Perspective: New directions in dynamical density functional theory

Michael te Vrugt and Raphael Wittkowski
Institut für Theoretische Physik, Center for Soft Nanoscience, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany
E-mail: raphael.wittkowski@uni-muenster.de

Abstract
Classical dynamical density functional theory (DDFT) has become one of the central modeling approaches in nonequilibrium soft matter physics. Recent years have seen the emergence of novel and interesting fields of application for DDFT. In particular, there has been a remarkable growth in the amount of work related to chemistry. Moreover, DDFT has stimulated research on other theories such as phase field crystal models and power functional theory. In this perspective, we summarize the latest developments in the field of DDFT and discuss a variety of possible directions for future research.

Keywords: dynamical density functional theory (DDFT), phase field crystal models, power functional theory, soft condensed matter, active and biological matter, nonequilibrium statistical mechanics, chemistry

1. Introduction
Classical dynamical density functional theory (DDFT) is a theory for the time evolution of the one-body density $\rho$ of a fluid, which is based on extending results from equilibrium density functional theory (DFT) \([1, 2]\) toward the nonequilibrium case. DDFT exists in deterministic and stochastic variants. Deterministic DDFT was first introduced phenomenologically by Evans [3] and later derived from microscopic particle dynamics by Marini Bettolo Marconi and Tarazona [4], Archer and Evans [5], Yoshimori [6], and Español and Löwen [7]. Stochastic DDFT was pioneered by Munakata [8], Kawasaki [9], and Dean [10]. Finally, Fraaije and coworkers [11, 12] have developed a DDFT for polymers. Nowadays, DDFT has been applied in a large and diverse number of fields ranging from simple [13] and colloidal [4] fluids to plasmas [14] and microswimmers [15]. A recent review can be found in [16].

Apart from its ‘older brother’ DFT, DDFT has two younger ‘siblings’—namely phase field crystal (PFC) models [17, 18] and power functional theory (PFT) [19, 20]. PFC models are simpler than DDFT (and can be derived from it [21]), whereas PFT is more complex and contains DDFT as a limiting case. The development of these two other theories is intimately connected to that of DDFT, and progress in DDFT has stimulated progress in these other theories. For example, the development of active DDFT [22] allowed to derive an active PFC model [23, 24], and improvements in DDFT allow also for more accurate PFT equations [25].
This perspective article complements our review [16] in two ways. First, we present articles on DDFT from the past two years, thereby also covering articles not included in the review because they are too recent. Second, we discuss perspectives for future work, thereby providing also a more speculative outlook on the new directions the field is developing towards.

This article is structured as follows: In section 2, we briefly review the derivation of DDFT and its relations to some other methods. Recent developments are explained in section 3. In section 4, we discuss possible future directions. We conclude in section 5.

### 2. A brief introduction to DDFT

#### 2.1. Density functional theory

DDFT is an extension of classical DFT, which describes the equilibrium state of a classical fluid. Classical DFT, in turn, originates from the more widely known quantum DFT developed by Hohenberg and Kohn [26], which allows to model the ground state of a many-electron system.

We start by briefly introducing DFT following [16, 27]. The microscopic description of a classical many-body system requires, in principle, knowledge of the exact phase-space distribution function. Classical DFT makes use of the fact that the state of an equilibrium fluid is completely determined once the one-body density $\rho$ is known. The equilibrium density $\rho_{\text{eq}}$ can be calculated from the grand-canonical free energy functional $\Omega$ (depending on the temperature $T$ and the chemical potential $\mu$) via the minimization principle (DFT equation)

$$\frac{\partial \Omega(T, \mu, \rho)}{\partial \rho(r)} \bigg|_{\rho = \rho_{\text{eq}}} = 0. \quad (1)$$

From the grand-canonical functional $\Omega$, the canonical free energy functional $F$ can be obtained via the Legendre transformation

$$\Omega(T, \mu, \rho) = F(T, \rho) - \mu \int d^3r \rho(r). \quad (2)$$

The free energy $F$ can be split into three parts:

$$F(T, \rho) = F_{\text{id}}(T, \rho) + F_{\text{exc}}(T, \rho) + F_{\text{ext}}(\rho). \quad (3)$$

The first term in equation (3) is the exactly known ideal gas free energy

$$F_{\text{id}}(T, \rho) = k_B T \int d^3r \rho(r) \left( \ln(\Lambda^3 \rho(r)) - 1 \right). \quad (4)$$

Here, $k_B$ is the Boltzmann constant and $\Lambda$ is the (irrelevant) thermal de Broglie wavelength. The third term in equation (3) is the external free energy

$$F_{\text{ext}}(\rho) = \int d^3r \rho(r) U_1(r) \quad (5)$$

depending on the external potential $U_1$. Finally, the excess free energy $F_{\text{exc}}$ describes interactions of the particles in the system and is not known exactly. (Parametric dependencies are suppressed from here on.)
2.2. Dynamical density functional theory

Now, we turn to the nonequilibrium case and present the derivation of DDFT following Archer and Evans [5]. The starting point is the Smoluchowski equation

\[
\frac{\partial}{\partial t} \hat{\Psi} (\{\vec{r}_i\}, t) = \Gamma \sum_{i=1}^{N} \vec{\nabla} \cdot (k_B T \vec{\nabla} \hat{\rho}_i + \vec{\nabla} U(\{\vec{r}_i\}, t)) \hat{\Psi} (\{\vec{r}_i\}, t)
\]

(6)

describing the dynamics of the distribution function \( \hat{\Psi} \) depending on the positions \( \vec{r}_i \) of the \( N \) particles (we consider spherical overdamped particles with two-body interactions only) and on time \( t \). Here, \( \Gamma \) is the mobility of a particle and \( U = U_1 + U_2 \) (with the pair-interaction potential \( U_2 \)) the total potential. The one-body density is defined as

\[
\rho(\vec{r}, t) = N \int d^3 r_2 \cdots \int d^3 r_N \hat{\Psi} (\{\vec{r}_i\}, t).
\]

Integrating equation (6) over the coordinates of all particles except for one and using equation (7) gives

\[
\frac{\partial}{\partial t} \rho(\vec{r}, t) = D \vec{\nabla}^2 \rho(\vec{r}, t) + \Gamma \vec{\nabla} \cdot (\rho(\vec{r}, t) \vec{\nabla} U_1(\vec{r}, t)) + \Gamma \vec{\nabla} \cdot \int d^3 r' \rho(2)(\vec{r}, r', t) \vec{\nabla} U_2(\vec{r}, r')
\]

(8)

with the diffusion constant \( D = \Gamma k_B T \), where we write \( \vec{r} \) for \( \vec{r}_1 \) and \( \vec{r}' \) for \( \vec{r}_2 \). Since equation (8) depends also on the unknown two-body density \( \rho^{(2)} \), we require a closure. For this purpose, one uses the adiabatic approximation, which corresponds to the assumption that the correlations in the system are the same as in an equilibrium system. This allows to insert the equilibrium relation

\[
\rho(\vec{r}) \vec{\nabla} \frac{\delta F^{\text{exc}} [\rho]}{\delta \rho(\vec{r})} = \int d^3 r' \rho^{(2)}(\vec{r}, r') \vec{\nabla} U_2(\vec{r}, r')
\]

(9)

into equation (8) to obtain the DDFT equation

\[
\frac{\partial}{\partial t} \rho(\vec{r}, t) = \Gamma \vec{\nabla} \cdot \left( \rho(\vec{r}, t) \vec{\nabla} \frac{\delta F^{\text{exc}} [\rho]}{\delta \rho(\vec{r}, t)} \right).
\]

(10)

Important alternative derivation routes start from the Langevin equations [4, 28] that describe the motion of the particles in the system or use the Mori–Zwanzig formalism [6, 7]. A complete overview is given in [16].

It is also worth mentioning here the most important limitations of DDFT (discussed in more detail in [16]):

(a) The adiabatic approximation required for the derivation of (deterministic) DDFT breaks down in a variety of contexts. For example, it does not capture shear flow\(^1\), which can bring a system arbitrarily far out of equilibrium without creating density gradients and therefore without creating adiabatic forces [20]. Colloidal many-body systems are governed by viscous and structural nonequilibrium forces not captured within the adiabatic approximation [20, 30]. Moreover, the adiabatic approximation leads to an underestimation of relaxation times [4, 31].

(b) DDFT usually employs grand-canonical free energy functionals, which leads to inaccuracies for systems with a small number of particles [32, 33].

---

\(^1\) Note that some extensions of DDFT do allow to model shear flow [29].
Free energy functionals used in practice are typically approximate. A possible consequence of this is that the system gets stuck in a local minimum of the free energy, leading to an arrested state that would not be predicted by a better functional [4].

Due to an underlying ergodicity assumption, DDFT predicts that hard particles in one dimension can pass through each other (which is unphysical) [25, 33].

### 2.3. Related approaches

**PFC models** [17, 18] are a closely related approach. They are based on an order parameter $\psi$ that is related to the density $\rho$ by $\rho = \rho_0 (1 + \psi)$, where $\rho_0$ is a spatially and temporally constant reference density. The governing equation of PFC models is given by

$$\frac{\partial}{\partial t} \psi(\vec{r}, t) = M \nabla^2 \frac{\delta F[\psi]}{\delta \psi(\vec{r}, t)}$$

(with a mobility $M$) and can be derived from equation (10) by making the approximation of a constant mobility. The free energy $F$ in PFC models is also considerably simpler than that of (D)DFT and can be derived by performing a Taylor expansion for the logarithm in equation (4) and a functional Taylor expansion combined with a gradient expansion for the excess free energy $F_{\text{exc}}$.

A detailed discussion of this derivation can be found in [16, 18, 34].

An extension of DDFT that has gained some popularity is PFT, which was developed by Schmidt and Brader [19] (see [16, 20, 35] for a review). PFT describes the nonequilibrium dynamics of many-body systems and is, like DFT, a formally exact variational theory. The variational principle is formulated here not for the density $\rho$, but for the current $\vec{J}$ that minimizes the so-called ‘power functional’. One can split the dissipative intrinsic part of this functional into an ‘ideal part’ (the part that is already present in DDFT) and an ‘excess part’ $P_{\text{exc}}$.

This leads to the governing equation [19]

$$\frac{\vec{J}(\vec{r}, t)}{\Gamma \rho(\vec{r}, t)} + \frac{\delta P_{\text{exc}}(\rho, \vec{J}, t)}{\delta \vec{J}(\vec{r}, t)} = -\nabla \frac{\delta F[\rho]}{\delta \rho(\vec{r}, t)}$$

of PFT, which reduces to equation (10) for $P_{\text{exc}} = 0$. (In PFT for Newtonian or quantum mechanics, one considers the power rate instead, which is minimized with respect to $\dot{\vec{J}}$ [36, 37]).

Given that PFT does not rely on the adiabatic approximation, it allows to avoid the problems related to limitation 1. For instance, PFT is capable of describing sheared systems and all relevant viscous and structural forces [20, 30, 38, 39].

The excess power functional $P_{\text{exc}}$ contains contributions that counteract the excessively fast relaxation predicted by the adiabatic part of the dynamics [20]. Notably, the functional $P_{\text{exc}}$ is non-local in space and time, and therefore allows to incorporate memory effects not present in DDFT. The presence of memory can give rise to interesting dynamics [40]. A further advantage of PFT is that it, in analogy to equilibrium DFT, is based on a formally exact variational principle [20]. PFT is also more accurate than PFC models (as a direct consequence of the fact that PFT is more accurate than DDFT and DDFT is more accurate than PFC models).

The relations between DFT, DDFT, PFC models, and PFT are visualized in figure 1. DFT is an exact theory (apart from approximations required for the free energy functional) for an equilibrium fluid. PFC models also allow to describe equilibrium systems, but with a more approximate free energy functional. If we go to the nonequilibrium case and use DDFT or PFC models, we are making an approximation (namely the adiabatic approximation), such that the theory is not
Figure 1. Relations of the various theories discussed in section 2. Different approaches can be used depending on the desired accuracy and the importance of nonequilibrium effects. The top right corner leaves room for future developments.

exact. PFT, finally, provides an exact nonequilibrium theory. For the three dynamical theories DDFT, PFC models, and PFT, we include also an active variant which is based on the same sorts of approximations, but will usually be applied to systems further away from equilibrium (namely active ones \([41, 42]\)).

A connection can also be established between DDFT and the path-integral approach. While equation (10) is deterministic, a very similar equation with a noise term (a stochastic DDFT) governs the dynamics of the microscopic density operator \([10]\). This theory, where \(F_{\text{exc}}\) takes a simple mean-field form, is an exact reformulation of the underlying Brownian dynamics (BD), and also the starting point for the derivation of deterministic DDFT in \([4]\). As demonstrated in \([43]\), stochastic DDFT can be re-written in path-integral form. Action functionals can be obtained within the Martin–Siggia–Rose (MSR) path-integral formalism \([44]\) (reviewed in \([45]\)). In the context of stochastic DDFT, the MSR formalism has been used to study mode-coupling theory and the glass transition \([46, 47]\). Recent applications can be found not only in works addressing this problem \([48, 49]\), but also in active matter physics \([50]\). Such methods have been used to study the ergodic-nonergodic transition \([47]\), whereas deterministic DDFT faces general problems with nonergodic systems \([33]\). However, path-integral formulations are also considerably more complex than the rather simple equation (10).

Another approach that is worth mentioning here is the general equation for the nonequilibrium reversible-irreversible coupling (GENERIC) developed by Grmela and Öttinger \([51, 52]\), which aims to provide a general structure for the dynamics of nonequilibrium systems. In a recent article based on earlier work \([53]\), Haussmann \([54]\) has established a connection between DDFT and the GENERIC formalism. It was also briefly remarked in \([55]\) that an extension of DDFT derived there is consistent with the GENERIC approach.

In theoretical models of fluids, the main alternative to field-theoretical approaches such as DDFT or PFC models are microscopic particle-based approaches such as BD or molecular dynamics (MD) simulations \([56, 57]\). Here, the equations of motion (Langevin equations or Newton’s equations) governing the individual constituents of a fluid are solved numerically. Such approaches are more accurate than DDFT, but also computationally far more expensive for a many-particle system. Consequently, BD and MD simulations can be used if the
microscopic details are important, whereas DDFT has advantages if one wishes to model larger length or time scales that are not accessible by particle-based simulations. Also, the more compact form of field-theoretical approaches makes it easier to gain qualitative insights. In practice, BD and MD simulations and DDFT can complement each other. For example, a comparison to BD or MD simulation results allows to test DDFT \[16\], and parameters of field theories can be obtained by fits to BD or MD simulation results \[40\].

3. Recent developments in DDFT

Since its original development, DDFT has found a very remarkable number of applications. A detailed overview has been given in our recent review article \[16\]. Since the purpose of the present manuscript is to highlight more recent developments and, in particular, future perspectives, we now briefly discuss the work on DDFT from the past two years, thereby covering (though not exclusively) articles not yet discussed in our review.

The amount of articles published on certain selected topics is visualized in figure 2. While for some topics the number of existing articles mainly originates from the work of a single author or research group, it is possible to identify certain trends. Perhaps the most interesting one is chemistry, which is addressed by a variety of authors in a variety of ways.

3.1. Epidemiology

Already in 2020, the worldwide outbreak of the coronavirus disease COVID-19 has motivated the application of DDFT to disease spreading. In the SIR-DDFT model (a combination of the susceptible-infected-recovered (SIR) model \[58\] with DDFT), repulsive particle interactions are used to represent social distancing measures \[59\]. The SIR-DDFT model has been extended to model governmental intervention strategies that can lead to multiple waves of a pandemic \[60\]. This extension represents the first DDFT with a time-dependent interaction potential. Moreover, a software package has been developed to simulate epidemic outbreaks in the SIR-DDFT model \[61\]. Yi et al \[62\] have proposed a way of combining the SIR-DDFT model with WiFi data in order to get estimates for values of the model’s parameters. Some further extensions were suggested in \[63\]. A brief overview was given in \[64\].

3.2. Chemistry

The SIR-DDFT model has the mathematical structure of a reaction-diffusion DFT (RDDFT) \[65, 66\], i.e. a reaction-diffusion equation \[67\] with the diffusion terms replaced by the right-hand side of equation (10). RDDFT has recently been used also to study actively switching Brownian particles \[68–70\]. Another active matter model based on RDDFT has been developed by Alston et al \[71\]. Finally, RDDFT has also been applied in actual chemistry to study catalytic oxidation \[72\], crystal nucleation \[73\], metal corrosion \[74\], reactions on catalytic substrates \[75\], and reactions on electrode surfaces \[76\].

As an example for such a theory, we discuss here the RDDFT for actively switching colloids by Moncho-Jordá and Dzubiella \[68\]. The model assumes soft Gaussian particles, which are well described by a simple mean-field free energy functional \[77\] (a fact that is also exploited in the SIR-DDFT model \[59\]). These particles can switch their size, which allows for a description as a two-component mixture of big and small particles with a diffusive contribution from DDFT and reaction terms for the switching process. By changing the switching rate, the phase behavior of the liquid can be controlled. Bley et al \[69\] report good agreement of the RDDFT to BD simulations.
Also apart from RDDFT, quite a number of recent applications of DDFT come from chemistry and chemical physics, broadly construed. In particular, DDFT has been used in electrochemistry to model systems and processes such as charging of electric double layers [78, 79] and supercapacitors [80, 81], counterions [82], dielectricity [83, 84], electrolytes [85–90], impedance response [91], and ion adsorption [92]. A further example is solvation dynamics [93, 94], which has a long tradition as an application of DDFT [95]. Finally, DDFT can be used to study nanoparticle separation [96], the release of molecules from nanoparticles [97], or porous surfaces [98], and wound healing [99].

DDFT for polymer systems [11, 12], which is already well established in chemical physics, should of course also be mentioned here. On the theoretical side, the microscopic construction of mobility functions was studied [100–102]. Further work considered Bayesian model calibration [103], the influence of correlations on polymer dynamics [104], memory effects [105, 106], micelle relaxation [107], and morphological phase transitions [108]. The relation to other relaxation models was briefly discussed in [109]. Finally, the MesoDyn software [110], which allows to simulate polymer systems based on DDFT, remains an important tool in the study of polymer dynamics [111–115].

3.3. Theoretical developments

While the majority of DDFT-related works from the past two years focuses on applications rather than on theoretical foundations, there has also been some progress on the theoretical side, which we discuss here. (See section 3.6 for a discussion of theoretical progress in PFC models and PFT.) One line of work is concerned with the fact that classical DFT is formulated in the grand-canonical ensemble, which is inappropriate for very small closed systems and somewhat inconsistent with the fact that DDFT has the form of a (particle-conserving) continuity equation. Work to address this issue has been directed at formulating a canonical DFT [116–119] and at extending DDFT towards the canonical case in a formalism known as ‘particle-conserving dynamics’ (PCD) [32]. Such approaches allow to address limitation 2 of DDFT mentioned in section 2.2.

Schindler et al [33], who developed a PCD for mixtures, have noted that this theory makes the unphysical prediction of allowing hard rods in one
dimension to pass through each other (limitation 4). This problem is solved in ‘order-preserving dynamics’ (OPD) [25], a variant of PCD based on an asymmetric interaction potential. Here, the ensemble averages are constructed in such a way that ‘unphysical’ particle configurations have probability zero. This theory employs a different equilibrium framework than standard DDFT, which turns out to affect the effects of the adiabatic approximation [25]. OPD has also been of interest for philosophers of physics. Since it treats observationally indistinguishable particle configurations in different ways, it is of relevance for the long-standing philosophical debate concerned with whether such distinctions are possible [120]. Wittmann et al [25] and te Vrugt [120] also discuss OPD in relation to PFT, where the form of the superadiabatic contribution might be affected by the fact that the adiabatic one has a different form in OPD.

More generally, DDFT has been discussed in philosophy in relation to the problem of thermodynamic arrow of time, i.e. the question how the irreversibility of macroscopic thermodynamics is compatible with the reversibility of the microscopic laws of physics [121–123], and to analyze the problem of scientific reduction [124]. In particular, [121] has the specific aim of developing a philosophy of DDFT.

Some of these discussions [121, 122] discuss DDFT in relation to the Mori–Zwanzig formalism [125–129], which allows to derive irreversible transport equations from reversible microdynamics and thus to understand irreversibility [122, 130]. This formalism has also been used to derive [6, 7] and extend [55, 131–133] DDFT. It is also important for more recent work. In particular, it plays a prominent role in Fang’s development of a DDFT for ferrofluids [134–137], in analyzing memory effects in polymers [105, 106], and in the study of crystal elasticity [54, 138, 139]. A stochastic theory related to stochastic DDFT was derived using the Mori–Zwanzig formalism in [140]. Since the Mori–Zwanzig formalism continues to be improved [141–144], it is likely to play an important role also in future work on DDFT.

3.4. Applications in new physical contexts

Simple and colloidal fluids remain a central field of application for DDFT, although more recent work on these systems has gone beyond ‘standard’ DDFT in several ways. For example, Marolt and Roth [145] have used DDFT to study colloids with Casimir and magnetic interactions. Jia and Kusaka [146] used an extended form of DDFT [132] to model nonisothermal hard spheres. The transport of soft Brownian particles was analyzed by Antonov et al [147]. Zimmermann et al [148] investigated the effects of barriers on the transport of colloids through microchannels. Archer et al [149, 150] modeled quasicrystals. Montañez-Rodriguez et al [151] studied diffusion on spherical surfaces. The nonequilibrium self-consistent generalized Langevin equation [152], an extension of DDFT, was applied to arrested density fluctuations by Lira-Escobedo et al [153, 154]. Density fluctuations were also modeled using an adiabatic approximation by Szamel [155]. Finally, Sharma et al [156] have studied the local softness parameter (which is useful for the description of caging) using DDFT.

In addition, stochastic DDFT [9, 10], commonly referred to as ‘Dean–Kawasaki equation’ (a name that is somewhat unfortunate as it fails to acknowledge the differences between Dean’s and Kawasaki’s approaches [16]), has remained an important tool in the study of interacting particles with stochastic dynamics. Recent examples include active matter [157, 158], chemotaxis [159, 160], electrolytes [85, 87–90], densely packed spheres [161], and proteins [162]. Satin [163] suggested a link between stochastic DDFT and theories of gravity.

Moreover, there have been several extensions of DDFT toward physical systems not previously considered in the context of DDFT. Building up on earlier work [134, 135], Fang [136, 137, 164] has recently derived a DDFT for
ferrofluids. Another example is the development of a DDFT for granular media [165, 166], Stanton et al [167] have modeled cellular membranes in DDFT. These can be described as a mixture of lipids and proteins. Finally, Wittmann et al [168] have derived a DDFT that allows to describe mechano-sensing in growing bacteria colonies.

DDFT is also frequently studied in relation to hydrodynamics. Several works have investigated the relation between DDFT and the Navier–Stokes equation [169–171]. Sterle and Gross [172] have derived a ‘hydrodynamic DFT’, which describes underdamped mixtures. An inertial DDFT with hydrodynamic interactions was studied by Goddard et al [173]. Moreover, DDFT allows to model drying colloidal films [174], droplets [175], flow in nanopores [92], hydrodynamics of ferrofluids [164], and polymer mixtures [176].

3.5. Mathematics and software

DDFT is of interest not only in physics and chemistry, but also for applied mathematics and software development. Recent work has considered stochastic DDFT (the Dean–Kawasaki equation) [177–183] and the McKean–Vlasov equation (a DDFT-type model) [184–187] from a mathematical perspective. Moreover, numerical methods were developed for DDFT [188–196] and PFC models [197–200]. DDFT was also used to test a new Brownian dynamics simulation method [201]. A particularly rapidly growing subfield is the application of machine learning, which can be used to learn static free energy functionals [103, 202–205] that can be used also in DDFT to overcome limitation 3 (inaccurate free energy functionals) from the list in section 2.2. However, machine learning is also used in the dynamical case [206–211]. An example of the latter type is multiscale modeling of proteins based on machine learning in [208], where the DDFT from [167] is used as a macroscale model.

3.6. Related theories: PFC models and PFT

Recent studies of PFC models have focused on active matter with [212–214] and without [215–221] inertia, amorphous solids [222], bifurcation diagrams [219, 220, 223–225], colored noise [226], cubic terms [227], crystals [228], dislocation lines [229], electromigration [230], grain boundaries [231, 232], mixtures [200, 220, 233–235], nucleation [236], solidification [237, 238], and stress tensors [239].

As an example, we discuss here two derivations of active PFC models from DDFT. First, Arold and Schmiedeberg [212, 213] have derived a theory for underdamped active particles by extending previous work on inertial DDFT [240]. Here, the free energy functional is chosen based on active PFC models. Second, te Vrugt et al [220] studied the construction of free energy functionals by deriving a PFC model for a mixture of active and passive particles from DDFT. Here, it was investigated in detail which approximations lead to which types of nonlinearities and coupling terms in the free energy functional.

The past two years have seen a significant amount of work on PFT and superadiabatic forces (forces that are not captured within the adiabatic approximation). On the one hand, the formalism has found several applications in the study of acceleration viscosities [241], active matter [242], the dynamics of the van Hove function [243, 244], shear flow [38], and superadiabatic demixing [245]. On the other hand, there have been more theoretical developments such as the derivation of Noether’s theorem for statistical mechanics [246–249] (which also served as the basis for a ‘force-based DFT’ [250]), a classification of nonequilibrium forces [30], a custom flow method [251], philosophical investigations of PFT [120, 121], and a reassessment of the original derivation of
PFT [252]. A method for calculating superadiabatic forces from first principles was recently proposed by Tschopp and Brader [253].

We here present one of these approaches in more detail, namely the extension of Noether’s theorem [254] to statistical mechanics by Hermann and Schmidt [246]. Noether’s theorem is commonly applied to a variational theory based on action functionals, where it yields conservation laws based on invariances (such as momentum conservation based on translational invariance). Hermann and Schmidt [246] exploited the fact that statistical mechanics in the form of DFT (equilibrium) and PFT (nonequilibrium) can also be based on variational principles. Making use of various invariances allows to derive hierarchies of sum rules, ranging from simple mechanical laws to complex nonequilibrium relations including memory. Hermann and Schmidt [246] also presents applications to active phase separation and sedimentation.

3.7. Overview articles

Finally, further overview articles covering (also) DDFT have been published; in particular an extensive review of PFT by Schmidt [20], a tutorial on active DDFT by Löwen [255], and several reviews on biology and medicine [256–261], coarse-graining [35, 262], electrochemistry [263–271], multiscale modeling [272], PFC models [273], and polymers [274–279] in which DDFT is mentioned. In our view, this large number of overview articles published in two years further highlights how timely the topic is.

4. Perspectives for the future

4.1. PFC models

The relation of PFC models to DDFT is a very complex one whose understanding demands further work. Actually, it is not even clear how to draw the boundary between them. Some authors see PFC models simply as a special case of DDFT [280], some see the difference in the fact that PFC models use a gradient expansion for the excess free energy [21], while others reserve the name ‘PFC’ for models that also have a constant mobility approximation and an expanded logarithm in the ideal gas free energy [34].

DFT functionals can, at least for hard particles, be derived pretty much ‘ab initio’. Fundamental measure theory (FMT) [281] provides highly accurate expressions for the free energy functional in hard-particle systems, such that, if we know the particle shapes (and other basic parameter such as the temperature), we can construct the DDFT equation (10) without having to adjust any free parameters. A comparison of several hard-sphere functionals can be found in [282]. In contrast, the free energy in PFC models is typically just assumed to have a very simple Swift–Hohenberg-type form [18, 283], and the parameters of this free energy can then be adjusted to fit a wide class of materials [34]. Nevertheless, a derivation of PFC models from DDFT does give microscopic expressions for all these parameters, and so in principle, assuming the free energy to be known for a certain interaction, PFC models also do not contain any free parameters. However, this option is almost never used in practice. This has to do with the fact that the predictions of DFT for the PFC parameters can turn out to be quite inaccurate as a consequence of the fact that the approximations made in the derivation of PFC models from DDFT (and perhaps also phase field models [285, 286], which are also connected to DDFT [287]), and in
general a better understanding of scientific reduction [124]. Recently, some work has been done in this direction. This includes a microscopic extension of the active PFC model toward mixtures [220], the development of a framework for obtaining gradient-based free energies from more general expressions [288], and in particular a systematic assessment of the derivation of PFC models from DDFT by Archer et al [34], who argued that the order parameter $\psi$ of PFC models should be interpreted not as the dimensionless deviation of the density from a reference value, but as the logarithm of the density.

4.2. Power functional theory

Since, as explained in section 2, PFT contains all of DDFT, but also adds additional structure, it can be quite complex. If one is interested in a model that allows to describe far-from-equilibrium processes but that is also easy to handle, one could also use PFC approaches to approximate the DDFT terms in equation (12). This would allow to obtain a model that combines the simplicity of the PFC approach with the ability of PFT to model far-from-equilibrium processes, and would allow, e.g. to study memory in active matter within the PFC framework (as done phenomenologically in [214]). Such a theory would fit in the currently empty spot at the top right of figure 1. A further interesting idea, suggested in [289], would be to combine PFT with RDDFT (see section 3) in order to model far-from-equilibrium effects in chemical reactions.

On the other hand, also the theoretical foundations of PFT merit further investigation. In particular, a recent article by Lutsko and Oettel [252] has highlighted certain issues in the original derivation of PFT by Schmidt and Brader [19]. More generally, the usefulness of PFT in practice strongly depends on the availability of a good approximation for the excess power functional. Something that would significantly increase the power of PFT would be the development of an analogon of FMT for the excess power functional, which provides an accurate expression obtained from first principles. Moreover, as discussed in [25, 120], the question whether a particular effect is to be classified as superadiabatic or not can strongly depend on the choice of the underlying equilibrium framework (e.g. on whether or not one uses OPD in one dimension), since this framework affects the effects of the adiabatic approximation.

4.3. Quantum mechanics

Although it is a classical theory, approaches based on DDFT can also be relevant for quantum systems. For example, DDFT can be used to close equations of motion in quantum hydrodynamics [290], and PFT has been extended to quantum systems [36]. However, quantum PFT has not found many applications up to now (an exception is [291]). Given the many interesting results of classical PFT, quantum PFT could allow for further insights into the dynamics of many-electron systems.

Moreover, generalized frameworks connecting classical and quantum descriptions can be developed based on Wigner functions [292]. These provide a phase-space description of quantum systems that (with certain caveats [293, 294]) reduces to the classical Liouville equation in the classical limit. This fact has been exploited to develop DDFT-like frameworks for hybrid quantum–classical systems [295, 296]. Such approaches represent a promising direction of research, in particular given that in the Wigner framework order parameters can be derived in a very similar way as in the classical case [297] and that the Wigner equations of motion for stochastic variants of quantum mechanics closely resemble classical Fokker–Planck equations [123]. Such approaches can also be used when spin interactions are relevant (such as in quantum ferrofluids [298]), since Wigner functions can also model spins [297, 299]. A further possible connection between
classical and quantum nonequilibrium DFT is the Runge–Gross theorem [300], which forms the basis of quantum mechanical time-dependent DFT, but which was also extended to classical mechanics by Chan and Finken [301].

4.4. Active matter

Active matter physics [41, 42], the study of systems that contain self-propelled particles, continues to be a rapidly growing subfield of soft matter physics in which a number of interesting effects are presumably still to be discovered. Active particles can be described in DDFT using a one-body density that depends also on the orientation of the particles. Apart from this, the general idea behind the derivation (see section 2) is still the same. Active DDFT has a number of interesting applications, in particular in the study of microswimmers [15, 302–304] (see [255] for an overview). Moreover, active DDFT serves as the basis for the derivation of active PFC models [23, 24, 220].

A conceptual challenge in modeling active particles using DDFT is that, as explained in section 2, DDFT is based on the assumption that the two-body correlations are the same as in an equilibrium system. Therefore, DDFT is based on a close-to-equilibrium assumption, which is problematic since active systems are far from equilibrium. This problem is, as mentioned in [305, 306], inherited by active PFC models. Dhont et al [307] have argued that active DDFT is inappropriate for particles with steep and short-ranged interactions. Moreover, DDFT models for microswimmers [15, 302] can become inaccurate at higher densities [308] since hydrodynamic interactions are modeled using a far-field approximation. PFT allows, in principle, to overcome the low-activity limitation as it does not require a close-to-equilibrium assumption, although the governing equation (12) of PFT in practice typically takes the form ‘DDFT equation + correction term’. Consequently, PFT has been successfully applied to active phase separation [242]. Microscopically derived active matter models generally require as an input knowledge (or assumptions) about the correlations in the system [309], and it is among the main virtues of DDFT that it provides such an input. Therefore, a promising direction would be to develop a DDFT-like theory based on correlations from a nonequilibrium steady state. Ideas of this form have been used in [310–312].

From a more ‘applied’ perspective, an interesting project could be the study of topological defects in active matter using DDFT. For equilibrium systems, it has been found that DFT provides a quantitatively accurate description (as compared to experiments) of the topology of confined smectics [313]. Given that topological defects are of central importance for the understanding of active matter systems [314], this suggests the investigation of defect dynamics in active matter systems as a further application of active DDFT. Since even the topology of equilibrium smectics remains a topic of active research [315, 316], the nonequilibrium case (that can be accessed by DDFT) promises even more interesting discoveries. A first step in this direction is the application of an active PFC model to this problem [317].

4.5. Biology

Closely related to active matter are biological applications of DDFT, which have a remarkable diversity. DDFT allows to understand biological systems across all scales. Ion channels [318, 319], which can be found in cell membranes, are a small-scale biological system that can be modeled in DDFT. Moreover, DDFT has been used to model the membranes themselves [167]. Going to larger scales, we arrive at DDFT models of entire cells as used in applications to cancer growth [320, 321], microswimmers [15, 255, 302–304], and bacteria [168]. In the SIR-DDFT model [59, 60], the considered ‘particles’ are humans. It even does
not have to stop there, since a (quantum-based) DFT has been applied to entire ecosystems [322]. This brief list should make clear the particular advantage DDFT has in biology—the same concept can be applied across all length scales, making DDFT an ideal tool for multiscale modeling.

4.6. Chemistry

When taking a look at the publications on DDFT from the past two years, it is notable that quite a number of them are in some way related to chemistry. Examples are the numerous applications of RDDFT [59–62, 64, 68–76] and the many works on electrochemistry [78–88, 91, 92, 263–266]. This is an interesting observation given that DDFT was developed as and is generally thought of as a theory for simple and colloidal fluids.

Since this trend is a rather recent development, DDFT has a lot of unexplored potential for chemistry. Essentially, any system in which chemical reactions occur in combination with other interactions—among the reactants or with other molecules in the environment—could get an improved description from DDFT. This includes, in particular, many biochemical reactions which take place in crowded environments [323]. Moreover, DDFT for ions can be used to improve the design of capacitors and batteries and in medical applications for studying ion channels. In the future, DDFT can therefore be expected to be relevant not only for basic research in statistical mechanics, but also for applications in biotechnology, nanotechnology, and chemical engineering.

5. Conclusions

In this article, we have summarized recent progress in the field of classical DDFT and outlined perspectives for the future. Interesting work remains to be done at the interface between DDFT and other closely related theories, namely PFC models and PFT. Moreover, DDFT has recently found quite a number of applications that are related to chemistry, which strongly suggests that this is a promising area for future work. Finally, DDFT is a powerful tool for the multiscale modeling of active and biological matter.

Data availability statement

No new data were created or analysed in this study.

Acknowledgments

We thank Rudolf Haussmann, Hartmut Löwen, Fabian Jan Schwarzendahl, and René Wittmann for helpful discussions. M t V thanks the Studienstiftung des deutschen Volkes for financial support. R W is funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation)—283183152.

ORCID iDs

Michael te Vrugt https://orcid.org/0000-0002-1139-3925
Raphael Wittkowski https://orcid.org/0000-0003-4881-9173

References

[1] Ebner C, Saam W F and Stroud D 1976 Density-functional theory of simple classical fluids: I. Surfaces Phys. Rev. A 14 2264–73
[2] Saam W F and Ebner C 1977 Density-functional theory of classical systems Phys. Rev. A 15 2566–8
[3] Evans R 1979 The nature of the liquid-vapour interface and other topics in the statistical mechanics of non-uniform, classical fluids Adv. Phys. 28 143–200
[4] Marini Bettolo Marconi U and Tarazona P 1999 Dynamic density functional theory of fluids J. Chem. Phys. 110 8032–44
[5] Archer A J and Evans R 2004 Dynamical density functional theory and its application to spinodal decomposition J. Chem. Phys. 121 4246–54
[6] Yoshimori A 2005 Microscopic derivation of time-dependent density functional methods Phys. Rev. E 71 031203
[7] Español P and Löwen H 2009 Derivation of dynamical density functional theory using the projection operator technique J. Chem. Phys. 131 244101
[8] Munakata T 1989 A dynamical extension of the density functional theory J. Phys. Soc. Japan 58 2434–8
[9] Kawasaki K 1994 Stochastic model of slow dynamics in supercooled liquids and dense colloidal suspensions Physica A 208 35–64
[10] Dean D S 1996 Langevin equation for the density of a system of interacting Langevin processes J. Phys. A: Math. Gen. 29 L613–7
[11] Fraaije J G E M 1993 Dynamic density functional theory for microphase separation kinetics of block copolymer melts J. Chem. Phys. 99 9202–12
[12] Fraaije J G E M, van Vlimmeren B A C, Maurits N M, Postma M, Evers O A, Hoffmann C, Altevogt P and Goldbeck-Wood G 1997 The dynamic mean-field density functional method and its application to the mesoscopic dynamics of quenched block copolymer melts J. Chem. Phys. 106 4260–9
[13] Archer A J 2005 Dynamical density functional theory: binary phase-separating colloidal fluid in a cavity J. Phys.: Condens. Matter 17 1405–27
[14] Diaw A and Murillo M S 2016 A dynamic density functional theory approach to diffusion in white dwarfs and neutron star envelopes Astrophys. J. 829 16
[15] Menzel A M, Saha A, Hoell C and Löwen H 2016 Dynamical density functional theory for microswimmers J. Chem. Phys. 144 024115
[16] te Vrugt M, Löwen H and Wittkowski R 2020 Classical dynamical density functional theory: from fundamentals to applications Adv. Phys. 69 121–247
[17] Elder K R, Katakowski M, Haataja M and Grant M 2002 Modeling elasticity in crystal growth Phys. Rev. Lett. 88 245701
[18] Emmerich H, Löwen H, Wittkowski R, Gruhn T, Töth G I, Tegez G and Gránásy L 2012 Phase-field-crystal models for condensed matter dynamics on atomic length and diffusive time scales: an overview Adv. Phys. 61 665–743
[19] Schmidt M and Brader J M 2013 Power functional theory for Brownian dynamics J. Chem. Phys. 138 214101
[20] Schmidt M 2022 Power functional theory for many-body dynamics Rev. Mod. Phys. 94 015007
[21] van Teefelen S, Backofen R, Voigt A and Löwen H 2009 Derivation of the phase-field-crystal model for colloidal solidification Phys. Rev. E 79 051404
[22] Wensink H H and Löwen H 2008 Aggregation of self-propelled colloidal rods near confining walls Phys. Rev. E 78 031409
[23] Menzel A M and Löwen H 2013 Traveling and resting crystals in active systems Phys. Rev. Lett. 110 055702
[24] Menzel A M, Ohta T and Löwen H 2014 Active crystals and their stability Phys. Rev. E 89 022301
[25] Wittmann R, Löwen H and Brader J M 2021 Order-preserving dynamics in one dimension—single-file diffusion and caging from the perspective of dynamical density functional theory Mol. Phys. 119 e186720
[26] Hohenberg P and Kohn W 1964 Inhomogeneous electron gas Phys. Rev. 136 B864–71
[27] Löwen H 1994 Melting, freezing and colloidal suspensions Phys. Rep. 237 249–324
[28] Marini Bettolo Marconi U and Tarazona P 2000 Dynamic density functional theory of fluids J. Phys.: Condens. Matter 12 A413–8
[29] Brader J M and Krüger M 2011 Density profiles of a colloidal liquid at a wall under shear flow Mol. Phys. 7 1029–41
[30] de las Heras D and Schmidt M 2020 Flow and structure in nonequilibrium Brownian many-body systems Phys. Rev. Lett. 125 018001
[31] Kawasaki K 2006 Interpolation of stochastic and deterministic reduced dynamics Physica A 362 249–60
[32] de las Heras D, Brader J M, Fortini A and Schmidt M 2016 Particle conservation in dynamical density functional theory J. Phys.: Condens. Matter 28 244024
[33] Schindler T, Wittmann R and Brader J M 2019 Particle-conserving dynamics on the single-particle level Phys. Rev. E 99 012605
[34] Archer A J, Ratliff D J, Rucklidge A M and Subramanian P 2019 Deriving phase field crystal theory from dynamical density functional theory: consequences of the approximations Phys. Rev. E 100 022140
[35] Schilling T 2022 Coarse-grained modelling out of equilibrium Phys. Rep. 972 1–45
[36] Schmidt M 2015 Quantum power functional theory for many-body dynamics J. Chem. Phys. 143 174108
[37] Schmidt M 2018 Power functional theory for Newtonian many-body dynamics J. Chem. Phys. 148 044502
[38] Jahreis N and Schmidt M 2020 Shear-induced deconfinement of hard disks Colloid Polym. Sci. 298 895–906
[39] de las Heras D and Schmidt M 2018 Velocity gradient power functional for Brownian dynamics Phys. Rev. Lett. 120 028001
[40] Treffenstädt L L and Schmidt M 2020 Memory-induced motion reversal in Brownian liquids Soft Matter 16 1518–26
[41] Marchetti M C, Joanny J F, Ramaswamy S, Liverpool T B, Prost J, Rao M and Simha R A 2013 Hydrodynamics of soft active matter Rev. Mod. Phys. 85 1143–89
[42] Bechinger C, Di Leonardo R, Löwen H, Reichhardt C, Volpe G and Volpe G 2016 Active particles in complex and crowded environments Rev. Mod. Phys. 88 045006
[43] Kawasaki K and Miyazima S 1997 Path integral formulation of dynamical density functional equation for dense fluids Z. Phys. B 103 423–31
[44] Martin P C, Siggs E D and Rose H A 1973 Statistical dynamics of classical systems Phys. Rev. A 8 423–37
[45] Hertz J A, Roudi Y and Sollich P 2016 Path integral methods for the dynamics of stochastic and disordered systems J. Phys. A: Math. Theor. 50 033001
[46] Kim B and Kawasaki K 2008 A fluctuation-dissipation relationship-preserving field theory for interacting Brownian particles: one-loop theory and mode coupling theory J. Stat. Mech. 2008 P02004
[47] Kim B, Kawasaki K, Jacquin H and van Wijland F 2014 Equilibrium dynamics of the Dean–Kawasaki equation: mode-coupling theory and its extension Phys. Rev. E 89 012150
[48] Das S P 2020 Dynamic transition in a Brownian fluid: role of fluctuation-dissipation constraints J. Stat. Mech. 2020 023208
[49] Kim B, Fuchs M and Krakoviack V 2020 Dynamics of a noninteracting colloidal fluid in a quenched Gaussian random potential: a time-reversal-symmetry-preserving field-theoretic approach J. Stat. Mech. 2020 023301
[50] Fodor E, Hayakawa H, Tailleur J and van Wijland F 2018 Non-Gaussian noise without memory in active matter Phys. Rev. E 98 062610
[51] Grmela M and Ottinger H C 1997 Dynamics and thermodynamics of complex fluids. I. Development of a general formalism Phys. Rev. E 56 6620–32
[52] Ottinger H C and Grmela M 1997 Dynamics and thermodynamics of complex fluids. II. Illustrations of a general formalism Phys. Rev. E 56 6633–55
[53] Haussmann R 2016 The way from microscopic many-particle theory to macroscopic hydrodynamics J. Phys.: Condens. Matter 28 113001
[54] Haussmann R 2022 Microscopic density-functional approach to nonlinear elasticity theory J. Stat. Mech. 2022 053210
[55] Wittkowski R, Löwen H and Brand H R 2013 Microscopic approach to entropy production J. Phys. A: Math. Theor. 46 355003
[56] Allen M P, Frenkel D and Talbot J 1989 Molecular dynamics simulation using hard particles Comput. Phys. Rep. 9 301–53
[57] Chen J C and Kim A S 2004 Brownian dynamics, molecular dynamics and Monte Carlo modeling of colloidal systems Adv. Colloid Interface Sci. 112 159–73
[58] Kermack W O and McKendrick A G 1927 A contribution to the mathematical theory of epidemics Proc. R. Soc. A 115 700–21
[59] te Vrugt M, Bickmann J and Wittkowski R 2020 Effects of social distancing and isolation on epidemic spreading modeled via dynamical density functional theory Nat. Commun. 11 5576
[60] te Vrugt M, Bickmann J and Wittkowski R 2021 Containing a pandemic: nonpharmaceutical interventions and the “second wave” J. Phys. Commun. 5 055008
[61] Jeggle J and Wittkowski R 2021 sir_ddft—a Rust implementation of the SIR-DDFT model with Python and JavaScript bindings (Zenodo) (http://doi.org/10.5281/zenodo.4702572)
[62] Yi F, Xie Y and Jameson K 2021 The case for small-scale, mobile-enhanced CoVID-19 epidemiology 2021 19th Int. Symp. on Modeling and Optimization in Mobile, Ad hoc and Wireless Networks (WiOpt 2021) (Philadelphia, PA: IEEE)
[63] Durán-Olivencia M A and Kalliadasis S 2021 More than a year after the onset of the CoVid-19 pandemic in the UK: lessons learned from a minimalistic model capturing essential features including social awareness and policy making medRxiv Preprint (https://doi.org/10.1101/2021.04.15.21255510) (Accessed 16 August 2021)
[64] Löwen H 2021 Abstand halten! Physikalische Modelle aus der Theorie der weichen Materie liefern neue Einblicke in die Ausbreitung von Infektionskrankheiten Phys. J. 20 18–19
[65] Lutsko J F 2016 Mechanism for the stabilization of protein clusters above the solubility curve: the role of non-ideal chemical reactions J. Phys.: Condens. Matter 28 244020
[66] Lutsko J F and Nicolis G 2016 Mechanism for the stabilization of protein clusters above the solubility curve Soft Matter 12 93–98
[67] Turing A M 1952 The chemical basis of morphogenesis Phil. Trans. R. Soc. B 237 37–72
[68] Moncho-Jordá A and Dzubiella J 2020 Controlling the microstructure and phase behavior of confined soft colloids by active interaction switching Phys. Rev. Lett. 125 078001
[69] Bley M, Dzubiella J and Moncho-Jordá A 2021 Active binary switching of soft colloids: stability and structural properties Soft Matter 17 7682–96
[70] Bley M, Hurtado P I, Dzubiella J and Moncho-Jordá A 2022 Active interaction switching controls the dynamic heterogeneity of soft colloidal suspensions Soft Matter 18 397–411
[71] Alston H, Parry A O, Voituriez R and Bertrand T 2022 Intermittent attractive interactions lead to microphase separation in nonmotile active matter Phys. Rev. E 106 034603
[72] Liu Y and Liu H 2020 Development of reaction-diffusion DFT and its application to catalytic oxidation of NO in porous materials AIChE J. 66 e16824
[73] Zong S, Wang J, Huang X, Wu H, Liu Q and Hao H 2022 Formation and stabilization mechanism of mesoscale clusters in solution IUCrJ 9 215–22
[74] Chen Z, Liu Y, Li W and Liu H 2022 Development of a BV-TDDFT model for metal corrosion in aqueous solution Chem. Eng. Sci. 248 117267
[75] Tang W, Yu H, Zhao T, Qing L, Xu X and Zhao S 2021 A dynamic reaction density functional theory for interfacial reaction-diffusion coupling at nanoscale Chem. Eng. Sci. 236 116513
[76] Liu Y 2020 Multiscale mechanisms of reaction-diffusion process in electrode systems: a classical density functional study Chem. Eng. Sci. 227 115899
[77] Louis A A, Bolhuis P G and Hansen J P 2000 Mean-field fluid behavior of the Gaussian core model Phys. Rev. E 62 7961–72
[78] Qing L, Zhao S and Wang Z-G 2021 Surface charge density in electrical double layer capacitors with nanoscale cathode–anode separation J. Phys. Chem. B 125 625–36
[79] Ma K, Janssen M, Lian C and van Roij R 2022 Dynamic density functional theory for the charging of electric double layer capacitors J. Chem. Phys. 156 084101
[80] Qing L and Jiang J 2022 Double-edged sword of ion-size asymmetry in energy storage of supercapacitors J. Phys. Chem. Lett. 13 1438–45
[81] Aslyamov T, Sinkov K and Akhatov I 2022 Relation between charging times and storage properties of nanoporous supercapacitors Nanomaterials 12 587
[82] Frusawa H 2020 Transverse density fluctuations around the ground state distribution of counterions near one charged plate: stochastic density functional view Entropy 22 34
[83] Qing L, Lei J, Zhao T, Qiu G, Ma M, Xu Z and Zhao S 2020 Effects of kinetic dielectric decrement on ion diffusion and capacitance in electrochemical systems Langmuir 36 4055–64
[84] Déjardin P-M 2022 Kinetic Yvon–Born–Green theory of the linear dielectric constant and complex permittivity of isotropic polar fluids Phys. Rev. E 105 024109
[85] Mahdisoltani S and Golestanian R 2021 Transient fluctuation-induced forces in driven electrolytes after an electric field quench New J. Phys. 23 073034
[86] Aslyamov T and Janssen M 2022 Analytical solution to the Poisson–Nernst–Planck equations for the charging of a long electrolyte-filled slit pore Electrochim. Acta 424 140555
[87] Frusawa H 2022 Stochastic density functional theory on lane formation in electric-field-driven ionic mixtures: flow-kernel-based formulation Entropy 24 500
[88] Frusawa H 2022 Electric-field-induced oscillations in ionic fluids: a unified formulation of modified Poisson–Nernst–Planck models and its relevance to correlation function analysis Soft Matter 18 4280–304
[89] Avni Y, Adar R M, Andelman D and Orland H 2022 Conductivity of concentrated electrolytes Phys. Rev. Lett 128 098002
[90] Avni Y, Andelman D and Orland H 2022 Conductance of concentrated electrolytes: multivalency and the Wien effect (arXiv:2207.10116)
[91] Tomlin R J, Roy T, Kirk T L, Marinescu M and Gillespie D 2022 Impedance response of ionic liquids in long slit pores J. Electrochem. Soc. accepted (https://doi.org/10.1149/1945-7111/ac89b5)
[92] Zhao T, Qing L, Long T, Xu X, Zhao S and Lu X 2021 Dynamical coupling of ion adsorption with fluid flow in nanopores AIChE J. 67 e17266
[93] Li Y, Zhao T, Qing L, Yu H, Xu X, Li P and Zhao S 2021 Solvation dynamics in simple fluids: effect of solute size and potential Chem. Eng. Sci. 232 116371
[94] Li Y, Qing L, Yu H, Peng Y, Xu X, Li P and Zhao S 2021 Dynamical density functional theory for solvation dynamics in polar solvent: heterogeneous effect of solvent orientation Chem. Eng. Sci. 246 116978
[95] Chandra A and Bagchi B 1991 Molecular theory of solvation and solvation dynamics in a binary dipolar liquid J. Chem. Phys. 94 8367–77
[96] Yu H, Wang Z, Long T, Li Y, Thushara D, Bao B and Zhao S 2022 Permeability and selectivity analysis for affinity-based nanoparticle separation through nanochannels AIChE J. 68 e17583
[97] Moncho-Jordá A, Jódar-Reyes A B, Kanduč M, Germán-Bellod A, López-Romero J M, Contreras-Cáceres R, Sarabia F, García-Castro M, Pérez-Ramírez H A and Ondrioza G
2020 Scaling laws in the diffusive release of neutral cargo from hollow hydrogel nanoparticles: paclitaxel-loaded poly (4-vinylpyridine) ACS Nano 14 15227–40
[98] Chang L-H and Yu H-Y 2020 Flow-driven release of molecules from a porous surface explored using dynamical density functional theory J. Taiwan Inst. Chem. Eng. 117 26–38
[99] Li R, Wang Z, Lian X, Hu X and Wang Y 2020 Antimicrobial rubber nanocapsule-based iodophor promotes wound healing CCS Chem. 2 245–56
[100] Li B, Daoulas K and Schmid F 2021 Dynamic coarse-graining of polymer systems using mobility functions J. Phys.: Condens. Matter 33 194004
[101] Mantha S, Qi S and Schmid F 2020 Bottom-up construction of dynamic density functional theories for inhomogeneous polymer systems from microscopic simulations Macromolecules 53 3409–23
[102] Schmid F and Li B 2020 Dynamic self-consistent field approach for studying kinetic processes in multiblock copolymer melts Polymers 12 2205
[103] Baptista R, Caob L, Chen J, Ghattas O, Li F, Marzouk Y M and Oden T J 2022 Bayesian model calibration for block copolymer self-assembly: likelihood-free inference and expected information gain computation via measure transport (arXiv:2206.11343)
[104] Chen X, Qi S, Zhang X and Yan D 2020 Influence of small-scale correlation on the interface evolution of semiflexible homopolymer blends ACS Omega 5 7593–600
[105] Rottler J and Müller M 2020 Kinetic pathways of block copolymer directed self-assembly: insights from efficient continuum modeling ACS Nano 14 13986–94
[106] Müller M 2022 Memory in the relaxation of a polymer density modulation J. Chem. Phys. 156 124902
[107] Pantelidou M S, García Daza F A, Avalos J B and Mackie A D 2022 Universal scaling for the exit dynamics of block copolymer from micelles at short and long time scales Macromolecules 55 914–27
[108] Martínez-Agustina F, Ruiz-Salgado S, Zenteno-Mateo B, Rubio E and Morales M A 2022 3D pattern formation from coupled Cahn–Hilliard and Swift–Hohenberg equations: morphological phases transitions of polymers, bock and diblock copolymers Comput. Mater. Sci. 210 111431
[109] Erukhimovich I Y, Krikisin Y A and Kadryavytsev Y V 2022 Block copolymers in high-frequency electric field: mean-field approximation Polym. Sci. A 64 121–7
[110] Altevogt P, Evers O A, Fraaije J G E M, Maurits N M and van Vlimmeren B A C 1999 The MesoDyn project: software for mesoscale chemical engineering J. Mol. Struct.: THEOChem 463 139–43
[111] Pang B, Jia Y, Dai Pang S, Zhang Y, Du H, Geng G, Ni H, Qian J, Qiao H and Liu G 2021 The interpenetration polymer network in a cement paste–waterborne epoxy system Cem. Concrl. Res. 139 106236
[112] Chae J E, Lee S Y, Baek S Y, Song K H, Park C H, Kim H-J and Lee K-S 2021 High-performance multiblock PEMs containing a highly acidic fluorinated-hydrophilic domain for water electrolysis J. Membr. Sci. 638 119694
[113] Slimane M, Gaye I, Ghoul M and Chebil L 2020 Mesoscale modeling and experimental study of quercetin organization as nanoparticles in the poly-lactic-co-glycolic acid/water system under different conditions Ind. Eng. Chem. Res. 59 4809–16
[114] Lee S Y, Park C H, Chae J E, Lee S, Lee H-J, Yoo S J, Kim J Y, Jang J H and Kim H-J 2021 Reinforced polymer blend membranes with liposome-like morphology for polymer electrolyte membrane fuel cells operating under low-humidity conditions Adv. Eng. Mater. 23 2001174
[115] Feng P and Wang L 2022 The effects of temperature on surfactant solution: a molecules dynamics simulation J. Phys.: Conf. Ser. 2194 012037
[116] Lutsko J F 2022 Classical density functional theory in the canonical ensemble Phys. Rev. E 105 034120
[117] de las Heras D and Schmidt M 2014 Full canonical information from grand-potential density-functional theory Phys. Rev. Lett. 113 238304
[118] White J A and Velasco S 2001 The Ornstein–Zernike equation in the canonical ensemble Europhys. Lett. 54 475
[119] White J A and González A 2002 The extended variable space approach to density functional theory in the canonical ensemble J. Phys.: Condens. Matter 14 L1907
[120] te Vrugt M 2021 How to distinguish between indistinguishable particles Br. J. Phil. Sci. accepted (https://doi.org/10.1086/718495)
[121] te Vrugt M 2021 The five problems of irreversibility Stud. Hist. Phil. Sci. 87 136–46
[122] te Vrugt M 2022 Understanding probability and irreversibility in the Mori–Zwanzig projection operator formalism Euro. Jnl. Phil. Sci. 12 41
[123] te Vrugt M, Töth G I and Wittkowski R 2021 Master equations for Wigner functions with spontaneous collapse and their relation to thermodynamic irreversibility J. Comput. Electron. 20 2209–31
[124] te Vrugt M, Needham P and Schmitz G J 2022 Is thermodynamics fundamental? (arXiv:2204.04352)
[125] Mori H 1965 Transport, collective motion and Brownian motion Prog. Theor. Phys. 33 423–55
[126] Nakajima S 1958 On quantum theory of transport phenomena: steady diffusion Prog. Theor. Phys. 20 948–59
[127] Zwanzig R 1960 Ensemble method in the theory of irreversibility J. Chem. Phys. 33 1338–41
[128] Grabert H 1982 Projection Operator Techniques in Nonequilibrium Statistical Mechanics (Springer Tracts in Modern Physics vol 95) 1st edn (Berlin: Springer)
[129] te Vrugt M and Wittkowski R 2020 Projection operators in statistical mechanics: a pedagogical approach Eur. J. Phys. 41 045101
[130] Zeh H-D 2007 The Physical Basis of the Direction of Time 5th edn (Berlin: Springer)
[131] Wittkowski R, Löwen H and Brand H R 2012 Extended dynamical density functional theory for colloidal mixtures with temperature gradients J. Chem. Phys. 137 224904
[132] Anero J G, Español P and Tarazona P 2013 Functional thermo-dynamics: a generalization of dynamic density functional theory to non-isothermal situations J. Chem. Phys. 139 034106
[133] Camargo D, de la Torre J A, Duque-Zumajo D, Español P, Delgado-Buscalioni R and Chejne F 2018 Nanoscale hydrodynamics near solids J. Chem. Phys. 148 064107
[134] Fang A 2019 First-principles magnetization relaxation equation of interacting ferrofluids with applications to magnetoviscous effects Phys. Fluids 31 122002
[135] Fang A 2020 Generic theory of the dynamic magnetic response of ferrofluids Soft Matter 16 10928–34
[136] Fang A 2022 Dynamical effective field model for interacting ferrofluids: I. Derivations for homogeneous, inhomogeneous and polydisperse cases J. Phys.: Condens. Matter 34 115102
[137] Fang A 2022 Dynamical effective field model for interacting ferrofluids: II. The proper relaxation time and effects of dynamic correlations J. Phys.: Condens. Matter 34 115103
[138] Ras T, Szafarczyk M and Fuchs M 2020 Elasticity of disordered binary crystals Colloid Polym. Sci. 298 803–18
[139] Ganguly S, Shrivastav G P, Lin S-C, Häring J, Haussmann R, Kahl G, Oettel M and Fuchs M 2022 Elasticity in crystals with a high density of local defects: insights from ultra-soft colloids J. Chem. Phys. 156 064501
[140] Uneyama T 2022 Application of projection operator method to coarse-grained dynamics with transient potential Phys. Rev. E 105 044417
[141] Glatzel F and Schilling T 2021 Comments on the validity of the non-stationary generalized Langevin equation as a coarse-grained evolution equation for microscopic stochastic dynamics J. Chem. Phys. 154 174107
[142] Meyer H, Voigtmann T and Schilling T 2019 On the dynamics of reaction coordinates in classical, time-dependent, many-body processes J. Chem. Phys. 150 174118
[143] te Vrugt M and Wittkowski R 2019 Mori–Zwanzig projection operator formalism for far-from-equilibrium systems with time-dependent Hamiltonians Phys. Rev. E 99 062118
[144] te Vrugt M, Hossenfelder S and Wittkowski R 2021 Mori–Zwanzig formalism for general relativity: a new approach to the averaging problem Phys. Rev. Lett. 127 231101
[145] Marolt K and Roth R 2020 Statics and dynamics of a finite two-dimensional colloidal system with competing attractive critical Casimir and repulsive magnetic dipole interactions Phys. Rev. E 102 042608
[146] Jia W and Kusaka I 2021 Density functional study of non-isothermal hard sphere fluids Mol. Phys. 119 e1875077
[147] Antonov A P, Ryabov A and Maas P 2021 Driven transport of soft Brownian particles through pore-like structures: effective size method J. Chem. Phys. 155 184102
[148] Zimmermann U, Löwen H, Kreuter C, Erbe A, Leiderer P and Smoltenburg F 2021 Negative resistance for colloids driven over two barriers in a microchannel Soft Matter 17 516–22
[149] Archer A J, Dotera T and Rucklidge A M 2022 Rectangle–triangle soft-matter quasicrystals with hexagonal symmetry Phys. Rev. E 106 044602
[150] Scacchi A, Somerville W R C, Buzzà D M A and Archer A J 2020 Quasicrystal formation in binary soft matter mixtures Phys. Rev. Res. 2 032043
[151] Montañéz-Rodríguez A, Quintana C and González-Mozuelos P 2021 Spectral analysis of the collective diffusion of Brownian particles confined to a spherical surface Physica A 574 126012
[152] Ramírez-González P and Medina-Noyola M 2010 General nonequilibrium theory of colloid dynamics Phys. Rev. E 82 061503
[153] Lira-Escobedo J, Vélez-Cordero J R and Ramírez-González P 2022 Spatially heterogeneous dynamics and locally arrested density fluctuations from first-principles Phys. Fluids 34 0333107
[154] Lira-Escobedo J, Vélez-Cordero J R and Ramírez-González P 2022 Ultra-slow and arrested density-fluctuations as precursor of spatial heterogeneity Phys. Fluids 34 011704
[155] Szamel G 2022 An alternative, dynamic density functional-like theory for time-dependent density fluctuations in glass-forming fluids J. Chem. Phys. 156 191102
[156] Sharma M, Nandi M K and Bhattacharyya S M 2022 Identifying structural signature of dynamical heterogeneity via the local softness parameter Phys. Rev. E 105 044604
[157] Martin D, O’Byrne J, Cates M E, Fodor E, Nardini C, Tailleur J and van Wijland F 2021 Statistical mechanics of active Ornstein–Uhlenbeck particles Phys. Rev. E 103 032607

[158] Zakine R, Fournier J-B and van Wijland F 2020 Spatial organization of active particles with field-mediated interactions Phys. Rev. E 101 022105

[159] Mahdisoltani S, Zinati R B A, Dufcet C, Gambassi A and Golestanian R 2021 Nonequilibrium polarity-induced chemotaxis: emergent Galilean symmetry and exact scaling exponents Phys. Rev. Res. 3 013100

[160] Ben Ali Zinati R, Dufcet C, Mahdisoltani S, Gambassi A and Golestanian R 2022 Stochastic dynamics of chemotactic colonies with logistic growth Europhys. Lett. 136 050003

[161] Frusawa H 2021 Non-hyperuniform metastable states around a disordered hyperuniform state of densely packed spheres: stochastic density functional theory at strong coupling Soft Matter 17 8810–31

[162] Goutaland Q, van Wijland F, Fournier J-B and Noguchi H 2021 Binding of thermalized and active membrane curvature-inducing proteins Soft Matter 17 5560–73

[163] Satin S E 2022 Correspondences of matter field fluctuations in semiclassical and classical gravity in the decoherence limit Class. Quantum Grav. 39 095004

[164] Fang A 2022 Consistent hydrodynamics of ferrofluids Phys. Fluids 34 013319

[165] Hurst T 2020 Granular media at multiple scales: mathematical analysis, modelling and computation PhD Dissertation University of Edinburgh

[166] Goddard B D, Hurst T D and Ocone R 2021 Modelling inelastic granular media using dynamical density functional theory J. Stat. Phys. 183 6

[167] Stanton L G, Oppelstrup T, Carpenter T S, Ingólfsson H I, Surh M P, Lightstone F C and Goslì J N 2021 Dynamic density functional theory of multicomponent cellular membranes (arXiv:2112.08651)

[168] Wittmann R, Schwarzenzal F J and Löwen H 2022 Mechano-sensing in growing bacteria colonies with dynamical density functional theory (in preparation)

[169] Qiao C, Zhao T, Yu X, Qing L, Bao B, Zhao S and Liu H 2021 On the relation between dynamical density functional theory and Navier–Stokes equation Chem. Eng. Sci. 230 116203

[170] Mills-Williams R 2020 Analysis and applications of dynamic density functional theory PhD Dissertation University of Edinburgh

[171] Zhao T, Qiao C, Xu X and Zhao S 2021 Self-consistent equations governing the dynamics of non-equilibrium binary colloidal systems Chem. Eng. Sci. 241 116623

[172] Sterle R and Gross J 2021 Hydrodynamic density functional theory from mixtures with a variational principle and its application to droplet coalescence J. Chem. Phys. 155 134101

[173] Goddard B D, Mills-Williams R D and Sun J 2020 The singular hydrodynamic interactions between two spheres in Stokes flow Phys. Fluids 32 062001

[174] He B, Martin-Fabiani I, Roth R, Tóth G I and Archer A J 2021 Dynamical density functional theory for the drying and stratification of binary colloidal dispersions Langmuir 37 1399–409

[175] Perez C M, Rey M, Goddard B D and Thijssen J H J 2021 Changing the flow profile and resulting drying pattern of dispersion droplets via contact angle modification (arXiv:2111.00464)

[176] Howard M P and Nikoubashman A 2020 Stratification of polymer mixtures in drying droplets: hydrodynamics and diffusion J. Chem. Phys. 153 054901

[177] Cornalba F, Shardlow T and Zimmer J 2020 From weakly interacting particles to a regularised Dean–Kawasaki model Nonlinearity 33 864

[178] Cornalba F, Shardlow T and Zimmer J 2021 Well-posedness for a regularised inertial Dean–Kawasaki model for slider particles in several space dimensions J. Differ. Equ. 284 253–83

[179] Le Doussal P 2022 Ranked diffusion, delta Bose gas and Burgers equation Phys. Rev. E 105 L012103

[180] Lee W and Yeo J 2020 Improved field theoretical approach to noninteracting Brownian particles in a quenched random potential J. Korean Phys. Soc. 77 719–34

[181] Helfmann L, Djurdjevac Conrad N, Djurdjevac A, Winkelmann S and Schütte C 2021 From interacting agents to density-based modeling with stochastic PDEs Commun. Appl. Math. Comput. Sci. 16 1–32

[182] Cornalba F and Fischer J 2021 The Dean–Kawasaki equation and the structure of density fluctuations in systems of diffusing particles (arXiv:2109.06500)

[183] Fehrman B and Gess B 2021 Well-posedness of the Dean–Kawasaki and the nonlinear Dawson–Watanabe equation with correlated noise (arXiv:2108.08858)

[184] Gomes S N, Pavliotis G A and Vaes U 2020 Mean field limits for interacting diffusions with colored noise: phase transitions and spectral numerical methods Multiscale Model. Simul. 18 1343–70

[185] Bechtold F and Coppini F 2021 A law of large numbers for interacting diffusions via a mild formulation Electron. J. Probab. 26 1–27

[186] Delgadino M G, Gvalani R S and Pavliotis G A 2021 On the diffusive-mean field limit for weakly interacting diffusions exhibiting phase transitions Arch. Ration. Mech. Anal. 241 91–148
[187] Zakine R and Vanden-Eijnden E 2022 Minimum action method for nonequilibrium phase transitions (arXiv:2202.06936)

[188] Carrillo J A, Kalliadasis S, Perez S P and Shu C-W 2020 Well-balanced finite-volume schemes for hydrodynamic equations with general free energy Multiscale Model. Simul. 18 302–41

[189] Carrillo J A, Castro M J, Kalliadasis S and Perez S P 2021 High-order well-balanced finite-volume schemes for hydrodynamic equations with nonlocal free energy SIAM J. Sci. Comput. 43 A828–58

[190] Kruk N, Carrillo J A and Koeppl H 2021 A finite volume method for continuum limit equations of nonlocally interacting active chiral particles J. Comput. Phys. 440 110275

[191] Mendes J, Russo A, Perez S P and Kalliadasis S 2021 A finite-volume scheme for gradient-flow equations with non-homogeneous diffusion Comput. Math. Appl. 89 150–62

[192] Bañás L, Gess B and Vieth C 2020 Numerical approximation of singular-degenerate parabolic stochastic PDEs (arXiv:2012.12150)

[193] Aduamoah M, Goddard B D, Pearson J W and Roden J C 2022 Pseudospectral methods and iterative solvers for optimization problems from multiscale particle dynamics BIT Numer. Math. 62 1703–43

[194] Goddard B D, Gooding B, Short H and Pavliotis G A 2020 Noisy bounded confidence models for opinion dynamics: the effect of boundary conditions on phase transitions IMA J. Appl. Math. 87 80–110

[195] Magaletti F, Gallo M, Perez S P, Carrillo J A and Kalliadasis S 2022 A positivity-preserving scheme for fluctuating hydrodynamics J. Comput. Phys. 463 111248

[196] Roden J C, Mills-Williams R D, Pearson J W and Goddard B D 2022 MultiShape: a spectral element method, with applications to dynamic density functional theory and PDE-constrained optimization (arXiv:2207.05589)

[197] Wang M, Huang Q and Wang C 2021 A second order accurate scalar auxiliary variable (SAV) numerical method for the square phase field crystal equation J. Sci. Comput. 88 33

[198] Wang L and Huang Y 2021 Error estimates for second-order SAV finite element method to phase field crystal model Electron. Res. Arch. 29 1735

[199] Coelho D L, Vitral E, Pontes J and Mangiavacchi N 2021 Numerical scheme for solving the nonuniformly forced cubic and quintic Swift–Hohenberg equations strictly respecting the Lyapunov functional J. Comput. Appl. Math. 407 114005

[200] Li Q and Mei L 2021 Numerical approximation of the two-component PFC models for binary colloidal crystals: efficient, decoupled and second-order unconditionally energy stable schemes J. Sci. Comput. 88 60

[201] Antonov A P, Schweers S, Ryabov A and Maass P 2022 Brownian dynamics simulations of hard rods in external fields and with contact interactions Phys. Rev. E 106 054606

[202] Lin S-C and Oettel M 2019 A classical density functional from machine learning and a convolutional neural network SciPost Phys. 6 025

[203] Lin S-C, Martius G and Oettel M 2020 Analytical classical density functionals from an equation learning network J. Chem. Phys. 152 021102

[204] Cats P, Kuipers S, de Wind S, van Damme R, Coli G M, Dijkstra M and van Roij R 2021 Machine-learning free-energy functionals using density profiles from simulations APL Mater. 9 031109

[205] Yatsyshin P, Kalliadasis S and Duncan A B 2022 Physics-constrained Bayesian inference of state functions in classical density-functional theory J. Chem. Phys. 156 074105

[206] Ahn D H et al 2020 Flux: overcoming scheduling challenges for exascale workflows Future Gener. Comput. Syst. 110 202–13

[207] Bhatia H et al 2021 Machine-learning-based dynamic-importance sampling for adaptive multiscale simulations Nat. Mach. Intell. 3 401–9

[208] Ingólfsson H I et al 2022 Machine learning–driven multiscale modeling reveals lipid-dependent dynamics of RAS signaling proteins Proc. Natl Acad. Sci. USA 119 e2113297119

[209] Zhao H, Braatz R D and Bazant M Z 2021 Image inversion and uncertainty quantification for constitutive laws of pattern formation J. Comput. Phys. 436 110279

[210] Zhao H, Storey B D, Braatz R D and Bazant M Z 2020 Learning the physics of pattern formation from images Phys. Rev. Lett. 124 060201

[211] Bhatia H et al 2021 Adaptable coordination of large multiscale ensembles: challenges and learnings at scale Generalizable Coordination of Large Multiscale Workflows: Challenges and Learnings at Scale (St. Louis, MO, United States, 14–19 November 2021)

[212] Arold D and Schmiedeberg M 2020 Active phase field crystal systems with inertial delay and underdamped dynamics Eur. Phys. J. E 43 47

[213] Arold D and Schmiedeberg M 2020 Mean field approach of dynamical pattern formation in underdamped active matter with short-ranged alignment and distant anti-alignment interactions J. Phys.: Condens. Matter 32 515403

[214] te Vrugt M, Jeggle J and Wittkowski R 2021 Jerky active matter: a phase field crystal model with translational and orientational memory New J. Phys. 23 063023
[215] Ophaus L, Kirchner J, Gurevich S V and Thiele U 2020 Phase-field-crystal description of active crystallites: elastic and inelastic collisions Chaos 30 123149
[216] Ophaus L, Knobloch E, Gurevich S V and Thiele U 2021 Two-dimensional localized states in an active phase-field-crystal model Phys. Rev. E 103 032601
[217] Huang Z-F, Menzel A M and Löwen H 2020 Dynamical crystallites of active chiral particles Phys. Rev. Lett. 125 218002
[218] Krause V and Voigt A 2021 Deformable active nematic particles and emerging edge currents in circular confinements (arXiv:2102.02108)
[219] Holl M P, Archer A J, Gurevich S V, Knobloch E, Ophaus L and Thiele U 07 2021 Localized states in passive and active phase-field-crystal models IMA J. Appl. Math. 86 896–923
[220] te Vrugt M, Holl M P, Koch A, Wittkowski R and Thiele U 2022 Derivation and analysis of a phase field crystal model for a mixture of active and passive particles Modelling Simul. Mater. Sci. Eng. 30 084001
[221] Frohoff-Hülsmann T, Holl M P, Knobloch E, Gurevich S V and Thiele U 2022 Stationary broken parity states in nonvariational models (arXiv:2205.14364)
[222] Abdalla S, Archer A J, Gránásy L and Tóth G I 2022 Thermodynamics, formation dynamics and structural correlations in the bulk amorphous phase of the phase-field crystal model J. Chem. Phys. 157 164502
[223] Holl M P, Archer A J and Thiele U 2020 Efficient calculation of phase coexistence and phase diagrams: application to a binary phase-field-crystal model J. Phys.: Condens. Matter 33 115401
[224] Knobloch E 2020 Dissipative systems Emerging Frontiers in Nonlinear Science ed P G Kevrekidis, J Cuevas-Maraver and A Saxena (Cham: Springer) pp 279–303
[225] Steinberg A B, Maucher F, Gurevich S V and Thiele U 2022 Exploring bifurcations in Bose–Einstein condensates via phase field crystal models Chaos 32 113112
[226] Ankudinov V, Starodumov I, Kryuchkov N P, Yakovlev E V, Yurchenko S O and Galenko P K 2021 Correlated noise effect on the structure formation in the phase-field crystal model Math. Methods Appl. Sci. 44 12185–93
[227] Chen Z, Hu Y, He X, Xiao T, Hao L and Ruan Y 2021 Phase-field crystal method for multiscale microstructures with cubic term Mater. Today Commun. 29 102935
[228] Backofen R, Sahlmann L, Willmann A and Voigt A 2021 A comparison of different approaches to enforce lattice symmetry in two-dimensional crystals Proc. Appl. Math. Mech. 20 e202000192
[229] Skogvoll V, Angheluta L, Skaugen A, Salvalaglio M and Viñals J 2022 A phase field crystal theory of the kinematics of dislocation lines J. Mech. Phys. Solids 166 104932
[230] Wang N, Guo H and Provatas N 2021 Connecting the phase-field-crystal model of electromigration with electronic and continuum theories Phys. Rev. Mater. 5 115002
[231] Blixt K H and Hallberg H 2022 Evaluation of grain boundary energy, structure and stiffness from phase field crystal simulations Modelling Simul. Mater. Sci. Eng. 30 014002
[232] Martine-La Boissonnière G, Choksi R and Lessard J-P 2022 Microscopic patterns in the 2D phase-field-crystal model Nonlinearity 35 1500–20
[233] Ankudinov V and Galenko P K 2022 Structure diagram and dynamics of formation of hexagonal boron nitride in phase-field-crystal model Phil. Trans. R. Soc. A 380 20200318
[234] Shuai X, Wang Z J, Mao H, Tang S, Kong Y and Du Y 2021 Atomic-scale study of compositional and structural evolution of early-stage grain boundary precipitation in Al–Cu alloys through phase-field-crystal simulation J. Mater. Sci. 56 12700–15
[235] Salvalaglio M, Voigt A, Huang Z-F and Elder K R 2021 Mesoscale defect motion in binary systems: effects of compositional strain and Cottrell atmospheres Phys. Rev. Lett. 126 185502
[236] Podmianczyk F and Gránásy L 2021 Nucleation and post-nucleation growth in diffusion-controlled and hydrodynamic theory of solidification Crystals 11 437
[237] Ankudinov V, Elder K R and Galenko P K 2020 Traveling waves of the solidification and melting of cubic crystal lattices Phys. Rev. E 102 062802
[238] Wang C and Wise S M 2021 A thermodynamically-consistent phase field crystal model of solidification with heat flux (arXiv:2107.05555)
[239] Skogvoll V, Skaugen A and Angheluta L 2021 Stress in ordered systems: Ginzburg–Landau-type density field theory Phys. Rev. B 103 224107
[240] Archer A J 2009 Dynamical density functional theory for molecular and colloidal fluids: a microscopic approach to fluid mechanics J. Chem. Phys. 130 014509
[241] Renner J, Schmidt M and de las Heras D 2022 Shear and bulk acceleration viscosities in simple fluids Phys. Rev. Lett. 128 094502
[242] Hermann S, de las Heras D and Schmidt M 2021 Phase separation of active Brownian particles in two dimensions: anything for a quiet life Mol. Phys. 119 e1902585
[243] Treffenstädt L L and Schmidt M 2021 Universality in driven and equilibrium hard sphere liquid dynamics Phys. Rev. Lett. 126 058002
[244] Treffenstädt L L, Schindler T and Schmidt M 2022 Dynamic decay and superadiabatic forces in the van Hove dynamics of bulk hard sphere fluids SciPost Phys. 12 133
[245] Geigenfeind T, de las Heras D and Schmidt M 2020 Superadiabatic demixing in nonequilibrium colloids Commun. Phys. 3 23
[308] Bickmann J, Bröker S and Wittkowski R 2022 Active Brownian particles in external force fields: field-theoretical models, generalized barometric law, and programmable density patterns (arXiv:2202.04423)
[309] Jeggle J, Stenhammar J and Wittkowski R 2020 Pair-distribution function of active Brownian spheres in two spatial dimensions: simulation results and analytic representation J. Chem. Phys. 152 194903
[310] Wittmann R and Brader J M 2016 Active Brownian particles at interfaces: an effective equilibrium approach Europhys. Lett. 114 68004
[311] Pototsky A and Stark H 2012 Active Brownian particles in two-dimensional traps Europhys. Lett. 98 50004
[312] Farage T F F, Krinninger P and Brader J M 2015 Effective interactions in active Brownian suspensions Phys. Rev. E 91 042310
[313] Wittmann R, Cortes L B G, Löwen H and Aarts D G A L 2021 Particle-resolved topological defects of smectic colloidal liquid crystals in extreme confinement Nat. Commun. 12 623
[314] Shankar S, Souslov A, Bowick M J, Marchetti M C and Vitelli V 2022 Topological active matter Nat. Rev. Phys. 4 380–98
[315] Monderkamp P A, Wittmann R, Cortes L B G, Aarts D G A L, Smallenburg F and Löwen H 2021 Topology of orientational defects in confined smectic liquid crystals Phys. Rev. Lett. 127 198001
[316] Monderkamp P A, Wittmann R, te Vrugt M, Voigt A, Wittkowski R and Löwen H 2022 Topological fine structure of smectic grain boundaries and tetratic disclination lines within three-dimensional smectic liquid crystals Phys. Chem. Chem. Phys. 24 15691–704
[317] Huang Z-F, Löwen H and Voigt A 2022 Defect dynamics in active smectics induced by confining geometry and topology Commun. Phys. 5 294
[318] Gillespie D 2008 Energetics of divalent selectivity in a calcium channel: the ryanodine receptor case study Biophys. J. 94 1169–84
[319] Gillespie D, Xu L, Wang Y and Meissner G 2005 (De)constructing the ryanodine receptor: modeling ion permeation and selectivity of the calcium release channel J. Phys. Chem. B 109 15598–610
[320] Chauviere A, Hatzikirou H, Kevrekidis I G, Lowengrub J S and Cristini V 2012 Dynamic density functional theory of solid tumor growth: preliminary models AIP Adv. 2 011210
[321] Al-Saedi H M, Archer A J and Ward J 2018 Dynamical density-functional-theory-based modeling of tissue dynamics: application to tumor growth Phys. Rev. E 98 022407
[322] Trappe M-I and Chisholm R A 2021 A mechanistic density functional theory for ecology across scales bioRxiv Preprint (https://doi.org/10.1101/2021.06.22.449359) (Accessed 16 August 2022)
[323] Minton A P 2001 The influence of macromolecular crowding and macromolecular confinement on biochemical reactions in physiological media J. Biol. Chem. 276 10577–80