Preface to the Second Edition

Seven years have past since the first edition of this book is published. This new edition is composed of 13 chapters. Actually, we have broken two chapters of the first edition into several ones, providing with additional sections. We also added new chapters, following fundamental concepts of the first edition. Thus we deal with several models in physics, chemistry and biology, taking regarding two mathematical structures, that is the duality and scaling. In this new edition, we added several topics in physics, particularly the theory of perfect fluids and that of static magnetic fields. Some parts, particularly, the chapters of chemotaxis and time realization are also modified according to the study after the first edition. Below we record the descriptions at the beginning of the chapters of the first edition.

Duality-Sealed Variation

Self-organization is a phenomenon widely observed in physics, chemistry, and biology. Usually, it is mentioned in the context of far-from-equilibrium of dissipative open systems describing the discharge of entropy, but the other aspect, formation of self-assembly, is sealed in the total set of stationary solutions of thermodynamically closed systems. This stationary problem is contained in a hierarchy of the mean field of many self-interacting particles, whereby the transmission of free energy is a leading factor. We can observe a unified structure of calculus of variation in these mathematical models, and obtain a guideline of mathematical analysis from it, especially in the total structure of stationary solutions and its roles in dynamics. Then we will see the features of self-organization achieved *near from equilibrium*.

Equations describing self-assembly have been classified into models (A), (B), and (C). Although model (C) equations indicate models other than those of model (A) or (B) equations, see [113], some of them are formulated as the (skew-) gradient system with semi-duality. In this part, first, we take a simplified system of

chemotaxis to confirm the above story, and then develop the abstract theory of Toland duality. Next, we examine the closed characters of model (A) and model (B) equations, and, finally, confirm the profiles of dual variation sealed in several model (C) equations.

Scaling–Revealing Hierarchy

Details of the self-organization are hierarchical achievements between self-assembly and dissipative structures [425]. The latter is top-down and occurs in a far-from-equilibrium formulation of an open system that involves dissipation of entropy and is characterized by periodic structures, spiral waves, traveling waves, self-similar evolutions, and so forth [269]. The former is, as described in the previous part, bottom-up and controlled by the stationary state of the closed system which is involved by condensates, collapses, spikes, quantizations, free energy transmissions, variational structures, and so forth. The control of the total set of stationary states to the global dynamics, however, is not restricted to thermodynamics. This profile is observed widely in mathematical models involved by the mean field hierarchy and sometimes referred to as the nonlinear spectral mechanics [364]. In more precise terms, there is a unified mathematical principle in each mean field hierarchy provided with the underlying physical principle, such as the conservation laws, decrease of the free energy, and so forth.

This part describes the *quantized blow-up mechanism* which is one of the leading principle of self-assembly. It arises in self-interacting fluid, turbulence in the context of the *propagation of chaos*, mean field hierarchy derived from the *friction–fluctuation* self-interaction in the molecular kinetics, and gauge field concerning *condensate* of microscopic states. Actually, this profile of quantization is revealed by a blow-up analysis which is one of the important products of the method of scaling and is valid even to the higher space dimension.

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Preface to the First Edition

In general, systems of nonlinear partial differential equations are formulated and studied individually according to specific physical or biological models of interest. There are, however, certain classes of Lagrangian systems for which the asymptotic behavior of the nonstationary solutions, including the blow-up mechanism, is controlled by their total sets of stationary solutions. In this book, we will show that these equations have their origin in mean field theory and that the associated elliptic problems are provided with mass and energy quantizations because of their scaling properties.

Mean field approximation has been adopted to describe macroscopic phenomena from microscopic overviews, with some success, though still in progress, in many areas of science, such as the study of turbulence, gauge field, plasma physics, self-interacting fluids, kinetic theory, distribution function method in quantum chemistry, tumor growth modeling, phenomenology of critical phenomena. In this last scientific area, phase transition, phase separation, and shape memory alloys are included.

However, in spite of such a wide range of scientific areas that are concerned with the mean field theory, a unified study of its mathematical structure has not been discussed explicitly in the open literature. The benefit of this point of view on nonlinear problems should have significant impact on future research, as will be seen from the underlying features of self-assembly or bottom-up self-organization which is to be illustrated in a unified way. The aim of this book is to formulate the variational and hierarchical aspects of the equations that arise in the mean field theory from macroscopic profiles to microscopic principles, from dynamics to equilibrium, and from biological models to models that arise from chemistry and physics.

One of the key concepts to be used repeatedly in our discussion in this book is the notion of duality, which has been the origin of the extension of functions to distributions [322] that provides a useful tool for the formulation of *weak solutions* in the theory of partial differential equations. In addition, Riesz' representation theorem [117] provides the formulation of duals for such important function spaces

as $C(K)' \cong M(K)$ and $L^1(\Omega)' \cong L^\infty(\Omega)$, where K and Ω are compact and open sets in R^n, respectively. Thus if a family of continuous approximate solutions is not compact but is provided with *a priori* estimates, say, in the L^∞ or L^1 norm, then the weak solution is realized as an L^∞ function or a measure, respectively, whereby several fundamental profiles caused by the nonlinearity can be observed (e.g., interface, shock, localization, concentration, condensate, blowup, self-similar evolution, traveling and spiral waves, …). Another concept of duality, namely, that of Hardy–BMO [344] is reflexive. It is represented by $L\log L(\Omega)' \cong Exp(\Omega)$ and $Exp(\Omega)' \cong L\log L(\Omega)$, where $\Omega \subset R^n$ is a bounded domain. The Hardy–BMO duality is associated with the mean field hierarchy through the *entropy* functional and the *Gibbs measure*. Thus this duality notion can be applied to the study of phenomena between particles and fields in the microscopic level as governed by the Boltzmann principle and the zeta function, respectively. Yet another duality concept that will be used in this book is operator theoretical. For example, for some given rectangular matrix A a column vector b, the duality of the linear model $Ax = b$ is the transposed operation that arises in the context of the Fredholm formulation concerning the existence and uniqueness of the solution. On the other hand, the linear inequality $Ax \geq b$ in convex analysis has an analogous duality formulation. For example, this formulation results from integrating a linear functional equation where the *Legendre transformation* takes on the role of the transposed operator [35]. This involutive operation is often referred to as the Fenchel–Moreau duality, which results in the more complicated dualities of Kuhn–Tucker and Toland. Here, the *Toland* duality is concerned with the functional represented by the difference of two convex functionals, such as the Helmholtz free energy. The field functional then is obtained in its dual form, and these two principal functionals are regarded as unfoldings of the *Lagrangian*.

This book consists of two main chapters. The first chapter is devoted to the study of variational structures, where the quantized blow-up mechanism observed in the chemotaxis system [364] is first described. Within this section, the free energy transmission, which results in the formation of self-assembly, is emphasized which means that the source of the emergence is the wedge of blow-up envelope, while entropy and mass are exchanged to create a clean self with the quantized mass. The leading principle derived from this study can be summarized as follows: dual variation sealed in the mean field hierarchy and scaling that reveals this hierarchy. In fact, the phenomenon of quantization is sealed in the total set of stationary solutions, referred to as the nonlinear spectral mechanics. The structure of dual variation controls, not only the local dynamics around the stationary state, but also the formation of self-assembly realized as a global dynamics including the blowup of the solution. This duality is associated with the convexity of the functional; and thus, our description involves convex analysis as mentioned above. We will examine the phenomena and logistics of both variational and dynamical structures of several problems including phase transition, phase separation, hysteresis in shape memory alloys which review the theory of nonequilibrium thermodynamics.

Chapter 2 is devoted to the discussion of the method of scaling for revealing the mathematical principles hidden in the mean field hierarchy subject to the second law of thermodynamics. More precisely, we will describe the quantized blow-up mechanism observed in self-gravitating fluid, turbulence, and self-dual gauge field. In particular, blow-up analysis, one of the most important applications of the method of scaling, is used to clarify this mechanism. This analysis consists of four ingredients, namely, scaling invariance of the problem, classification of the solution of the limit problem defined on the whole space and time, control of the rescaled solution at infinity, and hierarchical arguments. Meanwhile we will also describe the method of statistical mechanics for the study of macroscopic phenomena caused by the microscopic principles. In particular, we will reformulate the simplified system of chemotaxis as a fundamental equation of the material transport, the Smoluchowski–Poisson equation.

Unfortunately, a complete overview of the topics mentioned above is beyond the scope of this book, and the list of references is far from being sufficient. Furthermore, several important related topics are missing, among which are the complex Ginzburg–Landau free energy associated with superconductivity in low temperature [24, 269], Arnold's variational principle for describing the MHD equilibrium [12], the density function theory of quantum chemistry [48], kinetic equations in fluid dynamics [32], and the duality between Aleksandrov's problem in integral geometry and the optimal mass transport theory [281]. There are also several stationary problems in engineering associated with duality [131] which may be extended to the nonstationary problems of their own.

We take this opportunity to clarify several terminologies used in this book that are the concern of thermal phenomena associated with *dissipation*. First, we follow the classical concepts of equilibrium thermodynamics and classify thermal systems into isolated, closed, and open systems. This classification is also associated with the theory of equilibrium statistical mechanics. More precisely, these systems are provided with the microscopic structures of microcanonical, canonical, and grand canonical ensembles, respectively. A closed system here indicates the lack of transport of materials between the outer systems, whereby the transport of heat and that of the energy are permitted. In the open system, on the other hand, the transport of material between the outer systems is also permitted. Next, in view of the theory of nonequilibrium thermodynamics, we add one more aspect to the openness, that is the dissipation of entropy to the outer system [266]. Under this agreement, closedness is reformulated as a system provided with decreasing total free energy or that provided with increasing total entropy. Thus we have two kinds of closedness: physical closedness in terms of kinetic and/or material, and thermodynamical closedness described by two typical models discussed in detail in this book. Free energy *transmission* occurs in the latter case and could be the origin of "self-assembly".

In this connection, we note that the *dissipative system* is defined by the presence of an attractor in the theory of dynamical systems. Gradient system with compact semi-orbits is a typical dissipative system in this case [151]. We believe, however, that this definition of dissipative system does not describe what were observed by

[266]. More precisely, decrease of the free energy or increase of the entropy means thermodynamical *closedness*. It is formulated by the gradient system in the same two models as mentioned above, and, therefore, is never provided with the dissipation in the sense of nonequilibrium thermodynamics [266] in spite of the fact that these two models are typical dissipative systems in the theory of dynamical systems. To avoid this confusion, the above mentioned terminology of dissipative system in the theory of dynamical systems [151] is *not* used in this book. Actually, a recent paradigm asserts two aspects of self-organization, *far-from-equilibrium* (top-down self-organization) and *self-assembly* (bottom-up self-organization), emphasizing the role of their *hierarchical developments*, with the Hopf bifurcation casting the threshold [425]. Dissipation occurs in a state far-from-equilibrium, which results in a spiral wave, a traveling wave, a periodic structure, a self-similar development, and so forth; while self-assembly, we believe, is formed near-from-equilibrium of thermodynamically closed system induced by the stationary states, developing a condensate, a collapse, a blowup, a spike, and so forth.

This book is concerned with the formation of self-assembly. Its profile is provided with the "triple seal," of which basic concepts have already been described. First, several features of self-assembly, that is, one aspect of the self-organization are sealed in thermodynamically closed systems. Secondly, the dynamics of the closed system is sealed in the total set of stationary states. Finally, the stationary states themselves are sealed in the (skew-) Lagrangian, provided with the structure of dual variation. These features of the mean field hierarchy are certainly revealed by the method of scaling derived from the microscopic principle. In summary, formation of self-assembly arises in thermodynamically closed systems, and hence this process is subject to the calculus of variation. The closed system follows the microscopic principle. This principle controls the mean field hierarchy totally, and, therefore, fundamental profiles of the macroscopic mean field equation are revealed by the method of scaling. We would like to thank Prof. Tomohiko Yamaguchi for several stimulative discussions on nonequilibrium thermodynamics. Thanks are also due to Profs. Piotr Biler, Fumio Kikuchi, Futoshi Takahashi, and Gershon Wolansky for careful reading over the primary version of the manuscript.

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