

Multiphysics simulation of fluid–structure interaction

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YUE SUN

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ABSTRACT

Fluid–structure interaction (FSI) underpins the life and locomotion of living organisms, as well as the behavior of engineering systems. It encapsulates many complex physical phenomena in the coupled dynamics of solids immersed in fluids. Simulations have been an attractive complement to studying FSI, enabling us to uncover scientific discoveries that are inaccessible via theory or experiment. However, simulating FSI is a nontrivial task. The fundamental challenge lies in how to computationally represent both solids and fluids. As solid stress is induced by strain, solids are naturally modeled in a Lagrangian framework; while fluids are often described in an Eulerian framework, given that fluid stress is induced by strain rate. In addition to this natural dichotomy in the preferred discretization framework for solids and fluids, modeling multi-body interactions or capturing the material and geometric nonlinearity in solids further complicates FSI simulations. In this thesis, we explore the development of multiphysics simulation of FSI from three perspectives: experimental, numerical, and artistic.

In [Chapter 2](#), we examine the one-way FSI in the context of cryo-plunging experiments. We simulate plunge freezing for sample preparation in cryogenic electron microscopy and develop a computational framework to create three-dimensional (3D) “digital twins” of sample vitrification in liquid ethane. By integrating experimental protocols, adaptive mesh refinement, and parallelization, our 3D simulations provide a lens to visualize heat transfer during cryo-plunging and quantify the effects of plunging protocols on cooling rates. Validated against experimental data, this framework lays the groundwork for engineering fluid dynamics to improve cryo-vitrification.

In **Chapter 3**, we focus on the method development for simulating two-way FSI. We extend the lattice Boltzmann (LB) method to model finite-strain solids on one fixed Eulerian grid with the reference map technique (RMT). We introduce a new Eulerian boundary condition to model multiple moving deformable solids with different densities. The resulting LBRMT is fully explicit, and therefore suitable for parallelization. It is validated against benchmark problems and applied to simulate multi-body interactions between soft solids and fluids such as rotating and mixing. This general method offers a new computational approach to the LB community for simulating many-body FSI problems involving hundreds of deformable solids in fluids, using modest computational resources.

In **Chapter 4**, we explore an ancient art form, marbling, and examine how the use of thin tools to craft stable and intricate artwork on a viscosified fluid surface constitutes an intriguing FSI problem. Through a showcase of various marbling patterns, we uncover a physical explanation of the workings of marbling and the roles of interfacial tension, surfactants, and viscosity. Additionally, we introduce a basic computational framework for capturing sharp color interfaces inspired by the reference map technique.

Contents

TITLE PAGE	
COPYRIGHT	
ABSTRACT	iii
TABLE OF CONTENTS	vi
LIST OF FIGURES	viii
LIST OF TABLES	ix
DEDICATION	x
ACKNOWLEDGMENTS	xi
I INTRODUCTION	1
1.1 State-of-the-art numerical methods for fluid–structure interaction	3
1.2 Contribution of this thesis	9
2 SIMULATION OF SAMPLE VITRIFICATION IN CRYO-PLUNGING	13
2.1 Introduction	13
2.2 Experimental integration	19
2.3 Theoretical formulation	26
2.4 Numerical implementation	30
2.5 Results	32
2.6 Discussion	45
3 A FULLY-INTEGRATED LATTICE BOLTZMANN METHOD FOR FLUID–STRUCTURE INTERACTION	48
3.1 Introduction	48
3.2 Theoretical formulation	52
3.3 Numerical implementation	65
3.4 Results	80
3.5 Discussion	94

4	THE HYDRODYNAMICS OF MARBLING ART	97
4.1	Introduction	97
4.2	Marbling experiments	98
4.3	Theoretical formulation	102
4.4	Results	103
4.5	Outlook of numerical implementation	107
4.6	Discussion	110
5	CONCLUSION	112
APPENDIX A SUPPLEMENTARY MATERIAL FOR CHAPTER 2		115
A.1	Additional thermocouple experiments	115
A.2	Derivation of the convection–diffusion equation	116
A.3	Example cryoflo input file	118
A.4	Other average temperature calculations	120
A.5	Analytical model for entry temperature estimation	122
A.6	Movies	129
APPENDIX B SUPPLEMENTARY MATERIAL FOR CHAPTER 3		130
B.1	Unit conversions and parameter choices	130
B.2	Validation of the fluid solver	135
B.3	Derivation of mass and momentum conservation in the smooth flux correction	136
B.4	Simulation time and performance	138
B.5	Movies	140
APPENDIX C SUPPLEMENTARY MATERIAL FOR CHAPTER 4		141
C.1	Marbling patterns	141
REFERENCES		158

List of Figures

1.1	Illustration of fluid–structure interaction (FSI) numerical methods	4
2.1	Cryo-EM sample preparation steps and phase diagram of water	16
2.2	EM grid dimensions	21
2.3	Pipeline to convert Z-stack images to 3D voxels	22
2.4	Illustrations and photos of cryo-plunging experiments	24
2.5	Illustrations, photos and measurements of thermocouple experiments	25
2.6	Update of fluid and solid phases in simulation domain	30
2.7	Simulations of thermocouple experiments	35
2.8	Simulation of sample vitrification	37
2.9	Sample ID numbers on the EM grid	39
2.10	3D visualization of sample vitrification	41
2.11	Effects of different plunging protocols on cooling	43
3.1	Illustration of large solid deformation and lattice Boltzmann reference map technique	53
3.2	Diagram of the D_2Q_9 lattice model and the smooth flux correction boundary condition	57
3.3	Illustration of one-dimensional smooth flux correction	61
3.4	Illustration of the reference map extrapolation	69
3.5	Stencils for the reference map advection and solid stress computation	71
3.6	Diagram of wall boundary conditions	76
3.7	Schematics of simulation domain, custom data structures, and collision stress computation	78
3.8	Benchmark example of a soft solid in a lid-driven cavity	82
3.9	Bending, twisting, and stretching of anchored rotors	84
3.10	Settling and floating of a solid	87
3.11	Softness enhances mixing rate	90
3.12	Mixing of 506 ellipses	93
4.1	Setup for marbling experiments	100
4.2	Physics of spreading	104
4.3	Role of surfactants in spreading	105
4.4	Physics of (not) mixing	106
4.5	Example of a stable swirling pattern	107
A.1	Additional thermocouple experiments	115
A.2	Other calculations of average temperature	120

A.3	Numerical fit of environment temperature	125
A.4	Numerical fit of thermocouple temperature with different plunging speeds	128
B.1	Validation of the LBRMT fluid solver	135
B.2	Profiling and multithreading of the LBRMT	139
C.1	Marbling pattern: stone	142
C.2	Marbling pattern: French curl	143
C.3	Marbling pattern: gelgit	144
C.4	Marbling pattern: gelgit (free-style)	145
C.5	Marbling pattern: nonpareil	146
C.6	Marbling pattern: Icarus	147
C.7	Marbling pattern: collage of stone, gelgit, nonpareil, feather, and Icarus	148
C.8	Marbling pattern: bouquet	149
C.9	Marbling pattern: octopus	150
C.10	Marbling pattern: palm, flame, and octopus	151
C.11	Marbling pattern: Spanish waves	152
C.12	Marbling pattern: zebra on Spanish waves	153
C.13	Marbling pattern: Italian vein	154
C.14	Marbling pattern: overmarble	155
C.15	Marbling pattern: free-style	156
C.16	Marbled bookmarks	157

List of Tables

2.1	Geometric, physical, and thermal properties involved in the cryo-plunging simulation	20
2.2	Individual sample cooling time and rate	39
3.1	Summary of the velocity sets c_i and their weights w_i in D_2Q_9 model	56
3.2	Relevant LBRMT simulation parameters with their symbols and physical dimensions	67
A.1	Example input file to <code>cryoflo</code>	119
A.2	Relative errors compared with experiments at different plunging speeds	127
B.1	Conversions between the same quantity in the physical unit system and the LB unit system . . .	132
B.2	Timing and multithreading results of Section 3.4 simulations	138

TO MY MĀMA AND BÀBA.

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