The Mathematical Foundations of Mixing

Mixing processes occur in a variety of technological and natural applications, with length and time scales ranging from the very small – as in microfluidic applications – to the very large – for example mixing in the Earth's oceans and atmosphere. The diversity of problems can give rise to a diversity of approaches. Are there concepts that are central to all of them? Are there tools that allow for prediction and quantification?

The authors show how a range of flows in very different settings – micro to macro, fluids to solids – possess the characteristic of *streamline crossing*, a central kinematic feature of 'good mixing'. This notion can be placed on firm mathematical footing via Linked Twist Maps (LTMs), which is the central organizing principle of this book.

The authors discuss the definition and construction of LTMs, provide examples of specific mixers that can be analysed in the LTM framework and introduce a number of mathematical techniques – nonuniform hyperbolicity and smooth ergodic theory – which are then brought to bear on the problem of fluid mixing. In a final chapter, they argue that the analysis of linked twist maps opens the door to a plethora of new investigations, both from the point of view of basic mathematics as well as new applications, and present a number of open problems and new directions. Consequently, this book will be of interest to a broad spectrum of readers, from pure and applied mathematicians, to engineers, physicists, and geophysicists.

CAMBRIDGE MONOGRAPHS ON
APPLIED AND COMPUTATIONAL MATHEMATICS

22 The Mathematical Foundations of Mixing

The *Cambridge Monographs on Applied and Computational Mathematics* reflects the crucial role of mathematical and computational techniques in contemporary science. The series publishes expositions on all aspects of applicable and numerical mathematics, with an emphasis on new developments in this fast-moving area of research.

State-of-the-art methods and algorithms as well as modern mathematical descriptions of physical and mechanical ideas are presented in a manner suited to graduate research students and professionals alike. Sound pedagogical presentation is a prerequisite. It is intended that books in the series will serve to inform a new generation of researchers.

Also in this series:

1. A Practical Guide to Pseudospectral Methods, *Bengt Fornberg*
2. Dynamical Systems and Numerical Analysis, *A. M. Stuart and A. R. Humphries*
3. Level Set Methods and Fast Marching Methods, *J. A. Sethain*
4. The Numerical Solution of Integral Equations of the Second Kind, *Kendall E. Atkinson*
5. Orthogonal Rational Functions, *Adhemar Bultheel, Pablo González-Vera, Erik Hendiksen, and Olav Njastad*
6. The Theory of Composites, *Graeme W. Milton*
7. Geometry and Topology for Mesh Generation *Herbert Edelsfrunner*
8. Schwarz-Christoffel Mapping *Tofin A. Dirscoll and Lloyd N. Trefethen*
9. High-Order Methods for Incompressible Fluid Flow, *M. O. Deville, P. F. Fischer and E. H. Mund*
10. Practical Extrapolation Methods, *Avram Sidi*
11. Generalized Riemann Problems in Computational Fluid Dynamics, *Matania Ben-Artzi and Joseph Falcovitz*
12. Radial Basis Functions: Theory and Implementations, *Martin D. Buhmann*
13. Iterative Krylov Methods for Large Linear Systems, *Henk A. van der Vorst*
14. Simulating Hamiltonian Dynamics, *Ben Leimkuhler & Sebastian Reich*
15. Collacation Methods for Volterra Integral and Related Functional Equations, *Hermann Brunner*
16. Topology for Computing, *Afra J. Zomorodian*
17. Scattered Data Approximation, *H. Wendland*
18. Matrix Preconditioning Techniques and Applications, *K. Chen*

The Mathematical Foundations of Mixing

The Linked Twist Map as a Paradigm in Applications
Micro to Macro, Fluids to Solids

ROB STURMAN

School of Mathematics
University of Bristol
University Walk
Bristol, BS8 1TW
United Kingdom

JULIO M. OTTINO

Departments of Chemical and Biological Engineering
and Mechanical Engineering
Northwestern University
Evanston, Illinois 60208
USA

STEPHEN WIGGINS

School of Mathematics
University of Bristol
University Walk
Bristol, BS8 1TW
United Kingdom

CAMBRIDGE
UNIVERSITY PRESS

CAMBRIDGE
UNIVERSITY PRESS

Shaftesbury Road, Cambridge CB2 8EA, United Kingdom

One Liberty Plaza, 20th Floor, New York, NY 10006, USA

477 Williamstown Road, Port Melbourne, VIC 3207, Australia

314–321, 3rd Floor, Plot 3, Splendor Forum, Jasola District Centre, New Delhi – 110025, India

103 Penang Road, #05–06/07, Visioncrest Commercial, Singapore 238467

Cambridge University Press is part of Cambridge University Press & Assessment, a department of the University of Cambridge.

We share the University's mission to contribute to society through the pursuit of education, learning and research at the highest international levels of excellence.

www.cambridge.org
Information on this title: www.cambridge.org/9780521868136

First published 2006

A catalogue record for this publication is available from the British Library

ISBN 978-0-521-86813-6 Hardback

THOMASINA:
When you stir your rice pudding, Septimus, the spoonful of jam spreads itself round making red trails like the picture of a meteor in my astronomical atlas. But if you stir backward, the jam will not come together again. Indeed, the pudding does not notice and continues to turn pink just as before. Do you think this odd?

SEPTIMUS:
No.

THOMASINA:
Well, I do. You cannot stir things apart.

SEPTIMUS:
No more you can, time must needs run backward, and since it will not, we must stir our way onward mixing as we go, disorder out of disorder into disorder until pink is complete, unchanging and unchangeable, and we are done with it for ever.

Arcadia, Tom Stoppard

Contents

Preface

Where is mixing important?

Mixing processes occur in a variety of technological and natural applications, with length and time scales ranging from the very small (as in microfluidic applications), to the very large (mixing in the Earth's oceans and atmosphere). The spectrum is quite broad; the ratio of the contributions of inertial forces (dominant in the realm of the very large) to viscous forces (dominant on the side of the very small) spans more than twenty orders of magnitude.

Theoretical and experimental developments over the last two decades have provided a strong foundation for the subject, yet much remains to be done. Earlier work focused on mixing of liquids and considerable advances have been made. The basic theory can be extended in many directions and the picture has been augmented in various ways. One strand of the expansion has been an incursion into new applications such as oceanography, geophysics and applications to the design of new mixing devices, as in microfluidics. A second strand is incursion into new types of physical situations, such as mixing of dry granular systems and liquid granular systems (in which air is replaced by a liquid). These applications clearly put us on a different plane – new physics – since, in contrast to mixing of liquids, a complicating factor in the flow of granular material is the tendency for materials to segregate or demix as a result of differences in particle properties, such as density, size, or shape. Mixing competes with segregation: mixtures of particles with varying size (S-systems) or varying density (D-systems) often segregate leading to what, on first viewing, appear to be baffling results. This class of problems can also be attacked with extensions of the basic theory.

The diversity of problems can give rise to a diversity of approaches and a temptation to deepen work on application-driven tools. Specificity may dominate the picture. One could, however, take the opposite approach. Are there concepts that are central enough that they should be developed in more detail? Broadness competes with specificity. Would however this viewpoint allow for a more encompassing view that may otherwise be lost by generation of fragmented results?

Why is this book needed?

The purpose of this book is to focus on new developments in mathematics and take this broader view point – the objective is on general results rather than specifics. Even though the work is of a manifestly mathematical bent, we expect that the presentation will resonate with a diverse set of readers. We are aware however that the question ‘Is all this mathematics really necessary?’ will surface in many readers’ minds. The reason for the mathematics is to set a baseline, a clear picture as to where things come from. We recognize however, that in long stretches of the presentation things get manifestly technical, and we are also aware that we have to persuade the reader that going through the material is a good investment of time. We have therefore decided to provide help in navigating the book. Periodically we insert physical and heuristic explanations to go along with the mathematical descriptions. All chapters have mini-intros, a distillation of the contents of the chapters, and connections to fluid applications where possible.

What will this book cover?

It is also important to clarify what we will and will not do. Of all the components of mixing we will focus on only one – the kinematical aspects of mixing a fluid with itself. The objective here is to study a problem which is tractable from an analytical as well as a computational perspective. The broad objective, then, is to determine what characteristics of a flow enable it to efficiently stretch material lines and surfaces, and to analyse the simplest possible flows capable of ‘good mixing’. Making precise what we mean by ‘good mixing’ will occupy us for at least one chapter of the book. We shall focus primarily on kinematics, rather than on dynamics (in the sense of the dynamics of fluids). Our study is an analysis of the motion due to an imposed velocity field; i.e. the study of the following dynamical system:

$$\mathrm{d}x/\mathrm{d}t = v(x,t), \quad x = X \quad \text{at} \quad t = 0.$$

In general, we shall study the motion by a sort of minimal flow – the simplest non-trivial flow that encapsulates the characteristics of wide classes of flows – and expose the characteristics which make them good or poor mixing flows, rather than study the hydrodynamic forces which give rise to the flows themselves. The goal is to make recent dynamical systems theory accessible to users interested in the mixing of fluids.

It is then clear that *our presentation is a purposefully distorted view of mixing*. There is nothing in this view, for example, that accounts for turbulent flows. We argue however, that the baseline presented here is crucial to the understanding of more complicated cases of mixing.

At the starting point of any mixing process there exist two (or more) constituents which occupy distinct domains whose size is on the order of the system size itself. The objective of the mixing process is to reduce the length scales of these materials below a certain level, resulting in a 'homogeneous' system – a mixture. This length scale and the level of homogeneity are of course dependent upon the application in question. We distinguish three aspects. The first is essential; the other two may or may not be present. (1) *Mechanical mixing*: This is the stretching and folding part; the motion causes the interfaces between the materials to stretch, creating inter-material area between highly striated structures. The system, which at first contained a blob of one fluid in another, now appears as a stretched and folded filament with, in general, a wide distribution of striation thicknesses; (2) *Breakup*: If the filament has been sufficiently stretched, differences in the interfacial tension on opposite sides of an interface can cause the filament to break up into isolated droplets, reducing the length scale even further; in this step the properties of the materials matter; in the case of very viscous materials or in the case of very similar materials this aspect may be absent; (3) *Diffusion*: If the fluids are miscible, Brownian motion of individual fluid molecules, due to fluctuations in thermal energy, acts to homogenize the fluid at the molecular scale. This process does not take place if the materials are incompatible.

Thus not all of these mechanisms need be present in a given mixing process and, in many cases, breakup may be accompanied by its opposite – coalescence or unmixing. As a specific example, consider the mixing of two polymeric fluids with similar, but large, viscosities. Diffusion coefficients in such systems can be on the order of $10^{-8}\,\mathrm{cm}^2/\mathrm{sec}$. In this case, both breakup and diffusion are negligible, and the only means for mixing is stretching. In any case, the time required for molecular homogenization, T, can be estimated from simple dimensional analysis to be $T = L^2/D$, where D is the molecular diffusion coefficient and L is the length scale of the fluid domains. The most important factor which affects the time scale for final homogenization is the length scale of the fluid domains. The length scale is in turn determined by the extent of the stretching of the material domains which occurs due to the imposed motion. Thus, the most important part of understanding mixing is to understand how, and what types of flows are able, to generate efficient stretching.

How are the chapters related to one another?

The book is organized around the idea of the linked twist map (LTM). LTMs provide a minimal picture of mixing and one case for which nearly everything that can be known is known; for example, theorems from ergodic theory and conditions that guarantee mixing behaviour, measures of complexity, and geometrical properties. Results generally apply to infinite-time limits and one could argue that reality does not correspond to this case. As with every theory care is needed in interpreting its applicability. For example, a system having a horseshoe does not imply that good mixing will take place (by 'good' we invoke the notion of 'widespread' as opposed to 'localized'). On the other hand the absence of a horseshoe guarantees that no good mixing will occur. Most of the material presented is scattered throughout the mathematics literature. In particular we draw on four papers from the pure dynamical systems community, Devaney (1978), Burton & Easton (1980), Wojtkowski (1980), and Przytycki (1983) that were published around 25 years ago, mostly in arguably obscure and hard to find conference proceedings. Moreover their intended audience was a very different one from ours. Thus one of our main tasks, rather than to present a host of original dynamical systems theorems, is to distil the papers into the first unified and user-friendly presentation of these ideas and to show how these results and the mathematical details within the now classical proofs relate to contemporary mixing problems. The credit for the original pure mathematical results rests with the five authors listed above. In Chapters 1 and 2 we consider applications from a variety of fields; microfluidics, granular mixing as produced by tumbling, and transport in geophysical flows, for example, but we emphasize the 'universality' of the linked twist map approach to mixing across disciplines.

The book starts in full in Chapter 3, entitled 'The ergodic hierarchy'. This chapter is necessary because smooth ergodic theory is a technical subject requiring a mathematical background beyond that of most physicists, chemists, and engineers, yet we believe it is poised to play an important role in the subject of mixing in applications in the future. The situation is similar to that which existed for dynamical systems theory in the late 1970s and early 1980s. At that time the subject was relatively mathematically abstract and it required substantial extra effort on the part of physicists, chemists, and engineers to carry out the transference between 'abstract theorem' to a technique that could unlock the secrets of the specific nonlinear dynamical systems arising in applications. In smooth ergodic theory such a transference is only now beginning, but it promises to be equally as fruitful. Consider a specific example of the type of issue that techniques in smooth ergodic theory may address. The Smale horsehoe is the classic ‘chaotic dynamical system’, but it is only a set of ‘zero area’, and one would therefore expect that the probability of ‘observing’ the dynamics on this set would be zero. Experiments suggest otherwise – that the chaotic dynamics may persist beyond a set of zero area. Dynamical systems theory without smooth ergodic theory gives no indication that this might be the case. Smooth ergodic theory provides a framework for making these notions mathematically precise, and provides the techniques for extending results to sets of observational significance. In particular, the notion of the area of a set is dealt with quantitatively through the notion of measure and measurable sets. These notions allow one to give a probabilistic description of the dynamics, and also to quantify the idea of ‘observability’ in a way that lends itself to computation. Smooth ergodic theory also provides a framework for analysing a much more practical question – ‘When does Smale horseshoe-like behaviour occur on a set of non-zero area?’, or equivalently, ‘when is the horseshoe observable?’ By now Smale horseshoes have been shown to exist in literally hundreds of dynamical systems spanning many diverse areas of applications. However, their influence on ‘observable dynamics’ is unclear at best. One could view the linked twist maps studied in this monograph as being an example of a dynamical system exhibiting ‘horseshoe-like’ behaviour on a set of ‘full measure’, and ergodic theory provides the tools for carrying out the necessary analysis that quantifies this statement. But *mixing* is the motivating application for our studies, and ergodic theory enables us to characterize the mixing process mathematically and rigorously in a variety of ways. For example, it provides an ordered list of behaviours of increasing complexity; from ergodicity, through (measure-theoretic) mixing, to the Bernoulli property. We describe the main features of ergodicity, mixing, and the Bernoulli property in detail, as these are the most immediately applicable to the problem of fluid mixing. It should be noted that these definitions are very technical and differences between them may not be realizable in applications.

Chapter 4, ‘Existence of a horseshoe for the linked twist map’, builds on the definition and construction of a linked twist map on the plane. The underlying structure of complicated behaviour that arises in LTMs is that of the Smale horseshoe. This chapter presents a detailed construction of the horseshoe, and the implications of its existence for symbolic dynamics. The central element is revealing the existence of the invariant set of the LTM by a carefully chosen pair of quadrilaterals in the intersection of the two linked annuli. The invariant set is given by the images of the intersection of the quadrilaterals under infinite forward and backward time. The way in which the image of each quadrilateral intersects the original pair of quadrilaterals defines a *symbolic dynamics*, which gives a measure of the complexity of the system.

The horseshoe constructed is 'classical' in the sense that the chaotic invariant set is uniformly hyperbolic having measure zero. In this sense the linked twist maps provide a concrete example showing how nonuniform hyperbolicity arises in this class of dynamical systems. In later chapters we show how it can be analysed.

Chapter 5, 'Hyperbolicity', deals with one of the most fundamental aspects of dynamical systems theory, both from the point of view of pure dynamical systems – it represents one of the best-understood classes of dynamical system; and from the point of view of applied dynamical systems – one of the simplest models of complex and chaotic dynamics. We define uniform and nonuniform hyperbolicity, and go on to describe Pesin theory, which establishes a bridge between nonuniform hyperbolicity and the ergodic hierarchy. The theory of Pesin is central to our analysis. It relates non-zero Lyapunov exponents and nonuniform hyperbolicity. The method of invariant cone fields is introduced to prove the existence of non-zero Lyapunov exponents on a set of full measure. The special structure of the linked twist maps renders such calculations feasible. Once nonuniform hyperbolicity is established the theory of Pesin paves the way for conclusions about the existence of partitions into ergodic components and the Bernoulli property.

Chapter 6 is entitled 'The ergodic partition for toral linked twist maps' and discusses the application of Pesin theory in detail to linked twist maps defined on a torus. Here, drawing on three key papers from the ergodic theory literature, we give the proof that linked twist maps on the torus can be decomposed into (at most a countable number of) ergodic components.

Chapter 7 centres on 'Ergodicity and the Bernoulli property for toral linked twist maps'. Here we apply a global geometric argument, again from the ergodic theory literature, to extend the result of Chapter 6 to ergodicity and the Bernoulli property on a set of full measure for toral linked twist maps. Conditions are given such that these results hold. We give sufficient conditions for a toral linked twist map to enjoy the Bernoulli property. A key point – of significant practical importance – to notice is that different conditions are required for the co-rotating and counter-rotating cases.

In Chapter 8, these results are extended to planar linked twist maps. Linked twist maps on the plane are more directly applicable to fluid mixing, but introduce new technical difficulties in the mathematics.

Finally, in Chapter 9, we discuss a number of open problems. The analysis of linked twist maps only opens the door to a plethora of new investigations, both from the point of view of basic mathematics, as well as new applications. In fact, the latter drives the former as applications naturally suggest new types of linked twist maps, which we describe in detail. The sufficient conditions that we derive in earlier chapters leading to ergodicity and the Bernoulli property can be used as design parameters for optimizing mixing regions, and we show how this can be done.

In closing we remark again that in some sense this book can be read at two levels. Chapters 3 through 8 stand on their own as an analysis of the dynamics of linked twist maps on the torus and on the the plane, containing all of the necessary background and details. However, we believe that the real value of this approach comes in when one considers that linked twist maps embody the mixing paradigm of ‘crossing of streamlines’. When the range of examples showing this in Chapters 1 and 2 is considered then it becomes apparent that one has a new way of looking at the mixing process that leads to characterizing mixing properties on large regions of the domain in a way that has not been done before. The fact that the approach feeds immediately into optimization and design makes it even more compelling.

Acknowledgments

RS and SW gratefully acknowledge the financial support of the Office of Naval Research and the Engineering and Physical Sciences Research Council.
JMO wishes to acknowledge the financial support of the John Simon Guggenheim Memorial Foundation.
We thank James Springham for a careful reading of the text.
RS would like to thank Kathryn for much patience and support.