Organization Scheme

The book consists of 19 chapters, and all except the first are followed by exercises. These serve both to amplify the material already covered in each chapter and sometimes to introduce concepts not discussed elsewhere in the book. Some exercises are intended to help the student independently discover results that are otherwise well known in the literature. References cited in each chapter are collated (in alphabetical order by name of first author) at the end of each Part, instead of after each chapter. A number of illustrative (Fortran) programs are also available in connection with problems that require computational methods. In this electronic age, we have chosen to distribute this material via the national network; readers may log on to the *anonymous* user account on *flossie.che.wisc.edu* (IP number 128.104.170.10) and transfer source codes to their own machines. At the password prompt it is suggested that readers use their names (a password is not required) so that we may create a log record of the user community. The contents of the *anonymous* account have been subdivided along chapter lines. For example, the reader "John Doe" may access the boundary collocation program `mandr.for` of Chapter 13 by the following procedure:

```
% ftp flossie.che.wisc.edu
Name: anonymous
Anonymous user OK. Enter real ident... John Doe
* cd chapter13
* get mandr.for
* bye
```

In Chapter 1, we introduce characteristic scales for a range of problems in microhydrodynamics and the dimensional analysis leading to the governing equations for Stokes flow. In Chapter 2, we discuss a number of general properties of the Stokes equations, including fundamental theorems dealing with uniqueness and minimum energy dissipation. We also discuss the Lorentz reciprocal theorem, which is perhaps the theorem most often used in our book. The fundamental solution of the Stokes equations (the Green's dyadic for the Stokes equation is called the *Oseen tensor*) is derived along with the integral representation for the velocity and pressure fields.

The rest of the book is divided into three parts: Part II on the dynamics of a

single particle, Part III on hydrodynamic interactions, and Part IV on the computation of flow in complex geometries. Rather than attempt a comprehensive treatment of all aspects of viscous laminar flows, we shall focus our attention on a core set of themes for flow past a single particle that are readily generalized to encompass interactions between particles. We then show the connections between these analytical techniques and numerical techniques of Parts III and IV.

An understanding of the dynamics of a single particle is a prerequisite to everything else in the book, and many of the developments for multiparticle interactions are generalizations of results developed for a single particle. In Chapter 3, we derive the multipole expansion for a particle, starting from the integral representation for the velocity. For simple shapes, such as the sphere and ellipsoid, we show how the expansion can be truncated to obtain singularity solutions. The moments of the multipole expansion must be related to the given boundary conditions, and we show how this can be achieved by the use of the Faxén laws. We make a special effort to show the link between the singularity solutions and Faxén laws. The original derivation, by Faxén, required special properties of the sphere, thus obscuring the generality of this approach to particles of arbitrary shape.

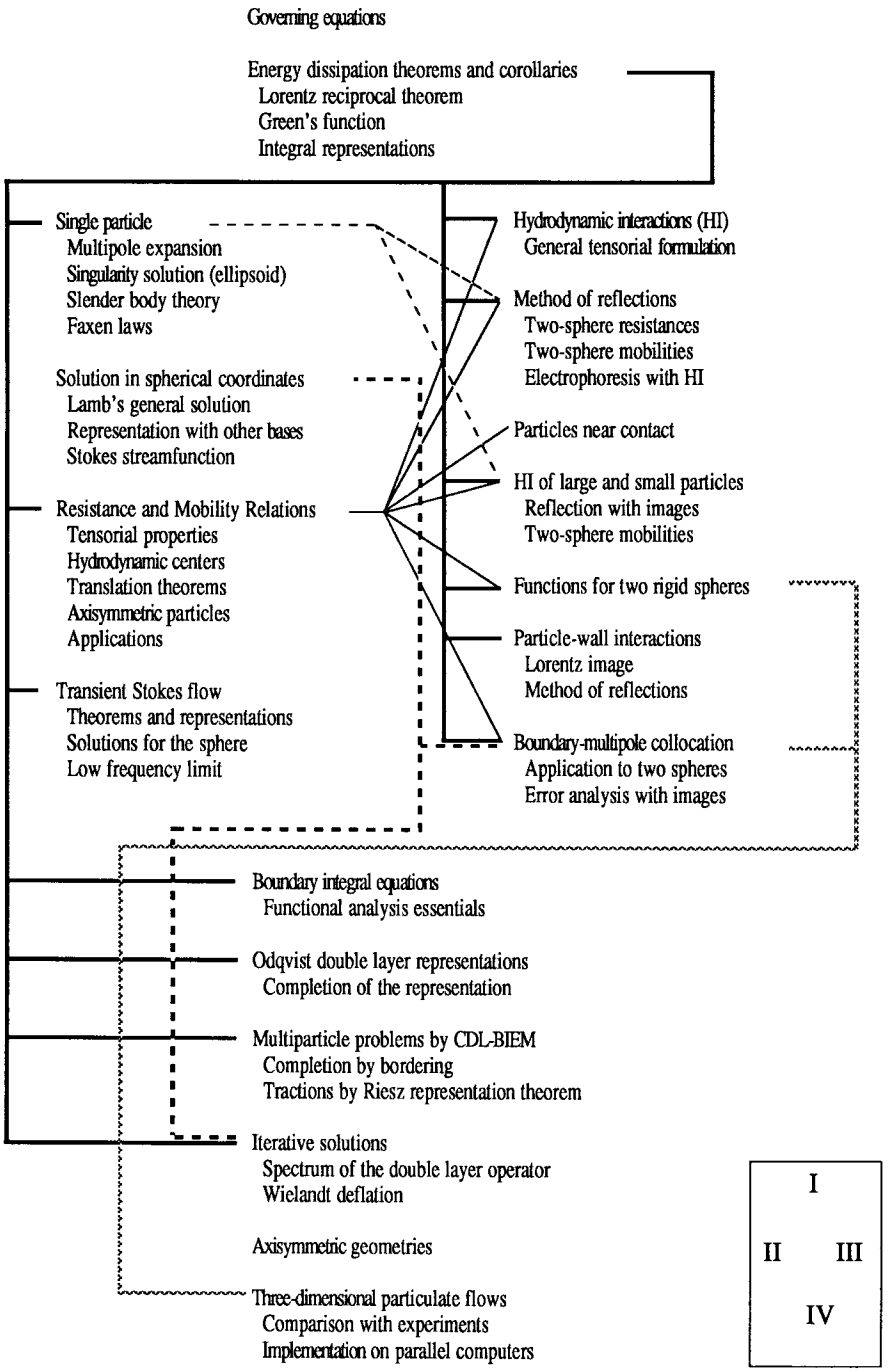
Chapter 4 discusses classical solution techniques for flow past a single sphere, including Lamb's general solution and the Stokes streamfunction. The connection with the more general multipole theory for a particle of arbitrary shape is brought out, thereby reinforcing the message that there is a unified structure for particulate Stokes flow.

The resistance and mobility relations for a single particle in unbounded flow are introduced in Chapter 5, along with inversion formulae for obtaining one set from another. Their use is illustrated with examples from the suspensions literature, including the rheology of a dilute suspension of spheroids and electrophoresis of a charged particle in an electric field. The examples illustrate how the resistance and mobility functions appear beyond the obvious context of trajectory calculations.

Chapter 6 presents an introduction to time-dependent Stokes flows, including the concepts of added mass and Basset forces. It is shown that in the limit of slow temporal variations, time-dependent effects appear at $O(\mathrm{Re}^{1/2})$, and a general method of obtaining the $O(\mathrm{Re}^{1/2})$ coefficient for particles of arbitrary shape is derived.

Part III, on hydrodynamic interactions, starts in Chapter 7 with general concepts of resistance and mobility relations between interacting particles of arbitrary shape. The rest of Part III is divided according to the separation between the particles.

For particles that are widely separated (Chapter 8), we use the method of reflections. The disturbance fields for each particle are written as multipole expansions, with the moment coefficients determined by the Faxén laws of Chapter 3. The iterative nature of the method is brought out with detailed examples on the interaction between spheres. For many-body problems the inversion from


Governing equations
Energy dissipation theorems and corollaries
Lorentz reciprocal theorem
Green's function
Integral representations
Single particle
Multipole expansion
Singularity solution (ellipsoid)
Slender body theory
Faxen laws
Solution in spherical coordinates
Lamb's general solution
Representation with other bases
Stokes streamfunction
Resistance and Mobility Relations
Tensorial properties
Hydrodynamic centers
Translation theorems
Axisymmetric particles
Applications
Transient Stokes flow
Theorems and representations
Solutions for the sphere
Low frequency limit
Hydrodynamic interactions (HI)
General tensorial formulation
Method of reflections
Two-sphere resistances
Two-sphere mobilities
Electrophoresis with HI
Particles near contact
HI of large and small particles
Reflection with images
Two-sphere mobilities
Functions for two rigid spheres
Particle-wall interactions
Lorentz image
Method of reflections
Boundary-multipole collocation
Application to two spheres
Error analysis with images
Boundary integral equations
Functional analysis essentials
Odqvist double layer representations
Completion of the representation
Multiparticle problems by CDL-BIEM
Completion by bordering
Tractions by Riesz representation theorem
Iterative solutions
Spectrum of the double layer operator
Wielandt deflation
Axisymmetric geometries
Three-dimensional particulate flows
Comparison with experiments
Implementation on parallel computers
I
II
III
IV

resistance to mobility relations becomes cumbersome, so a direct computational procedure for both resistance and mobility problems is derived.

In Chapter 9, we review methods for calculating the interaction between two nearly touching particles. For surfaces in relative motion (squeezing flows and shearing flows) we discuss the singular behavior of the resistance functions and show that these leading terms come from the dominant contributions in the gap region. The higher order nonsingular terms in these problems, as well as the resistance functions for surfaces moving in tandem as a rigid body, have contributions from all regions of the flow; in general, these terms can be obtained only by numerical techniques.

In Chapter 10, we consider interactions between large and small particles, especially at separation lengths that fall between the two grossly different sizes. The method of reflections is still applicable, but we can no longer truncate the multipole expansion for the reflections at the larger particle. We show how the reflections can be done by image methods, and a number of examples involving interactions between large and small spheres are given.

The interactions between two spheres deserve special attention because of the great interest and the large number of applications in suspensions research. In Chapter 11 we present a summary of all known analytical results for the entire collection of resistance and mobility functions that relate the force and hydrodynamic dipole moment (torque and stresslet) for two unequal spheres in a linear flow field. Several examples are given to illustrate the use of the formulae and tables.

The treatment of hydrodynamic interactions between a small particle and a wall is derived in Chapter 12 by a limiting process of the interaction between a small and large particle. By this manner, we derive the image of a point force (Stokeslet) near a plane wall and obtain the *Lorentz reflection principle* for the plane wall in a natural way. The extension to a planar fluid-fluid interface, *Lee's reflection lemma*, is also synthesized in this fashion. Here again, our goal is to use methods that emphasize the unified framework for Stokes flow.

For interactions between particles of simple shape, we show that boundary collocation applied to a truncated multipole expansion for each particle yields an effective numerical method (Chapter 13). The basis must be chosen so that contributions from the higher basis elements decay rapidly, and this point is illustrated with examples for spheroids of extreme aspect ratios. The convergence of the method is illustrated by comparison with the exact solution for the point force near a sphere. This problem serves as an excellent model for particle-particle interactions because moments of all orders are excited in the sphere.

We call Part IV "Foundations of Parallel Computational Microhydrodynamics." For complex geometries, the only way to capture the details of the particle or container boundary shape is to bring the Stokes singularities to the particle surface. The resulting class of numerical techniques is known as the *boundary integral (equation) methods.* Their distinct advantage over spatial methods, such as finite elements or finite differences, is *the reduction of dimensionality.* That

is, instead of a three-dimensional PDE, we solve a two-dimensional (boundary) integral equation, in which the unknowns are densities of the Stokes singularities distributed over the boundary of the fluid domain, and even infinite fluid domains without a container boundary cause no problems. Furthermore, although the mathematical theory places a smoothness requirement on the surface, this restriction can be loosened in the actual numerical procedure.

By going to a two-dimensional formulation, we reduce both the amount of work for discretization and the number of variables needed for getting some required numerical resolution. Yet at first glance it may appear that our emphasis on boundary methods goes against current trends in computational technology. For example, the emergence of fast and inexpensive processors suggests that the most interesting innovations will occur in parallel computational architectures. Indeed, fundamental physical barriers, such as the speed of light and the size of an atom, place a limitation on the speed and integration of a single processor. It is unlikely that in the future a single superprocessor would be orders of magnitude faster than those available today. Therefore the obvious trend to follow is parallel processing, which presents certain requirements on the algorithms to be implemented. It is easy to visualize how the equations from the finite element method or the finite difference method, which are just relations connecting only near neighbors, are implemented on parallel computers. Clearly these methods inherently possess a certain "graininess" that corresponds to a multiprocessor architecture. Boundary methods, on the other hand, lead to dense systems for the following reason. The fields emanating from the Stokes singularities on one boundary element propagate in all directions with a fairly persistent algebraic decay, so that each element interacts with all other elements to some extent. The mapping of such dense systems to parallel architectures is a nontrivial problem. Moreover, for the more popular boundary integral formulation for Stokes flow based on the single layer potential, we obtain the ill-posed Fredholm integral equation of the first kind and the associated ill-conditioning in the discretized equations. The onset of this ill-conditioning can be predicted using the techniques developed in Chapter 17 and represents a significant barrier to the application of this approach to complex geometries.

With this environment in mind, the emphasis of Part IV is on the construction of a new boundary integral method, which we call the Completed Double Layer Boundary Integral Equation Method (CDL-BIEM). The name is derived from the fact that Stokes double layer densities are employed, but since the double layers alone do not form a complete basis, a completion procedure is necessary. Using techniques from linear operator theory, we show that the solution of the general mobility problem of N particles in either a bounded or unbounded domain can be cast in terms of a fixed point problem, in which some finite power of the linear operator is a contraction mapping (the spectral radius of the operator is less than one). Furthermore, the three steps in the computational procedure (pre-processing or creation of the fixed point problem, iterative solution of the discretized problem, and post-processing to extract the physical variables of interest) can be formulated as parallel algorithms.

We will draw upon the developments of Parts II and III to show that in many-body suspension problems the interactions between elements on different particles are very small, in the sense that the eigenvalues determining the spectral radius are perturbed only slightly by hydrodynamic interactions between the particles. Thus we raise the proposition of attacking large-scale suspension simulations by a network of parallel processors, with each processor powerful enough to handle all boundary elements on a given particle. *In essence, we recover the nearest neighbor property of the spatial methods, only now the fundamental entity is not an element or a node, but the collection of elements on a particle.* The resulting iterative strategy will involve asynchronous iterations, accelerating the convergence relative to synchronous iterations similarly as the Gauss–Seidel iterations do in comparison with Gauss–Jacobi iterations. The many successes obtained to date with this new approach suggest that CDL-BIEM will be an important tool in our efforts to describe the motion of complex microstructures through a viscous fluid, although the full impact of the method may not be realized until it becomes popular with the research community.

Chapter 14 lists the mathematical background for comprehension of the material covered, to the extent that the reader should be able to apply the theory and algorithms presented for obtaining numerical results. We go over Fredholm integral equations of the first and the second kind, and some smoothness requirements for the kernels, which, for our application, imply smoothness requirements for the surface. The kernels encountered are *weakly singular*, so that an extension of the Fredholm theory, namely, the *Fredholm–Riesz–Schauder* theory for compact operators, is necessary. The fact that the integral operators are compact will be exploited in two ways. First, it implies that CDL-BIEM is a well-posed problem. Second, the spectrum of a compact operator is discrete, which in our case will be used to show that, even before discretization, the integral equations of CDL-BIEM can be solved by Neumann series expansion, in practice replaced by direct (Picard) iterations (also called *successive substitution*) corresponding to truncating the Neumann series.

The next two chapters put the integral representations for Stokes flow in the framework of linear operator theory. Chapter 15 presents the theory of Odqvist for a single particle, while Chapter 16 extends the theory to multiparticle problems in both bounded and unbounded domains. The range and the null space of the double layer integral operator are explored, and we show that in the multiparticle setting, no new null solutions are created by interactions between surfaces. The setting for multiparticle problems brings out another nontrivial result as well. In the analysis of the stress field generated by a double layer distribution on a Lyapunov-smooth container surface, we encounter improper integrals. Using just the techniques of classical functional analysis, the obvious way out is to increase the smoothness condition on the parametric representation of the surface, from Lyapunov-smooth to the class Bh (Hölder-continuous second derivatives), and this is the path followed by Odqvist. Thus, contrary to our physical intuition, Odqvist's theory requires a Bh-smooth container surface but only a Lyapunov-smooth particle surface. Our analysis in Section 16.2 of

the more general multiparticle setting offers a new line of proof, which shows that the theory applies to Lyapunov-smooth containers and that the earlier asymmetric result is simply an artifact of the mathematical technique. The framework of linear operator theory is fully exploited in the construction of a direct procedure for calculating surface tractions for particles undergoing rigid-body motions. The proof requires the combined use of the Riesz representation theorem for linear functionals and the Lorentz reciprocal theorem.

Chapter 17 is perhaps the most important one in Part IV, from a conceptual point of view. The spectrum of the integral operator is analyzed and the procedure for shifting the outermost eigenvalues ($7N$ of them for an N-particle system plus seven more if the domain is bounded) inward, by the procedure known as *Wielandt deflation*, is explained. The final result is an iterative scheme, based on the fact that the Neumann series will converge and Picard iterations therefore are feasible. Physical results, such as the translational and rotational velocities of the particles, turn out to be exactly the projection of the solution onto the eigenspace of the deflated eigenvalues. In addition, the surface tractions for each particle are also obtained as an iterative solution of the adjoint problem. We show that multiple Wielandt deflations can be implemented as a parallel algorithm, provided that the basis for the eigenspace is orthonormal. Since this is not true in general, we show how the Gram matrix may be inverted analytically by projection methods, so that the Gram–Schmidt orthogonalization process is also readily implemented as a parallel operation.

In Chapter 18 (Fourier analysis for axisymmetric geometries) and Chapter 19 (three-dimensional geometries), we illustrate the method with numerical examples. Only relatively simple discretization schemes are considered. In part this is because of our belief that true optimization of codes for parallel processing must reflect the coupling between architecture and algorithm. Thus we focus our efforts on results that we feel will apply to a broad class of parallel computers. These examples include comparisons with other numerical methods and experimental data. An illustrative range of particle geometries, such as sharp corners and grooves is examined, and dense linear systems up to 10,000 $\times$ 10,000 in size are explored without difficulty. We stop at the frontiers of computational microhydrodyanmics research. For very large systems of equations, communication becomes a bottleneck, even for Jacobi iterations. A promising strategy for asynchronous iterations that minimizes communication bottlenecks is outlined.