–Stokes equations. In the last section we discuss in detail the slip condition at solid–liquid interfaces, and present experimental and computational results as well as conceptual models of slip. We also revisit the lubrication problem and present the Reynolds–Vinogradova theory for hydrophobic surfaces.

In Chapter 11 we focus on water and its properties in various forms; this is one of the most actively investigated areas because of its importance in nature. The anomalies that exist in the bulk properties of water make it very interesting and challenging for research, and a vast deal of literature is already available. Even though water has been studied for more than 100 years now, its properties are far from understood. With the advances in fabrication of nanochannels that are only a few molecular diameters in critical dimension, the properties of water in confined nanochannels have recently received a great deal of attention. In this chapter, after introducing some definitions and atomistic models for water, we present the static and dynamic behavior of water in confined nanochannels.

In Chapter 12 we discuss the fundamentals and simulation of electroosmotic flow in nanochannels. The basic theory was covered in Chapter 7, so here the limitations of the continuum theory for electroosmotic flow in nanochannels are identified by presenting a detailed comparison between continuum and MD simulations. Specifically, the significance of the finite size of the ions and the discrete nature of the solvent molecules are highlighted. A slip boundary condition that can be used in the hydrodynamic theory for nanochannel electroosmotic flows is presented. Finally, the physical mechanisms that lead to the charge inversion and flow reversal phenomena in nanochannel electroosmotic flows are discussed.

In Chapter 13 we focus on functional fluids and on functionalized devices, specifically nanotubes. The possibility to target and precisely control the electrooptical as well as the mechanical properties of microstructures in a dynamic way using external fields has opened new horizons in microfluidics research including new concepts and protocols for micro- and nanofabrication. On the more fundamental level, systematic studies of paramagnetic particles or charged particles and their dynamics offer insight into the role of Brownian noise in microsystems as well as conceptual differences between deterministic and stochastic modeling. This is studied in the first

part of this chapter. In the second part of the chapter we study carbon nanotubes and their properties. Carbon nanotubes with diameters as small as 5–10 Å are comparable to the diameters encountered in biological ion channels. By *functionalizing* carbon nanotubes, it is possible to tune the surface properties of carbon nanotubes to investigate the function of a variety of ion channels. To enable such advances, it is important to understand how water, ions, and various electrolytes interact with carbon nanotubes and functionalized nanotubes.

In Chapter 14 we discuss representative numerical methods for continuum based simulations. The significant geometric complexity of flows in microsystems suggests that finite elements are more suitable than finite differences, while high-order accuracy is required for efficient discretization. To this end, we focus on spectral element and meshless methods in stationary and moving domains. We also discuss methods for modeling particulate microflows and focus on the force coupling method, a particularly fast approach suitable for three-dimensional simulations. These methods represent three different classes of discretization philosophies and have been used with success in diverse applications of microsystems.

In Chapter 15 we discuss theory and numerical methodologies for simulating gas flows at the mesoscopic and atomistic levels. Such a description is necessary for gases in the transition and free-molecular regimes. First, we present the Direct Simulation Monte Carlo (DSMC) method, a stochastic approach suitable for gases. We discuss limitations and errors in the steady version of DSMC and subsequently present a similar analysis for the unsteady DSMC. In order to bridge scales between the continuum and atomistic scales we present the Schwarz iterative coupling algorithm and apply it to modeling microfilters. We then give an overview of the Boltzmann equation, describing in some detail gas-surface interactions, and include benchmark solutions for validation of numerical codes and of macromodels. A main result relevant to accurately bridging microdynamics and macrodynamics is the Boltzmann inequality, which we also discuss in the last section on lattice Boltzmann methods (LBM). These methods represent a “minimal” discrete form of the Boltzmann equation, and they are applicable to both compressible and incompressible flows; in fact, the majority of LBM applications focuses on incompressible flows.

In Chapter 16 we discuss theory and numerical methodologies for simulating liquid flows at the atomistic and mesoscopic levels. The atomistic description is necessary for liquids contained in domains with dimension of fewer than ten molecules. First, we present the Molecular Dynamics (MD) method, a deterministic approach suitable for liquids. We explain details of the algorithm and focus on the various potentials and thermostats that can be used. This selection is crucial for reliable simulations of liquids at the nanoscale. In the next section we consider various approaches in coupling atomistic with mesoscopic and continuum level. Such coupling is quite difficult, and no fully satisfactory coupling algorithms have been developed

yet, although significant progress has been made. An alternative method is to embed an MD simulation in a continuum simulation, which we demonstrate in the context of electroosmotic flow in a nanochannel. In the last section we discuss a new method, developed in the late 1990s primarily in Europe: the dissipative particle dynamics (DPD) method. It has features of both LBM and MD algorithms and can be thought of as a coarse-grained version of MD.

In Chapter 17 we turn our attention to simulating full systems across heterogeneous domains, i.e., fluid, thermal, electrical, structural, chemical, etc. To this end, we introduce several reduced-order modeling techniques for analyzing microsystems. Specifically, techniques such as generalized Kirchhoff networks, black box models, and Galerkin methods are described in detail. In black box models, detailed results from simulations are used to construct simplified and more abstract models. Methods such as nonlinear static models and linear and nonlinear dynamic models are described under the framework of black box models. Finally, Galerkin methods, where the basic idea is to create a set of coupled ordinary differential equations, are described. The advantages and limitations of the various techniques are highlighted.

Finally, in Chapter 18 we discuss the application of these techniques to several examples in microflows. First, we present circuit and device models and their application to lab-on-a-chip systems. Then, we discuss reduced-order modeling of squeezed film damping by applying equivalent circuit, Galerkin, mixed-level, and black box models. Next, we present a compact model for electrowetting. Finally, we summarize some of the software packages that are available for reduced-order simulation.

We are very grateful to Prof. Chih-Ming Ho who agreed to provide a foreword to our book. We would like to thank all our colleagues from many different countries who have allowed us to use their work in the previous and this new and expanded edition of the book. We also want to thank Ms. Madeline Brewster at Brown University for her assistance with all aspects of this book, and our students who helped with formatting the figures, especially Vasileios Symeonidis, Pradipkumar Bahukudumbi, and Aveek Chatterjee. AB would like to thank his students I. Ahmed, P. Bahukudumbi, Prof. P. Dutta, Dr. J. Hahm, H.J. Kim, S. Kumar, Dr. J.H. Park, and Prof. C. Sert. The last author (NRA) would like to acknowledge the help of all his students, especially Chatterjee, De, Joseph, and Qiao for letting him use some of the results from their thesis work. NRA is very grateful to Profs. Karniadakis and Beskok for the opportunity to co-author this book with them. NRA would like to thank Profs. Dutton (Stanford), Hess (UIUC), Karniadakis (Brown), Law (Stanford), Pinsky (Stanford), Senturia (MIT), and White (MIT) for mentoring his career.

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Providence, Rhode Island, USA	George Em Karniadakis
College Station, Texas, USA	Ali Beskok
Urbana, Illinois, USA	Narayan R. Aluru

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