Research profile

Working group “Theory of active soft matter”

See `https://www.uni-muenster.de/Physik.TP/~wittkowski/research.pdf` for an update.

Contents

1 Fields of research

We mainly work on the theory of **active matter** and **statistical physics**. The focus of our research is on the theory of **active soft matter**.

1.1 Active matter

Active matter is a fascinating class of materials that has constituents that convert energy into directed motion. Examples for these **active particles** (often called **self-propelled particles**) range from molecular motors to motile microorganisms (swimming bacteria, migrating cancer cells,...) to populations of animals or humans. We are particularly interested in systems of active nano- and microparticles, i.e., **active soft matter**.

Today, it is even possible to fabricate artificial active nano- and microparticles, which are also called **nano-/micromachines** or **nano-/microrobots**. There exists a number of realizations of such particles that utilize different propulsion mechanisms and are supplied with energy, e.g., by fuel, light, or ultrasound. These synthetic active particles are a relatively new and unexplored topic of research with a high potential for intriguing **applications in medicine and materials science**. Therefore, they constitute a main topic of our research.

For example, artificial **active colloidal particles** could be applied in **targeted drug delivery**. Resembling remote-controlled nano- or microscaled submarines, they could transport drugs to a specific target in the body of a patient and thus reduce adverse drug reactions, e.g., in chemotherapies. Another example is **noninvasive surgery**, where the particles move through the vasculature to a target and perform surgical interventions at the cellular scale to avoid damage of healthy tissue.

Moreover, suspensions of artificial active colloidal particles and soft materials like gels with embedded active colloidal particles form **active materials** that, being intrinsically nonequilibrium systems and thus not subject to the laws of thermodynamics, can have properties that cannot be found in conventional materials. For example, many **exceptional effects and materials properties** have been observed in active materials. Some of them are analogous to quantum effects and other of them cannot even be observed in quantum systems. They include motility-induced phase separation, reversed Ostwald ripening, non-state-function pressure, low-Reynolds-number turbulence, superfluidity, negative viscosities, negative interfacial tension, anomalous Casimir forces, anomalous sound modes, programmable self-organization, and an active tunnel effect. (Several of them are discoveries of our own research; see section 3 for details.) Another important feature of active materials is the **tunability** of their properties. Since their properties originate from the activity of the particles, which in turn originates from the energy supply, it is possible to control the properties of active materials simply by tuning their energy source (e.g., light intensity or ultrasound intensity). In this way, their unusual effects can be switched on and off and their materials properties can be tuned in a wide parameter range as desired. Active materials should even be able to resemble neural networks and to form **programmable and intelligent matter**.

1.1.1 Research objectives

We study active systems ranging from individual to many interacting active particles and how their behavior can be controlled by external fields. Our main goals are **exploring the fundamental properties of active matter** and solving crucial problems to **turn the envisaged applications of active matter in medicine and materials science into reality**. The main projects of our current research are described in the following.

1.1.2 Acoustically propelled microparticles

Microparticles with a symmetry-broken shape or anisotropic acoustic properties have been found to exhibit active propulsion when they are exposed to ultrasound. Since such acoustically propelled microparticles can be biocompatible and able to move in various liquids and soft materials, this type of active colloidal particles has a particularly high potential for future medical applications. Their propulsion mechanism makes them also to an ideal candidate for applications in materials science. However, the properties of these particles are still mostly unexplored.

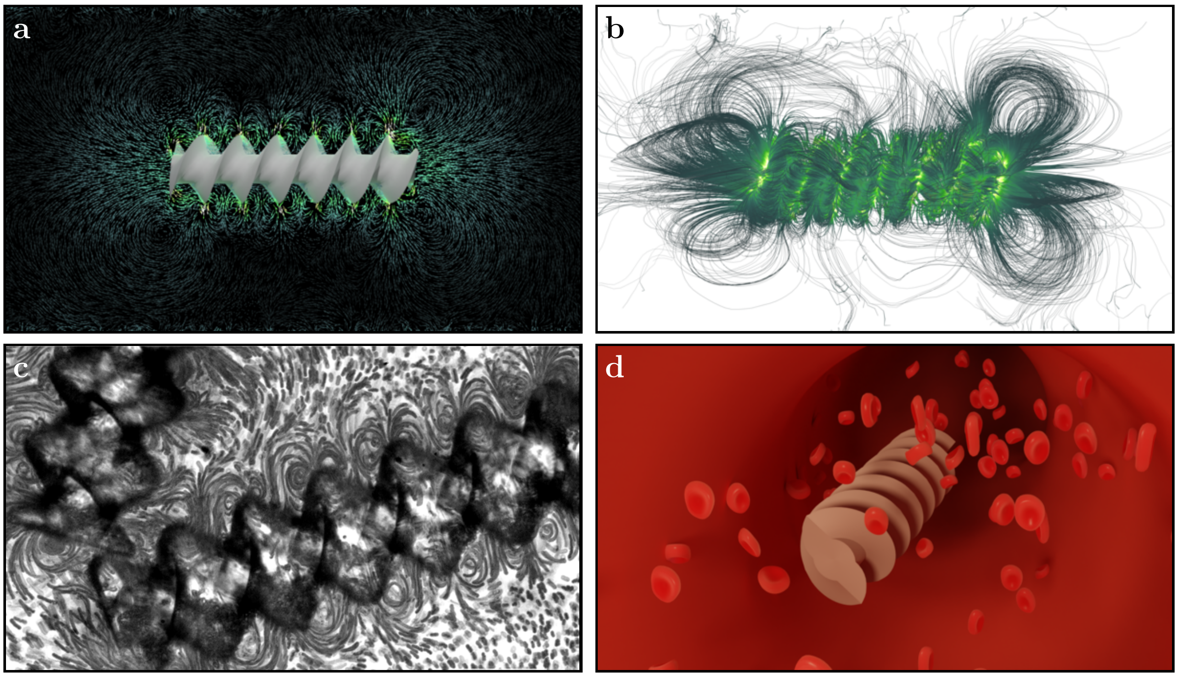

Figure 1: A screw-shaped ultrasound-propelled microparticle. Our simulation results with **(a)** velocity field and **(b)** streamlines for the flow field around the particle obtained with `AcoDyn`, **(c)** experimental results, and **(d)** illustration of a potential medical application [Sci. Adv. **9**, eadh526 (2023)].

Therefore, we study the properties of acoustically propelled microparticles and their collective dynamics. Important aims of our research are to **develop better particle designs** (e.g., to reach a faster propulsion at a harmless sound intensity) and to **develop biocompatible methods for navigating the particles and controlling their collective dynamics** (as it is necessary for most medical applications and offers further control over the properties of active materials).

Since sound leads to motion of the particles and their distribution affects the sound propagation, suspensions of sound-propelled microparticles can be expected to constitute a class of **responsive and adaptive new active materials with nonlinear acoustic properties** that could exhibit even memory effects. They are thus relevant for applications such as acoustic filters and might enable the realization of **programmable and even intelligent active materials**. Utilizing the nonlinear acoustic properties of the aforementioned suspensions, we want to develop acoustic neurons for **acoustics-based artificial neural networks** (counterparts to optical neural networks). The latter could be applied, e.g., in hearing aids for distinguishing speech from background noise without requiring electricity.

Our long-term goal is to take the step from fundamental research to **actual medical and technical applications** of acoustically propelled particles.

1.1.3 Refractive light-propelled microparticles

We have **developed a new type of light-propelled microparticles** [J. Phys. Photonics **5**, 022501 (2023), section 30] whose propulsion does not rely on reflection or absorption of light but on symmetry-broken light refraction that results in a momentum transfer from the light field to the particle. Furthermore, these particles allow for a partial decoupling of particle shape and propulsion. For this purpose, the particles are transparent and have a symmetry-broken refractive index profile. Advantages of these refractive light-propelled microparticles compared to other types of light-propelled particles are that light can propagate deep into a suspension of the particles and there is no heating due to light absorption. This makes our particles an ideal choice for the realization of light-propelled active materials and enables **applications in photonics**. However, their properties are still mostly unexplored.

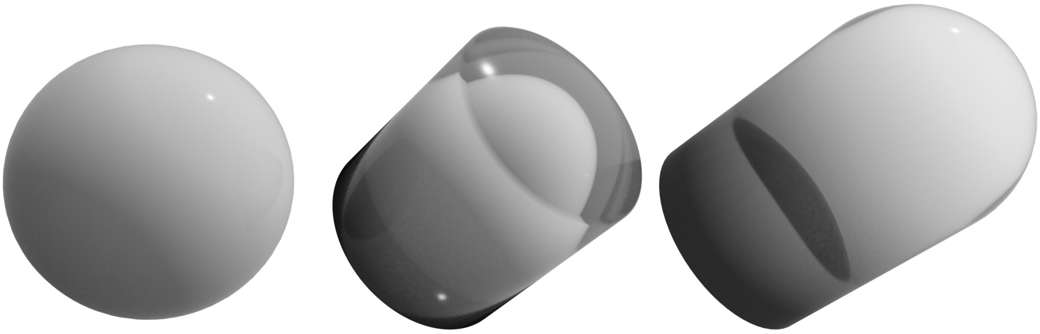

Figure 2: Light-propelled microparticles with a symmetry-broken refractive index profile (depicted in grayscale).

Therefore, we study the properties of refractive light-propelled microparticles and their collective dynamics. We **improve the particle design** and explore the properties of suspensions of the particles, which are light-responsive and constitute **a new class of nonlinear optical materials**. Important aims of our research are to apply these materials in **optical neural networks** (especially **reservoir computing**) and to further develop them from responsive to adaptive to **programmable and intelligent matter**.

1.1.4 Acoustically and optically propelled microparticles

In the future, we will also combine acoustic propulsion (see section 1.1.2) and refractive light propulsion (see section 1.1.3) to obtain active particles and smart materials with an even higher complexity and additional applications. Examples for such applications are **programmable acoustic holograms, metamaterials, and photonic crystals**.

1.1.5 Epidemiology

As populations of animals or humans can also be considered as active matter, we also work on modeling the spread of infectious diseases. For example, we have developed the popular **SIR-DDFT model**, which is a compartmental model that takes effects of social distancing and self-isolation into account. We aim at **developing further epidemiological models** and to obtain new insights into the spread of infectious diseases and how it is affected by public health interventions.

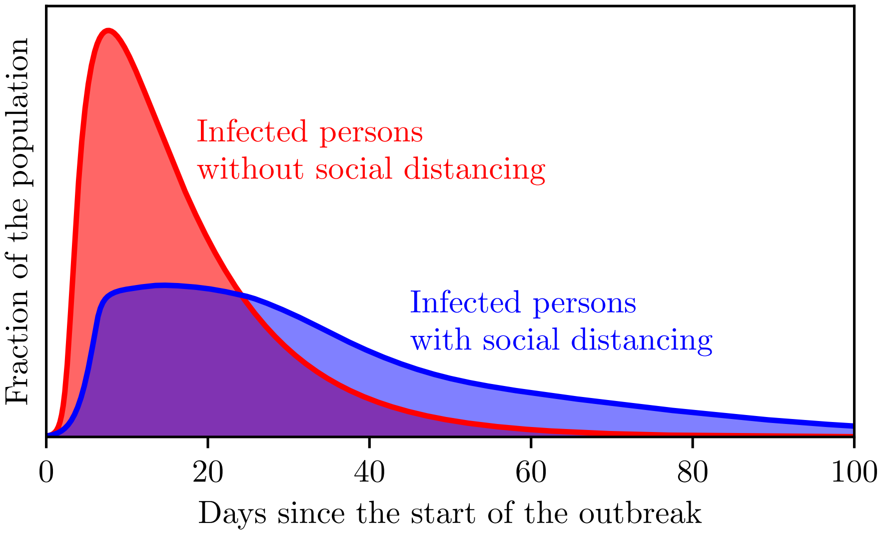

Figure 3: Flattening of the infection curve by social distancing as predicted by our SIR-DDFT model, which takes effects of social distancing and self-isolation into account [Nat. Commun. **11**, 5576 (2020)].

1.2 Statistical physics

Statistical physics is a branch of physics that deals with the mathematical description and analysis of **many-particle systems**. Since nearly everything consists of smaller constituents and is thus a many-particle system, the methods of statistical physics are extremely powerful. They can be applied to nearly all fields of physics and beyond physics (biology, medicine, economics,...).

1.2.1 Research objectives

In our research, we strongly deal with **far-from-equilibrium many-particle systems**. We mainly focus on **classical** systems. However, in some of our research publications, we have studied **quantum-mechanical** and **cosmological** systems. Thus, our research and methodology can cover many-particle systems from the smallest to the largest scales.

Our main goals are the **further development of methods** of statistical physics, the **development of new scientific software** dealing with many-particle systems, the **development of new models** for many-particle systems, and the **investigation of fundamental problems** of statistical physics. The main projects of our current research are described in the following.

1.2.2 Further development of methods

We further develop important methods of statistical physics. For example, we have already strongly enhanced **classical dynamical density functional theory**, the **Mori-Zwanzig projection operator formalism**, the **interaction-expansion method**, and **phase-field-crystal models**. In the case of the Mori-Zwanzig projection operator formalism, we have extended it towards quantum-mechanical or classical far-from-equilibrium systems with an explicitly time-dependent Hamiltonian and towards general relativistic systems.

Since we strongly deal with these methods and have contributed to their development, we have already published **1-2 review articles on each of these methods** (see section 3). The two review articles in *Advances in Physics* are widely seen as the **standard references** in the fields of classical dynamical density functional theory and phase-field-crystal models, respectively. The review article on the interaction-expansion method is the standard reference on this topic.

1.2.3 Development of scientific software

We develop new scientific software. Examples are our **acoustofluidic computer simulation software package** `AcoDyn`, which solves the compressible Navier-Stokes equations numerically using the finite volume method and is two orders of magnitude faster than the popular finite volume simulation package `OpenFOAM`. Another example is our **generic particle simulation framework** `FIPS` for safe (especially data-race free) and parallel molecular dynamics simulations. It can simulate different types of dynamics (e.g., Newtonian, Langevin, and Brownian dynamics) and does not require manual code modifications when simulating systems such as active particles and particles with nonreciprocal interactions, which are currently of large scientific interest but not directly supported by other molecular dynamics simulation software packages.

For other software that we have already developed and published, see `https://www.uni-muenster.de/Physik.TP/~wittkowski/publications.pdf`.

1.2.4 Development of models

In our research, e.g., on active matter, we apply many methods of statistical physics. We mainly use them to **develop new models** for the nonequilibrium dynamics of active matter and to reveal with these models the unusual emerging properties of active matter. For example, we have (together with coworkers) developed many of the **most important models** of active matter physics: **Active Model B**, **Active Model H**, **Active Model I**, and **Active Model I+** (see section 3). Since our methods are applicable also to other fields of physics and even to many fields beyond physics, we also address problems outside of our main field of research (active matter); see section 1.3 for details. For example, we have developed the **SIR-DDFT model** for the spreading of infectious diseases in populations that received much attention in physics and medicine (see section 3).

In general, we have a focus on the **microscopic derivation of predictive field theories**, i.e., the systematic derivation of a needed model (describing a system on a mesoscopic or macroscopic scale) from the equations of motion of the constituting particles. The equations for these “microscopic” particles (atoms, molecules, colloids, animals, humans,..., galaxies) are usually known or easy to write down. The system of interest and the variables/observables the wanted model shall include can be freely chosen as needed. Our derivations based on this **systematic coarse-graining** are predictive in the sense that they provide not only the wanted model but also equations that predict the values of all (materials) parameters that occur in the model.

A central question of our work is **how the properties of many-particle systems arise from the properties of the underlying constituents**.

1.2.5 Investigation of fundamental problems

Occasionally, we address fundamental problems of statistical physics, such as spontaneous collapse models in the context of the quantum-classical transition and their relation to the emergence of thermodynamic irreversibility.

1.3 Further fields of research

Our fields of research beyond active matter and statistical physics are mainly fields that overlap with active matter physics, being an interdisciplinary field of research in the large intersection area of physics, chemistry, biology, and medicine, or that have a particularly high relevance for our research on active matter:

1. **Acoustofluidics:** In the context of acoustically propelled microparticles (see section 1.1.2), we strongly deal with acoustofluidics.

2. **Artificial intelligence:** We deal with acoustics-based (see section 1.1.2), optical (see section 1.1.3), and phononic (see further below in the present list) artificial neural networks. We also apply machine-learning methods.

3. **Biophysics:** We investigate, e.g., swimming microorganisms, the migration of cancer cells, and the mechanical properties and time evolution of biological tissue.

4. **Engineering:** With our work on fluid dynamics, acoustofluidics, microrobots, and active materials (see other items in the present list and section 1.1), our work has a strong relation to engineering.

5. **Fluid dynamics:** In the context of acoustically propelled microparticles (see section 1.1.2), we strongly deal with acoustofluidics. In the context of materials based on light-propelled microparticles (see section 1.1.3), we deal with optofluidics. We also, e.g., address the hydrodynamics of microswimmers and the rheology of (active) soft matter.

6. **Materials science:** We investigate and develop, e.g., active and soft materials with extraordinary properties (see section 1.1).
7. **Medical physics:** With our work towards medical applications of ultrasound-propelled microparticles (see section 1.1.2) and our work in biophysics, we also contribute to medical physics.
8. **Phononics:** Transferring our experience with simulating sound propagation in acoustofluidics to solid media, we want to develop complex phononic structures for phononic chips with new functionalities. For example, we want to develop phononic neural networks.
9. **Photonics:** In the context of light-propelled microparticles (see section 1.1.3), we strongly deal with photonics.
10. **Quantum physics:** We study analogies between active matter systems and quantum systems and have discovered some of these analogies (e.g., the active tunnel effect). We have also published articles on nonequilibrium quantum many-particle systems and order-parameters for quantum liquid crystals. In a current collaboration with Artur Widera (Kaiserslautern), we study a new class of nonequilibrium quantum systems with potential relevance for **quantum technology** (e.g., quantum computing).
11. **Soft matter:** We intensively studied different types of soft matter, e.g., colloidal suspensions and liquid crystals.

In addition, we have already published articles addressing topics from the following fields, to which our methods are applicable as well (see section 1.2.4):

12. **Miscellaneous I:** Nanotechnology, Plasma physics, Solid state physics, Cosmology,...

We are also interested in and currently deal with the following application-oriented topics:

13. **Miscellaneous II:** 3D printing, Volumetric displays,...

For our corresponding publications, see
`https://www.uni-muenster.de/Physik.TP/~wittkowski/publications.pdf`.

2 Methods of research

We apply a wide range of methods of **theoretical physics** and **computational physics**. They include analytical methods (mainly **analytical modeling**) and numerical methods (mainly **computer simulations**). We also **further develop methods** and we **develop scientific software**. For a complete overview about the methods that we apply or further develop, see
`https://www.uni-muenster.de/Physik.TP/~wittkowski/methods.pdf`.

2.1 Analytical modeling

In the context of analytical modeling, we focus on the **microscopic derivation of predictive field theories** for nonequilibrium many-particle systems by **systematic coarse-graining**. We apply, e.g., classical dynamical density functional theory, the Mori-Zwanzig projection operator formalism, the interaction-expansion method, and phase-field-crystal models. See section 1.2.4 for details.

2.2 Computer simulations

In the context of computer simulations, we perform **particle-based simulations** and **field-based simulations**. Our particle-based simulations correspond to simulating the equations of motion of a many-particle system on a microscopic level by numerically solving the equations of motion of the constituting particles. Here, our focus is on **molecular-dynamics simulations**, including Newtonian, Langevin, and Brownian dynamics. We use them, e.g., to simulate the Brownian dynamics of active or passive colloidal particles. Our field-based simulations correspond to simulating a system on a usually mesoscopic or macroscopic level by numerically solving the equations associated with a field-theoretical model for the system. Here, our focus is on the **finite element method** and the **finite volume method**. We use them, e.g., for our acoustofluidic and fluid dynamics simulations. Often, we perform simulations based on own analytical models that we have derived previously (see section 2.1).

Our methods cover **microscopic, mesoscopic, and macroscopic scales** and include methods that address systems on particular scales as well as **scale-bridging methods** that allow to map smaller onto larger scales.

2.3 Further development of methods

We are involved in the **further development of methods** (see section 1.2.2).

2.4 Development of scientific software

We are also involved in the **development of scientific software** (see section 1.2.3).

3 Results of research

3.1 Examples for our largest scientific achievements

1. We **strongly contributed to the investigation of active matter** and published **review articles** dealing with active matter:
   Reviews: J. Phys. Condens. Matter **35**, 313001 (2023)
   Eur. Phys. J. Spec. Top. **222**, 3023-3037 (2013)

2. We discovered several new **effects and materials properties in active matter**, e.g.:
   a) **Shape-induced gravitaxis**
   Nat. Commun. **5**, 4829 (2014)

    b) **Programmable self-organization**
    Sci. Adv. **2**, e1501850 (2016)
    Phys. Rev. Lett. **131**, 168203 (2023)
    c) **Anomalous sound modes**
    New J. Phys. **23**, 063023 (2021)
    d) **Active tunnel effect**
    Nat. Commun. **14**, 1302 (2023)

3. We further developed several important **methods of statistical physics** and published frequently cited **review articles** on each of these methods (see section 1.2.2):
    a) **Classical dynamical density functional theory**
    Reviews: Adv. Phys. **69**, 121-247 (2020)*
    J. Phys. Condens. Matter **35**, 041501 (2023)
    b) **Interaction-expansion method**
    Review: J. Phys. Condens. Matter **35**, 313001 (2023)*
    c) **Mori-Zwanzig projection operator formalism**
    Review: Eur. J. Phys. **41**, 045101 (2020)
    d) **Phase-field-crystal models**
    Review: Adv. Phys. **61**, 665-743 (2012)*

    Three of our review articles (marked by *) are widely seen as the **standard texts** on the respective methods.

4. We derived a large number of **new models** (see section 1.2.4), including very popular ones, e.g.:
    a) **Active Model B**
    Nat. Commun. **5**, 4351 (2014)
    b) **Active Model H**
    Phys. Rev. Lett. **115**, 188302 (2015)
    c) **Active Models I and I+**
    Nat. Commun. **14**, 1302 (2023)
    d) **SIR-DDFT model**
    Nat. Commun. **11**, 5576 (2020)

    The active-matter models a)-c) belong to the **most important models of active matter physics** and model d), describing the spread of infectious diseases, received **much attention in physics and medicine**.

5. We developed several **scientific software packages** with advantages compared to previously existing software, such as **AcoDyn** for orders of magnitude faster acoustofluidic simulations and **FIPS** for safer and more flexible molecular dynamics simulations (see section 1.2.3).

6. We invented **refractive light-propelled microparticles** (see section 1.1.3):
    J. Phys. Photonics **5**, 022501 (2023), section 30

7. We studied the **orientation-dependent propulsion of anisotropic microparticles that are exposed to a traveling sound wave** and showed that they can move lateral, parallel, and even antiparallel to the sound wave, which makes them relevant for a number of medical applications:
   ACS Nano **16**, 3604-3612 (2022)

8. We developed a medically relevant **method for guiding acoustically propelled microparticles** collectively to a target:
   Nanoscale Adv. **4**, 2844-2856 (2022)

3.2 Further results

See `https://www.uni-muenster.de/Physik.TP/~wittkowski/results.pdf`.

4 Collaborations

Our research is performed in a large network of national and international cooperations with **theorists and experimentalists**. We also collaborate with **companies** (Fassisi GmbH, SonoPrint GmbH,...). For an overview, see
`https://www.uni-muenster.de/Physik.TP/~wittkowski/cooperations.pdf`.

Through the wide thematic and methodic range of our work, there are many opportunities for collaborations with researchers from various fields of physics and other disciplines. Even if the fields of interest of a researcher are far away from our main fields of research, one intensive discussion was so far always sufficient to develop ideas for interesting joint projects. This is why, e.g., we have published an article in *Physical Review Letters* together with Sabine Hossenfelder (Frankfurt) on cosmology, we collaborate with colleagues from the Department of Chemistry at the University of Münster within the CRC 1459 “Intelligent Matter”, and we recently wrote a MSCA COFUND (EU) proposal together with colleagues from medicine and business information systems.

5 Technology transfer

We are involved in technology transfer through **patent applications** (one filed, one currently in progress) for our inventions and a planned **spin-off company**. One patent application deals with light-based particle sorting, the other one with **sustainable electronics**. Details are omitted here for reasons of confidentiality.

6 Special features of the research

1. **Thematic broadness:** Our research is highly interdisciplinary. Since our methods are widely applicable, we have contributed to a wide range of fields (see section 1).

2. **Methodic broadness:** We use a wide range of analytical and numerical methods that allows us to perform research in many fields of physics and beyond physics (see section 2).

3. **Method synergy:** We strongly combine analytical modeling and computer simulations (see sections 2.1 and 2.2). In addition, we collaborate with experimentalists (see section 4).

4. **Method development:** We further develop several important methods of statistical physics (see section 1.2.2).

5. **Model development:** We derive a large number of new models (see section 1.2.4).

6. **Software development:** We develop scientific software (see section 1.2.3).

7. **Wide range of scales:** Our research and methodology cover systems from the smallest to the largest scales. We mainly focus on **classical** systems, but also have investigated **quantum-mechanical** and **cosmological** systems (see section 1). The systems we investigate, the methods we apply, and the methods we further develop cover all these scales.

8. **Wide range of collaborations:** We have a large network of national and international cooperations with researchers (theoreticians and experimenters) at universities, research institutions, and companies (see section 4).

9. **Flexible contributions and enhanced interdisciplinarity:** The broadness of our fields and methods of research allow us to adapt our research to local opportunities for collaborations and local needs, to react quickly to new research trends and challenges, and to easily participate in initiatives for coordinated research funding programmes. We can therefore establish new connections between different research fields/departments and thus enhance their interdisciplinary networking.

10. **Technology transfer:** We are involved in technology transfer through patent applications and a planned spin-off company (see section 5).

11. **International recognition:** We are internationally recognized for our contributions to active matter physics, statistical physics, analytical modeling, classical dynamical density functional theory, the Mori-Zwanzig projection operator formalism, the interaction-expansion method, and phase-field-crystal models.

12. **Leading on the theory of sound-propelled microparticles:** To the best of our knowledge, we are worldwide the first and still the main theory group with a strong focus and a significant number of publications on sound-propelled microparticles. (There are many groups working experimentally in this field.) We are especially a leading research group on computer simulations of sound-propelled microparticles. Most of the existing simulation-based articles on sound-propelled microparticles have been published by us and we have performed the most complex computer simulations in this field so far.

13. **Efficient computational fluid dynamics and acoustofluidics:** Our self-developed software package `AcoDyn` allows much faster computer simulations in

the fields of fluid dynamics and acoustofluidics than widely used conventional software such as `COMSOL Multiphysics` or `OpenFOAM`. For example, in our acoustofluidic computer simulations on sound-propelled microparticles, `AcoDyn` is two orders of magnitude faster than `OpenFOAM` so that we can perform more elaborate and complex simulations than the other researchers in this field.