

Think Before You Compute

Every fluid dynamicist will at some point need to use computation. Thinking about the physics, constraints and the requirements early on will be rewarded with benefits in time, effort, accuracy and expense. How these benefits can be realised is illustrated in this guide for would-be researchers and beginning graduate students to some of the standard methods and common pitfalls of computational fluid mechanics. Based on a lecture course that the author has developed over 20 years, the text is split into three parts. The quick introduction enables students to solve numerically a basic nonlinear problem by a simple method in just three hours. The follow-up part expands on all the key essentials, including discretisation (finite differences, finite elements and spectral methods), time-stepping and linear algebra. The final part is a selection of optional advanced topics, including hyperbolic equations, the representation of surfaces, the boundary integral method, the multigrid method, domain decomposition, the fast multipole method, particle methods and wavelets.

E. J. HINCH has been a teacher and researcher in fluid mechanics and applied mathematics at the University of Cambridge for over 45 years. He is the author of *Perturbation Methods* (Cambridge University Press, 1991) and has been awarded the Fluid Dynamics prizes of the European Mechanics Society and the American Physical Society Division of Fluid Dynamics.

Cambridge Texts in Applied Mathematics

All titles listed below can be obtained from good booksellers or from Cambridge University Press. For a complete series listing, visit www.cambridge.org/mathematics.

Flow, Deformation and Fracture

G. I. BARENBLATT

Geometric and Topological Inference

JEAN-DANIEL BOISSONNAT, FRÉDÉRIC CHAZAL & MARIETTE YVINEC

Introduction to Magnetohydrodynamics (2nd Edition)

P. A. DAVIDSON

An Introduction to Stochastic Dynamics

JINQIAO DUAN

Singularities: Formation, Structure and Propagation

J. EGGERS & M. A. FONTELOS

Stochastic Modelling of Reaction-Diffusion Processes

RADEK ERBAN & S. JONATHAN CHAPMAN

Microhydrodynamics, Brownian Motion and Complex Fluids

MICHAEL D. GRAHAM

Discrete Systems and Integrability

J. HIETARINTA, N. JOSHI & F. W. NIJHOFF

An Introduction to Polynomial and Semi-Algebraic Optimization

JEAN BERNARD LASSERRE

An Introduction to Computational Stochastic PDEs

GABRIEL J. LORD, CATHERINE E. POWELL & TONY SHARDLOW

Self-Exciting Fluid Dynamos

KEITH MOFFATT & EMMANUEL DORMY

Numerical Linear Algebra

HOLGER WENDLAND

Think Before You Compute
A Prelude to Computational Fluid Dynamics

E. J. HINCH
University of Cambridge



Cambridge University Press
978-1-108-47954-7 — Think Before You Compute
E. J. Hinch
Frontmatter
[More Information](#)

CAMBRIDGE
UNIVERSITY PRESS

University Printing House, Cambridge CB2 8BS, 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
79 Anson Road, #06–04/06, Singapore 079906

Cambridge University Press is part of the University of Cambridge.

It furthers the University's mission by disseminating knowledge in the pursuit of education, learning, and research at the highest international levels of excellence.

www.cambridge.org

Information on this title: www.cambridge.org/9781108479547

DOI: 10.1017/9781108855297

© E. J. Hinch 2020

This publication is in copyright. Subject to statutory exception and to the provisions of relevant collective licensing agreements, no reproduction of any part may take place without the written permission of Cambridge University Press.

First published 2020

Printed in the United Kingdom by TJ International Ltd, Padstow Cornwall

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

ISBN 978-1-108-47954-7 Hardback

ISBN 978-1-108-78999-8 Paperback

Cambridge University Press has no responsibility for the persistence or accuracy of URLs for external or third-party internet websites referred to in this publication and does not guarantee that any content on such websites is, or will remain, accurate or appropriate.

Contents

	<i>Preface</i>	<i>page xi</i>
	PART I A FIRST PROBLEM	1
1	The driven cavity	3
	1.1 The problem	3
	1.2 Know your physics	3
	1.3 Know your PDEs	5
	1.4 Special physics of the corner	6
	1.5 Nondimensionalisation	7
	1.6 Steady vs transient calculations	7
	1.7 Pressure!	8
2	Streamfunction-vorticity formulation	9
	2.1 Formulation	9
	2.2 Finite differences (simple)	10
	2.3 Poisson problem	13
	2.4 Test the code	16
	2.5 Code quality	19
	2.6 Simple graphs	20
	2.7 Vorticity evolution	21
	2.8 Time-step instability	22
	2.9 Accuracy consistency	24
	2.10 Results	27
3	Primitive variable formulation	35
	3.1 Formulation	35
	3.2 Pressure equation	35
	3.3 Algorithm 1 with pressure equation	36
	3.4 Incompressibility as a constraint: split time-step	38

3.5	Algorithm 2 by projection – spurious pressure modes	40
3.6	Algorithm 3 with a staggered grid	42
3.7	Results from algorithm 3	46
PART II GENERALITIES		51
4	Finite differences	53
4.1	Higher orders	53
4.1.1	Central differencing	53
4.1.2	One-sided differencing	54
4.1.3	Nonequispaced points	55
4.2	Compact fourth-order Poisson solver	56
4.2.1	One-dimensional version	56
4.2.2	Two dimensions	56
4.3	Upwinding	58
4.4	Other grids	59
4.5	Conservative schemes	60
5	Finite elements	64
5.1	The two ideas	64
5.2	Representations in one dimension	65
5.2.1	Constant elements	65
5.2.2	Linear elements	65
5.2.3	Quadratic elements	65
5.2.4	Cubic elements	66
5.2.5	Basis functions	67
5.3	Representations in two dimensions	67
5.3.1	Constant elements	68
5.3.2	Linear elements	68
5.3.3	Quadratic elements	69
5.3.4	Cubic elements	70
5.3.5	Basis functions	71
5.3.6	Rectangles	71
5.4	Variational statement of the Poisson problem	72
5.5	Details in one dimension	73
5.6	Details in two dimensions	74
5.7	Galerkin formulation	78
5.8	Diffusion equation	80
5.8.1	Weak formulation	80
5.8.2	In one dimension	80
5.8.3	In two dimensions	81

5.9	Navier–Stokes equation	81
5.9.1	Weak formulation	81
5.9.2	Time integration	82
5.9.3	Pressure problem – locking	82
5.9.4	Pressure problem – spurious modes	84
6	Spectral methods	86
6.1	The two ideas	86
6.2	Global vs local	87
6.3	Choice of spectral basis functions	89
6.4	Chebyshev polynomials	90
6.5	Rates of convergence	90
6.6	Gibbs phenomenon	91
6.7	Discrete Fourier Transform	93
6.8	Aliasing	94
6.9	Fast Fourier Transform (FFT)	96
6.10	Differential matrix	97
6.11	Navier–Stokes	98
6.12	Bridging the gap	99
7	Time integration	100
7.1	Stability	100
7.2	Forward Euler	102
7.3	Backward Euler	103
7.4	Midpoint Euler	104
7.5	Crank–Nicolson	104
7.6	Leapfrog	105
7.7	Runge–Kutta	105
7.8	Multistep methods	106
7.9	Symplectic integrators	107
7.10	Navier–Stokes	108
8	Linear algebra	110
8.1	LAPACK	111
8.2	Gaussian elimination	112
8.2.1	Pivoting	113
8.2.2	LU decomposition	114
8.2.3	Errors	115
8.3	QR decomposition	115
8.3.1	QR by Gram–Schmidt	116
8.3.2	QR by Givens rotations	117
8.3.3	QR by Householder reflections	118

8.4	Sparse matrices	119
8.5	Conjugate gradients	119
8.6	Eigenproblems	121
8.7	Power iteration	122
8.8	Jacobi	122
8.9	Main method	122
	PART III SPECIAL TOPICS	125
9	Software packages and FREEFEM++	127
9.1	Poisson problem	128
9.2	Driven cavity	131
10	Hyperbolic equations	136
10.1	Simplest, but unstable	137
10.2	Lax–Friedricks, too stable	139
10.3	Upwinding	142
10.4	Crank–Nicolson	142
10.5	Lax–Wendroff	144
10.6	Angled Derivative	145
10.7	Propagation of discontinuities	148
10.8	Flux limiters	149
10.9	Nonlinear advection	151
10.10	Godunov method	153
11	Representation of surfaces	156
11.1	Curves in two dimensions	157
11.1.1	Splines	157
11.2	Surfaces in three dimensions	158
11.2.1	Redistributing points	158
11.2.2	Curvature	159
11.3	Volume of Fluid (VoF) method	162
11.4	Diffuse interface method	163
11.5	Level sets	165
11.5.1	Fast Marching Method	165
12	Boundary integral method	167
12.1	Integral equation for Laplace equation	167
12.1.1	Greens functions	168
12.1.2	Eigensolutions	169
12.1.3	Singular integrals	169
12.2	Discretisation	169

12.2.1	Evaluation of the matrix elements	170
12.2.2	Avoiding the eigensolution	171
12.2.3	Tests	171
12.2.4	Costs	172
12.3	Free-surface potential flows	173
12.4	Stokes flows	173
13	Fast Poisson solvers	175
13.1	Multigrid method	175
13.1.1	A V-cycle	176
13.1.2	Accuracy and costs	177
13.2	Fast Fourier Transforms	178
13.3	Domain decomposition	180
13.3.1	Costs	182
14	Fast Multipole Method	183
14.1	Trees, roots and leaves	184
14.2	Barnes–Hut algorithm	184
14.3	Fast Multipole algorithm	186
14.3.1	Upward pass	186
14.3.2	Downward pass	187
14.3.3	Errors	187
14.3.4	Costs	188
15	Nonlinear considerations	190
15.1	Finding steady states	190
15.1.1	Finding the Jacobian	191
15.1.2	Example of the limit cycle of the Van der Pol oscillator	192
15.2	Parameter continuation	193
15.3	Searching for singularities of physical problems	193
15.3.1	Use of computer algebra	195
16	Particle methods	197
16.1	Molecular dynamics	197
16.2	Lattice Gas	199
16.3	Lattice Boltzmann	201
16.4	Dissipative particle dynamics	204
16.5	Stokesian dynamics	205
16.5.1	Hydrodynamic interactions	205
16.5.2	Brownian motion	207
16.6	Force Coupling Method	209

16.7	Granular media simulations	211
16.8	Smooth Particle Hydrodynamics	212
17	Wavelets	217
17.1	Continuous Wavelet Transform	218
17.2	Discrete Wavelet Transform	220
17.3	Fast Wavelet Transform	221
17.4	Daubechies wavelets	224
	<i>Index</i>	226

Preface

This book, based on a graduate course in Cambridge, is aimed at students starting research into fluid mechanics who are thinking about computing a flow, as one amongst other tools of investigation. It is an educational book for beginners, using the simplest methods appropriate, rather than an advanced text for those already familiar with the methods. It is certainly not a research monograph about the very latest techniques. It is for those using a little computing for research in fluid mechanics. It is not for those researching into computational methods, either proving their mathematical properties or creating new methods.

The book is designed for students who have taken an undergraduate course on fluid mechanics and an undergraduate course on computing simple numerical methods, designed to lead those students to some understanding of computing flows. The course on fluid mechanics should have discussed the incompressible Navier–Stokes equation, the Reynolds number, boundary layers, vorticity and streamfunctions. The course on numerical methods should have included simple finite differencing of differential equations and iterative solutions. This book will then develop numerical methods appropriate to fluid mechanics. On the other hand, the book will not develop fluid mechanics. This means that no examples are included of numerical calculations in acoustics, aeronautics, compressible flows, combustion and reactions, biology, atmospheres, oceans, geology, non-Newtonian fluids and many industries. It is important to point out the many models of turbulence are also not included.

The book is divided into three parts. Part I is short and composed of three chapters. It tackles a very simple problem in fluid mechanics by very simple numerical methods. By making everything simple, students should be able to obtain results for a nonlinear flow after just one week of lectures. Some MATLAB code is available on my website,¹ so that students do not even have

¹ www.damtp.cam.ac.uk/user/hinch/teaching/CMIFM_Handouts/***.m, where *** is PoissonTest, StrfnVort and PrimVarb.

to spend time coding the programs themselves. But more than quick results, the first part delivers a far-from-hidden message of the need to think about what one is doing. There are issues of understanding the formulation of the question, of designing and monitoring the accuracy, of noting where time is consumed, of handling instabilities, of producing evidence that the answer is correct. There is also the special numerical issue in fluid mechanics of how to find the pressure. The simple problem tackled in Part I is the driven cavity, a square domain with a prescribed tangential velocity on the top surface. The simple numerical methods used are finite differences, central in space and forward in time, and successive over-relaxation of Gauss–Seidel iteration to solve a Poisson problem.

Part II gives a more detailed treatment of the general issues, such as turning a continuous partial differential equation into a finite discrete problem, i.e. discretisation by finite differences, finite elements and spectral methods, and general issues of time-stepping and solving large sparse systems of linear equations. Topics covered under discretisation include conservative formulations, a compact fourth-order Poisson solver, problems with pressure in finite elements, local vs global representations and the need for a pseudospectral approach. While time-stepping is only a discretisation in time, it deserves a more careful examination. There are issues of controlling the accuracy, not being too stable and sometimes avoiding excessive expensive evaluations of derivatives. While fluid mechanics is strictly nonlinear, large linear problems occur in the Poisson problem to find pressure or in considering the linear stability of a flow; hence the chapter on linear algebra. Students are strongly recommended not to code up finite elements or solvers for linear algebra but rather to use safe professionally written packages. The two chapters on these topics are included to explain what the packages are doing, so that the correct package can be used wisely.

Part III is an incomplete collection of specialised topics. The first chapter of Part III gives a quick introduction to one particular finite element package, `FREEFEM++`. I selected this package having tried several, because I have found that in less than an hour students can learn to use it to compute a flow. Solving hyperbolic equations numerically is unwise, and Chapter 10 illustrates the problems that arise with seemingly good schemes; only the one-dimensional case is presented. Some fluid mechanics problems involve moving boundaries. Chapter 11 discusses various representations of surfaces. This is followed by a chapter on the boundary integral method, which for potential flow and Stokes flow only uses data on the surface and so is highly suited for computing moving boundary problems. A Poisson problem typically consumes much of the time in computing a flow, so fast methods have been

developed to solve it. For simple geometry, the multigrid method is probably the fastest, while in complex geometries domain-decomposition is particularly good with parallel computing. When the forcing of the Poisson problem is by many point sources, a fast multipole method can be useful, but only when there is a very large number of sources. While fluid mechanics is essentially about a continuum medium, particle descriptions naturally occur, whether one studies molecules moving in a gas, colloidal particles in a suspension, dry grains in a flowing granular medium or parcels of fluid in a Lagrangian description. Chapter 16 describes all these. The final chapter gives a quick introduction to wavelets, which have been found useful for analysing flows and identifying isolated regions of great activity.

A cautionary remark. One of the difficulties in computing flows is that every branch of fluid mechanics has its special physics, and that special physics should be reflected in some special numerics. Note the implication that there is no universal method or package applicable to every fluids problem. In fact I would go further to say that even for a particular problem there is no best method, one should always be able to dream up something better.

And finally I must acknowledge the enormous assistance of my colleagues Stephen Cowley, Paul Dellar and Paul Metcalfe in developing the graduate lecture course in Cambridge over a period of years.