

# Contents

**Acknowledgment — VII**

**Preface — IX**

## **Part I: Foundations and examples of complex heterogeneous systems**

### **1 Introduction and motivation — 3**

1.1 Notation, definitions, and dimensionless formulations — 11

### **2 Fundamental building blocks for CHeSs — 16**

- 2.1 Thermodynamic principles as a systematic pillar — 16
  - 2.1.1 Key concepts: system, heat, work, energy, and entropy — 16
  - 2.1.2 Efficiency: heat engines and generalizations — 26
  - 2.1.3 Fluctuations — 30
- 2.2 Complexity — 33
  - 2.2.1 McCabe's complexity: cyclomatic complexity — 35
- 2.3 Algorithmic Information Content (AIC) — 38
  - 2.3.1 The Turing machine — 38
  - 2.3.2 Definition of AIC — 39
- 2.4 Networks and graphs: from the theory of systems to CHeSs — 41
- 2.5 From thermodynamics to information — 44
  - 2.5.1 Maxwell's demon — 46
- 2.6 Percolation: criticality and phase transitions — 48
- 2.7 Nonequilibrium CHeSs: GENERIC and Variational Principles — 51
  - 2.7.1 Attempts inspired by GENERIC: dilute solutions from minimal energy and maximum dissipation — 52
- 2.8 Smart Interacting CHeSs: autonomy, decision, strategy, and learning — 53
  - 2.8.1 Learning interaction strategies: the fictitious play — 74
  - 2.8.2 Framework for decision dynamics: kinematic evolution and utility functions — 82

### **3 Examples of CHeSs: toward reliable and systematic descriptions — 88**

- 3.1 Nonequilibrium CHeSs: transport in solids — 88
  - 3.1.1 Applications and limits of phase field formulations — 92
- 3.2 Universal CHeSs: coarsening in heterogeneous media — 93
  - 3.2.1 Interfacial dynamics in heterogeneous media: coarsening rates — 93
- 3.3 Information/data processing systems as CHeSs: from PC over DC and HPC to QC — 98

3.3.1	PC as a CHeS —	<b>98</b>
3.3.2	DC as a CHeS —	<b>100</b>
3.3.3	HPC as a CHeS —	<b>102</b>
3.3.4	QC as a CHeS —	<b>103</b>
<b>4</b>	<b>CHeSs and measurements: state and parameter estimation —</b>	<b>105</b>
4.1	CHeS identification and description: stochastic models and filters —	<b>105</b>
4.1.1	CHeSs as stochastic input/output models —	<b>105</b>
4.1.2	CHeSs as a filter —	<b>112</b>
4.2	Concepts of parameter estimation —	<b>113</b>
4.2.1	Least Squares Estimator (LSE) —	<b>114</b>
4.2.2	Maximum Likelihood Estimator (MLE) —	<b>125</b>
4.3	State prediction of CHeSs by measurements: Kalman filter —	<b>128</b>
4.3.1	The Kalman filter problem formulation —	<b>129</b>
4.3.2	The discrete-time Kalman filter algorithm —	<b>131</b>
4.3.3	Derivation of the discrete-time Kalman filter —	<b>132</b>
<b>5</b>	<b>Reliability and degradation in CHeSs —</b>	<b>134</b>
5.1	Introduction —	<b>134</b>
5.2	Fundamental concepts —	<b>135</b>
5.3	Serial arrangement: $N$ independent systems —	<b>136</b>
5.4	Parallel arrangement: $N$ independent systems —	<b>137</b>
5.5	Reliability in CHeSs: serial and parallel combinations —	<b>138</b>
5.5.1	Software reliability —	<b>139</b>
<b>6</b>	<b>Multiscale CHeSs: upscaling, effective properties, and macroscopic descriptions —</b>	<b>142</b>
6.1	Introduction —	<b>142</b>
6.2	Network/graph-based upscaling: flow/circuit laws —	<b>142</b>
6.3	Upscaling based on homogenization theory: asymptotic two-scale expansion —	<b>145</b>
6.4	Properties of the effective conductivity tensor (6.22) —	<b>148</b>
6.4.1	(A) Symmetry and positive definiteness —	<b>148</b>
6.4.2	(B) Simple upper and lower bounds —	<b>150</b>
6.5	Upscaling for slowly varying microstructure —	<b>155</b>
6.6	Hydraulic conductivity: Darcy's law —	<b>157</b>
6.6.1	Stokes flow through deterministic pore spaces: formal derivation —	<b>157</b>
6.7	Convection diffusion problems —	<b>160</b>
6.8	CHeSs showing fractal designs: theory and examples —	<b>162</b>
6.8.1	Characterizations of fractals and generalizations to CHeSs —	<b>164</b>
6.8.2	Investigating fractal CHeSs —	<b>172</b>

- 6.8.3 Cross-shaped fractals: Surface areas, porosities, and capacities in CHeSs — 172

## **7 Quantum algorithms describing CHeSs — 177**

- 7.1 Introduction — 177
- 7.2 Mathematical framework for quantum systems — 177
- 7.3 Solving multiscale problems on a quantum computer — 178
- 7.3.1 Quantum algorithms required for multiscale problems — 179
- 7.3.2 Multiscale problems' benefit from quantum computers — 190

## **8 Electrochemical CHeSs — 195**

- 8.1 Energy storage and fuel cell systems — 195
- 8.1.1 CHeSs describing energy storage systems — 195
- 8.1.2 Fuel cell systems representing electrochemical CHeSs — 196
- 8.2 Optimal material design as interacting CHeSs — 199
- 8.3 Battery modeling — 205
- 8.3.1 Thermodynamic consistency: nonequilibrium formulation for electrolytes — 206
- 8.3.2 System (8.16) satisfies the principles of GENERIC — 209
- 8.3.3 Examples belonging to system (8.16) — 211
- 8.3.4 Charge transport formulations for Li-batteries — 214
- 8.3.5 Fundamental and Self-consistent Battery Equations (FSBEs): binary and neutrally dilute electrolytes with active Li-hosts — 218
- 8.3.6 Two-phase composite Li-battery — 218
- 8.3.7 Current-driven FSBE: linearization and 1D analytic solutions — 226
- 8.3.8 Nonlinear and self-consistent Li-transport in concentrated polymer solutions — 231

## **Part II: Rigorous mathematical methods: CHeSs relevant applications**

### **9 Electrochemical CHeSs: from well-posedness to battery failure/blow-up — 239**

- 9.1 Well-posedness of a binary electrolyte for  $\mathbf{v} = 0$  — 239
- 9.1.1 Conditions for blow-up in finite time — 243

### **10 Rigorous upscaling of CHeSs: the two-scale convergence method — 247**

- 10.1 Introduction — 247
- 10.2 The classical two-scale convergence method — 248
- 10.2.1 Two-scale convergence of conductivity problems — 250

<b>11</b>	<b>CHeSs governed by interparticle forces — 254</b>
11.1	Introduction — <b>254</b>
11.2	Upscaling of a hard-sphere particle system — <b>254</b>
11.2.1	Main results: effective macroscopic transport in strongly heterogeneous materials — <b>257</b>
11.2.2	Proof of the main results — <b>258</b>
11.3	Locating obstacles in transport problems: forward and inverse problems — <b>260</b>
11.3.1	Forward problem $\mathcal{F}$ — <b>261</b>
11.3.2	Inverse problem $\mathcal{I}$ — <b>262</b>
11.3.3	Data inferred barycenter: optimality constraints — <b>263</b>
11.4	Computational method: constrained gradient descent — <b>266</b>

**Bibliography — 269**

**Index — 277**