

Contents

	<i>Preface</i>	<i>page ix</i>
1	Introduction	1
2	Nonequilibrium Thermodynamics and Continuum Mechanics	5
	2.1 Thermodynamics	5
	2.2 Continuum Mechanics	7
	2.3 Nonequilibrium Thermodynamics	9
	2.4 Multicomponent Fluids and Coupled Transport Processes	19
	2.5 Spin Angular Momentum	25
3	Statistical Mechanical Foundations	31
	3.1 Fundamentals of Classical Mechanics	31
	3.2 The Liouville Equation	34
	3.3 Time Evolution	35
	3.4 Response Theory	38
	3.5 Green–Kubo Methods for Linear Transport	51
	3.6 Fluctuation Theorems	54
4	Temperature and Thermodynamic Fluxes	59
	4.1 Temperature	59
	4.2 Pressure Tensor and Heat Flux Vector	62
	4.3 Method of Planes Techniques for Inhomogeneous Fluids	76
	4.4 Volume Averaged Form of the Local Pressure Tensor	91
	4.5 Inclusion of Electrostatic Forces	92
5	Homogeneous Flows for Atomic Fluids: Theory	104
	5.1 The SLLOD Equations of Motion	104
	5.2 Dynamical Maps and the Relationship to Periodic Boundary Conditions	129

vi	Contents	
	5.3	Thermostats 136
	5.4	Further Considerations of the SLLOD Equations of Motion 147
6	Homogeneous Flows for Atomic Fluids: Applications	150
	6.1	Time-independent Flow 150
	6.2	General Homogeneous Flows 163
	6.3	Mixed Shear and Planar Elongational Flows 174
	6.4	Thermodynamic, Rheological and Structural Results for Simple Fluids under Shear and Extensional Flows 177
	6.5	TTCF Algorithms for Shear and Elongational Flows 190
7	Homogeneous Heat and Mass Transport	203
	7.1	Single Component Heat Transport 204
	7.2	Diffusion 210
	7.3	Multicomponent Heat Transport 214
	7.4	Evaluation of Thermodynamic Quantities 219
	7.5	Heat Transport for Molecular Fluids 223
8	Homogeneous Flows for Molecular Fluids	229
	8.1	Explicit and Coarse-grained Molecular Models 229
	8.2	Molecular Representation of the Pressure Tensor 239
	8.3	Molecular SLLOD 243
	8.4	Momentum and Internal Energy Balance in the Presence of a Homogeneous Thermostat 245
	8.5	Molecular Thermostats 247
	8.6	Molecular SLLOD Algorithms for Shear Flow 251
	8.7	Molecular SLLOD Algorithms for Elongational Flow 253
	8.8	Results for Molecular Fluids 254
9	Inhomogeneous Flows for Atomic Fluids	266
	9.1	Sinusoidal Transverse Field (STF) Method 267
	9.2	Poiseuille Flow 277
	9.3	Couette Flow 289
10	Confined Molecular Fluids	294
	10.1	Molecular Fluids 294
	10.2	Spin Coupling, Flow Reduction and Manipulation on the Nanoscale 302
	10.3	Binary Mixtures 303

11	Generalised Hydrodynamics and Slip	306
	11.1 Generalised Hydrodynamics	306
	11.2 Predicting Slip	325
	<i>Bibliography</i>	335
	<i>Index</i>	355