Energetic Methods for Multi-Component Reactive Mixtures

Modelling, Stability, and Asymptotic Analysis

Weierstrass Institute Berlin, September 13–15, 2023

This workshop is devoted to the mathematical analysis of PDE models for multi-component systems and reactive mixtures with applications to

- chemical reaction–diffusion processes,
- biological transport and cross-diffusion phenomena,
- multi-phase and viscoelastic flows in hydrodynamics.

A key challenge is the interaction between different constituents and the treatment of effects such as heat conduction and compressibility. Robust methods based on an energy or entropy structure are discussed and developed.

The organizers,

Katharina Hopf,
Ansgar Jüngel,
and Michael Kniely

WIAS
Weierstrass Institute for
Applied Analysis and Stochastics

DFG Deutsche Forschungsgemeinschaft

1 General Information

1.1 Workshop Dinner and Lunch

The dinner will take place at the restaurant Tapas y Más, Neue Grünstraße 17-18, 10179 Berlin, which is about 10 minutes by foot from WIAS. The dinner is covered within the conference fee and includes the meal and one drink per person.

Here are some places to have lunch, most of which are in close vicinity to WIAS:

- Lunch Time – pizza, pasta, and salads
- Chupenga – burritos, tacos, etc.
- Little Green Rabbit – fresh salads, hearty soups, and baked potatoes
- MALOA Poké Bowl – Hawaiian bowls
- Nanoosh – falafel wraps, Mediterranean salads, and hummus
- Frittenwerk – french fries meet diverse street food creations
- Fontana di Trevi – antipasti, pasta, pizza, and main dishes
- Thu My Marie Concept – Asian fusion cuisine
- Food trucks on Spittelmarkt (only Wednesday and Friday) – Asian dishes, baked potatoes
- Bakery Steinecke – snacks, cakes, and coffee
- Q Burger – creative burgers (10 minutes to walk)
- Huong Sen – Vietnamese cuisine (10 minutes to walk)

1.2 Poster Session

- Christine Keller (WIAS Berlin, Germany)
  Continuum-based modeling of biological ion channels
- Muhammad Uzair Qureshi (Technische Universität Berlin, Germany)
  Reduced order model for catalyst characterization chambers by an asymptotic expansion for the small sample limit
- Lina Sophie Schmitz (Leibniz Universität Hannover, Germany)
  Soap film bridge driven by an electrostatic force

2 Schedule

Wednesday, September 13

08:30–09:05	Registration
09:05–09:15	Opening
09:15–10:05	Miroslav Bulíček (Charles University, Prague, Czech Republic) *Coupling Navier–Stokes–Fourier with the Johnson–Segalman stress-diffusive viscoelastic model: global-in-time large-data analysis*
10:05–10:25	Milan Pokorný (Charles University, Prague, Czech Republic) *Existence analysis of a stationary compressible fluid model for heat-conducting and chemically reacting mixtures*
10:25–11:00	Coffee Break
11:00–11:50	Ewelina Zatorska (Imperial College London, United Kingdom) *Two-phase flows: challenges and insights*
11:50–12:10	Justyna Ogorzały (Military University of Technology, Warsaw, Poland) *The compressible Navier–Stokes equations with slip boundary conditions of friction type*
12:10–13:40	Lunch Break
13:40–14:30	Julian Fischer (ISTA, Klosterneuburg, Austria) *A rigorous approach to the Dean–Kawasaki equation of fluctuating hydrodynamics*
14:30–14:50	Stefanos Georgiadis (KAUST, Thuwal, Saudi Arabia) *The Maxwell–Stefan system: old and new*
14:50–15:10	Bao Quoc Tang (Universität Graz, Austria) *Equilibration for chemically reacting flows with Maxwell–Stefan diffusion*
15:10–15:45	Coffee Break
15:45–16:35	Virginie Ehrlacher (École des Ponts ParisTech & INRIA, France) *Boundary stabilization of cross-diffusion systems in moving domains*
16:35–16:55	Jean Cauvin-Vila (École des Ponts ParisTech & INRIA, France) *A moving-interface cross-diffusion model for thin film deposition*
17:00–18:00	Poster Session (small snacks are provided)

Thursday, September 14

09:15–10:05	Cleopatra Christoforou (University of Cyprus, Nicosia) *A hydrodynamic model of flocking type: BV weak solutions and long-time behaviour*
10:05–10:25	Felisia Angela Chiarello (Università degli Studi dell'Aquila, Italy) *On the singular limit problem for a class of first order nonlocal lane-changing traffic flow models*
10:25–11:00	Coffee Break
11:00–11:50	Vincent Giovangigli (École Polytechnique, Palaiseau, France) *Asymptotic stability for a multicomponent reactive flow diffuse interface model*
11:50–12:10	Yadong Liu (Universität Regensburg, Germany) *On a diffuse interface model for incompressible viscoelastic two-phase flows*
12:10–13:40	Lunch Break
13:40–14:30	Benoît Perthame (Sorbonne Université, Paris, France) *Analysis of models of living tissues and free boundary problems*
14:30–14:50	Dennis Trautwein (Universität Regensburg, Germany) *Existence and approximation of a viscoelastic Cahn–Hilliard model for tumour growth*
14:50–15:10	Christoph Hurm (Universität Regensburg, Germany) *Strong nonlocal-to-local convergence of the Cahn–Hilliard equation and its operator*
15:10–15:45	Coffee Break
15:45–16:35	Klemens Fellner (Universität Graz, Austria) *Oscillatory solutions to a nonlinear Becker–Döring type model for prion dynamics*
16:35–16:55	Annamaria Massimini (Technische Universität Wien, Austria) *Analysis of a Poisson–Nernst–Planck–Fermi system for charge transport in ion channels*
17:00–18:00	Coffee & Discussion
18:30–22:00	Workshop Dinner (buffet-style dinner at Tapas y más)

Friday, September 15

09:15–10:05	Agnieszka Świerczewska-Gwiazda (University of Warsaw, Poland) *Asymptotic analysis: from high friction gas dynamics to diffusion models*
10:05–10:25	Alex Rossi (FAU Erlangen-Nürnberg, Germany) *Stability of stationary solutions to Allen–Cahn type opinion formation models*
10:25–11:00	Coffee Break
11:00–11:50	Robert Lasarzik (WIAS Berlin, Germany) *Energy-variational solutions for different viscoelastic fluid models*
11:50–12:10	Manuel Landstorfer (WIAS Berlin, Germany) *Modeling and validation of material and transport models for electrolytes*
12:10–12:15	Closing
12:15–13:00	Get Together (small snacks are provided)

3 Abstracts (in alphabetical order)

Miroslav Bulíček (Charles University, Prague, Czech Republic)

Coupling Navier–Stokes–Fourier with the Johnson–Segalman stress-diffusive viscoelastic model: global-in-time large-data analysis

We focus on a large-data and global-in-time theory for weak solution to a system of partial differential equations describing an unsteady flow of an incompressible heat-conducting rate-type viscoelastic stress-diffusive fluid filling up a mechanically and thermally isolated container of any dimension. To overcome the principle difficulties connected with ill-posedness of the diffusive Oldroyd-B model in three dimensions, we assume that the fluid admits a strengthened dissipation mechanism, at least for excessive elastic deformations. All the relevant material coefficients are allowed to depend continuously on the temperature, whose evolution is captured by a thermodynamically consistent equation. We present a huge zoo of models for which, just based on the energy and the entropy inequality, one can deduce well-sounded existence theory for a weak solution.

Jean Cauvin-Vila (École des Ponts ParisTech & Institut National de Recherche en Informatique et en Automatique, France)

On a moving-interface cross-diffusion model for thin film deposition

We propose an extension of the one-dimensional model introduced in [1] to describe a vapor deposition process used for the fabrication of thin film layers in the photovoltaic industry. In the process, a wafer is introduced in a hot chamber where chemical elements are injected under gaseous form. As the latter deposit on the substrate, a heterogeneous solid layer grows upon it. We are interested in two essential features of the problem: the evolution of the surface of the film and the diffusion of the various species in both phases, due to high temperature conditions. Our model consists of two cross-diffusion systems coupled by a moving interface through which chemical reactions occur. More precisely, we consider the moving-boundary domain $\Omega(t) = (0, X(t)) \cup (X(t), 1)$ and n different chemical species represented by their densities of molar concentration $\boldsymbol{c}(t,x) = (c_i(t,x))_{1\leq i\leq n}$, subject to nonnegativity and volume-filling constraints. The dynamics in the solid (resp. gas) phase is modelled by a size-exclusion (resp. Stefan–Maxwell) cross-diffusion matrix, while the interface reactions are modelled by the Butler–Volmer formulas, given, for some constant reference chemical potentials $\boldsymbol{\mu}^{*,g}, \boldsymbol{\mu}^{*,s}$, by

$$F_i = c_i(X^-)e^{\frac{1}{2}(\mu_i^{*,g}-\mu_i^{*,s})} - c_i(X^+)e^{-\frac{1}{2}(\mu_i^{*,g}-\mu_i^{*,s})}.$$

These formulas appear as flux boundary data at X^-, X^+ of the respective cross-diffusion systems and the model is completed by the interface evolution formula

$$X' = -\sum_{i=1}^{n} F_i.$$

In this communication, I will introduce the model in full detail and present its dissipative structure, using ideas from [2]. I will also characterize the stationary states and discuss long-time asymptotics. Then, I will introduce a finite volume approximation of the system. Although such schemes were previously designed for each respective cross-diffusion system in a fixed domain, the main novelty of our scheme is the treatment of the moving interface. The resulting discrete nonlinear system is shown to admit a solution that preserves the full structure of the continuous system, namely: mass conservation, nonnegativity, volume-filling constraints and decay of the discrete free energy. Numerical simulations illustrate these properties and suggest that the scheme also preserves the long-time asymptotics. A concise presentation of the scheme can be found in [3].

Acknowledgments: The authors acknowledge support from the french ANR project COMODO (ANR-19-CE46-0002) which funds the Ph.D. of Jean Cauvin-Vila.

[1] A. Bakhta, V. Ehrlacher, *Cross-diffusion systems with non-zero flux and moving boundary conditions*, ESAIM Math. Model. Numer. Anal. **52** (2018), no. 4, 1385–1415.

[2] A. Glitzky, A. Mielke, *A Gradient Structure for Systems Coupling Reaction–Diffusion Effects in Bulk and Interfaces*, Z. Angew. Math. Phys. **64** (2013), no. 1, 29–52.

[3] C. Cancès, J. Cauvin-Vila, C. Chainais-Hillairet, V. Ehrlacher, *Structure Preserving Finite Volume Approximation of Cross-Diffusion Systems Coupled by a Free Interface* in Franck, E. et al. (eds.), *Finite Volumes for Complex Applications X–Volume 2, Hyperbolic and Related Problems*, Springer Proc. Math. Stat., vol. 433, Springer, Cham, 2023 (to appear). arXiv:2303.15817.

Felisia Angela Chiarello (Università degli Studi dell'Aquila, Italy)

On the singular limit problem for a class of first order nonlocal lane-changing traffic flow models

In this talk, we will present a nonlocal-to-local convergence result with applications to traffic models. In particular, we will consider a system of two (or more) nonlocal balance laws characterized by lane-changing functions on the right-hand sides and exponential kernels in the nonlocal terms of the flux functions, i.e.

$$
\begin{aligned}
\partial_t \boldsymbol{\rho}^1(t,x) + \partial_x\Big(V_1(\mathcal{W}[\boldsymbol{\rho}^1](t,x))\boldsymbol{\rho}^1(t,x)\Big) &= S\big(\boldsymbol{\rho}(t,x), \mathcal{W}[\boldsymbol{\rho}](t,x), x\big) && (t,x) \in (0,T)\times\mathbb{R}\\
\partial_t \boldsymbol{\rho}^2(t,x) + \partial_x\Big(V_2(\mathcal{W}[\boldsymbol{\rho}^2](t,x))\boldsymbol{\rho}^2(t,x)\Big) &= -S\big(\boldsymbol{\rho}(t,x), \mathcal{W}[\boldsymbol{\rho}](t,x), x\big) && (t,x) \in (0,T)\times\mathbb{R}\\
\boldsymbol{\rho}(0,x) &= \boldsymbol{\rho}_0(x) && x \in \mathbb{R}\\
\mathcal{W}[\rho](t,x) &= \tfrac{1}{\eta}\displaystyle\int_x^\infty \exp\left(\tfrac{x-y}{\eta}\right)\rho(t,y)\,\mathrm{d}y && (t,x) \in (0,T)\times\mathbb{R}
\end{aligned}
$$

with the nonlocal operator $\mathcal{W}$ defined for $\rho \in C([0,T]; L^1_{\text{loc}}(\mathbb{R})) \cap L^\infty((0,T); L^\infty(\mathbb{R}))$,

$$\mathcal{W}[\boldsymbol{\rho}](t,x) = (\mathcal{W}[\boldsymbol{\rho}^1], \mathcal{W}[\boldsymbol{\rho}^2])(t,x)$$

and $\boldsymbol{\rho} = (\boldsymbol{\rho}^1, \boldsymbol{\rho}^2)$. Here, the exponential kernels are approximations of the Dirac distribution and the coupling between the equations of the system is only through the right-hand sides. We will analytically prove that the solution of the nonlocal system converges to the solution of the corresponding local one when the kernels of the nonlocal terms approach the Dirac delta. Numerical illustrations supporting the main results will be also shown.

Acknowledgments: F.A.C. is member of Gruppo Nazionale per l'Analisi Matematica, la Probabilità e le loro Applicazioni (GNAMPA) of the Istituto Nazionale di Alta Matematica (INdAM). F.A.C. was partially supported by 'INdAM-GNAMPA Project', code CUP_E53C22001930001.

[1] F. A. Chiarello, A. Keimer, *On the singular limit problem for a class of first order nonlocal lane-changing traffic flow models*. In preparation.

Cleopatra Christoforou (University of Cyprus, Nicosia)

A hydrodynamic model of flocking type: BV weak solutions and long-time behaviour

In this talk, we present some results on the existence and time-asymptotic flocking of weak solutions to a hydrodynamic model of flocking-type with an all-to-all interaction kernel in a one-space dimension. An appropriate notion of entropy weak solutions with bounded support is given to capture the behavior of solutions with initial data that has finite total mass confined in a bounded interval and initial density uniformly positive therein. We show global in time existence of entropy weak solutions with concentration for any initial data of bounded variation having the structure above. In addition, we will describe a recent result on the time-asymptotic limit for such solutions, showing the asymptotic decay towards flocking profiles without any further restrictions on the data. Joint work with Debora Amadori (Univ. of L'Aquila).

Virginie Ehrlacher (École des Ponts ParisTech & Institut National de Recherche en Informatique et en Automatique, France)

Boundary stabilization of cross-diffusion systems in moving domains

This work is motivated by a collaboration with the French Photovoltaic Institute. The aim of the project is to propose a model in order to simulate and optimally control the fabrication process of thin film solar cells. The production of the thin film inside of which occur the photovoltaic phenomena accounting for the efficiency of the whole solar cell is done via a Physical Vapor Deposition (PVD) process. More precisely, a substrate wafer is introduced in a hot chamber where the different chemical species composing the film are injected under a gaseous form. Molecules deposit on the substrate surface, so that a thin film layer grows by

epitaxy. In addition, the different components diffuse inside the bulk of the film, so that the local volumic fractions of each chemical species evolve through time. The efficiency of the final solar cell crucially depends on the final chemical composition of the film, which is freezed once the wafer is taken out of the chamber. A major challenge consists in optimizing the fluxes of the different atoms injected inside the chamber during the process for the final local volumic fractions in the layer to be as close as possible to target profiles. Two different phenomena have to be taken into account in order to correctly model the evolution of the composition of the thin film: 1) the cross-diffusion phenomena between the various components occuring inside the bulk; 2) the evolution of the surface. As a consequence, the underlying model reads as a cross-diffusion system defined on a moving boundary domain. The complete optimal control problem of the fluxes injected in the hot chamber is currently out-of-reach in terms of mathematical analysis. The aim of this talk is to theoretically investigate a simpler problem, which is the boundary stabilization of the model used to simulate the PVD process. We show first exponential stabilization and then finite-time stabilization in arbitrary small time of the linearized system around uniform equilibria, provided the underlying cross-diffusion system has an entropic structure with a symmetric mobility matrix. This stabilization is achieved with respect to both the volumic fractions of the different chemical species composing the thin film and the thickness of the latter. The feedback control is derived using the backstepping technique, adapted to the context of a time-dependent domain. In particular, the norm of the backward backstepping transform is carefully estimated with respect to time.
This is joint work with Jean Cauvin-Vila and Amaury Hayat.

Klemens Fellner (Universität Graz, Austria)

Oscillatory solutions to a nonlinear Becker–Döring type model for prion dynamics

Prions are able to self-propagate biological information through the transfer of structural information from a misfolded/infectious protein in a prion state to a protein in a non-prion state. Prions cause diseases like Creuzfeldt–Jakob. Prion-like mechanisms are associated to Alzheimer, Parkinson, and Huntington diseases. We present a fundamental bi-monomeric, nonlinear Becker–Döring type model, which aims to explain experiments in the lab of Human Rezaei showing sustained oscillatory behaviour over multiple hours, [1]. Besides two types of monomers, our model suggests a nonlinear depolymerisation process as crucial for the oscillatory behaviour. Since then, experimental evidence seems to confirm this process. We provide details on the mechanism of oscillatory behaviour and show numerical simulations. This is joint work with Marie Doumic (CNRS & École Polytechnique), Mathieu Mezache (CNRS), Human Rezaei (INRA), J. L. Velázquez (U Bonn).

[1] M. Doumic, K. Fellner, M. Mezache, H. Rezaei, *A bi-monomeric nonlinear Becker–Döring type system to capture oscillatory aggregation kinetics in prion dynamics*, J. Theoret. Biol. **480** (2019), 241–261.

Julian Fischer (Institute of Science and Technology Austria (ISTA), Klosterneuburg)

A rigorous approach to the Dean–Kawasaki equation of fluctuating hydrodynamics

Fluctuating hydrodynamics provides a framework for approximating density fluctuations in interacting particle systems by suitable SPDEs. The Dean–Kawasaki equation – a strongly singular SPDE – is perhaps the most basic equation of fluctuating hydrodynamics; it has been proposed in the physics literature to describe the fluctuations of the density of N diffusing weakly interacting particles in the regime of large particle numbers N. The strongly singular nature of the Dean–Kawasaki equation presents a substantial challenge for both its analysis and its rigorous mathematical justification: Besides being non-renormalizable by approaches like regularity structures, it has recently been shown to not even admit nontrivial martingale solutions. In this talk, we give an overview of recent quantitative results for the justification of fluctuating hydrodynamics models. In particular, we give an interpretation of the Dean–Kawasaki equation as a "recipe" for accurate and efficient numerical simulations of the density fluctuations for weakly interacting diffusing particles, allowing for an error that is of arbitarily high order in the inverse particle number. Based on joint works with Federico Cornalba, Jonas Ingmanns, and Claudia Raithel.

Stefanos Georgiadis (King Abdullah University of Science and Technology & Technische Universität Wien, Saudi Arabia & Austria)

The Maxwell–Stefan system: old and new

In this talk, we focus on the Maxwell–Stefan system, describing diffusive phenomena in a multicomponent gas mixture. After introducing the model, we give an overview of the existing results regarding local-in-time existence and uniqueness of strong solutions and global-in-time existence and asymptotic behavior of weak solutions. We, then, present some new results regarding the absence of anomalous dissipation and the uniqueness of weak solutions. Finally, we discuss its non-isothermal analogue, called Maxwell–Stefan–Fourier, for which one can prove global-in-time existence of weak solutions and weak-strong uniqueness.

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Vincent Giovangigli (École Polytechnique, Palaiseau, France)

Asymptotic stability for a multicomponent reactive flow diffuse interface model

We investigate the asymptotic stability of constant equilibrium states for a multicomponent reactive flow diffuse interface model of Korteweg type. The model is obtained with simplifying assumptions from general Cahn–Hilliard fluid equations derived from the kinetic theory of dense gas mixtures and the BBGKY hierarchy. An augmented formulation is introduced with an extra unknown representing the gradient of density. The stability properties of the linearized augmented system as well as the validity of the gradient constraint are key arguments in the proof of asymptotic stability.

Christoph Hurm (Universität Regensburg, Germany)

Strong nonlocal-to-local convergence of the Cahn–Hilliard equation and its operator

We prove convergence of a sequence of weak solutions of the nonlocal Cahn–Hilliard equation to the strong solution of the corresponding local Cahn–Hilliard equation. The analysis is done in the case of sufficiently smooth bounded domains with Neumann boundary condition and a $W^{1,1}$-kernel. The proof is based on the relative entropy method. Additionally, we prove the strong L^2-convergence of the nonlocal operator to the negative Laplacian together with a rate of convergence.

Acknowledgments: This work was partially supported by the Graduiertenkolleg 2339 *IntCom-Sin* of the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) – Project-ID 321821685. The support is gratefully acknowledged.

[1] H. Abels, C. Hurm. *Strong nonlocal-to-local convergence of the Cahn-Hilliard equation and its operator*. In preparation.

[2] E. Davoli, H. Ranetbauer, L. Scarpa, L. Trussardi, *Degenerate nonlocal Cahn-Hilliard equations: well-posedness, regularity and local asymptotics*. Ann. Inst. H. Poincaré Anal. Non Linéaire **37** (2020), no. 3, 627–651.

[3] E. Davoli, L. Scarpa, L. Trussardi, *Local asymptotics for nonlocal convective Cahn-Hilliard equations with $W^{1,1}$ kernel and singular potential*. J. Differential Equations **289** (2021), 35–58.

[4] E. Davoli, L. Scarpa, L. Trussardi, *Nonlocal-to-local convergence of Cahn-Hilliard equations: Neumann boundary conditions and viscosity terms*, Arch. Ration. Mech. Anal. **239** (2021), no. 1, 117–149.

Christine Keller (Weierstraß-Institut Berlin, Germany)

Continuum-based modeling of biological ion channels

Ion channels in cell membranes are of ultimate importance in physiology. They control a large fraction of biological processes and are mainly investigated by current-voltage experiments. To support the interpretation of measured results, we develop a model- framework based on non-equilibrium thermodynamics that accounts for various important aspects, e.g., finite-volume effects and the surface charges of the channel. Julia-based numerical simulations are performed to compute current-voltage relations, with varying ion concentrations, applied voltages, and channel properties.

Manuel Landstorfer (Weierstraß-Institut Berlin, Germany)

Modeling and validation of material and transport models for electrolytes

In this talk, I will show some general aspects of modeling ionic species in liquid electrolytes which are subject to solvation effects. Based on non-equilibrium thermodynamics, the derivation for a material model of an incompressible solvation mixture is thus sketched. I will show how such a material model can be validated in thermodynamic equilibrium on various electrochemical measurement techniques and deduce some results regarding the modeling perception. Building on this, I will discuss several models for ionic flux relations, including Nernst–Planck-type fluxes and Onsager-type cross-diffusion models. I will show some shortcomings of the classical Nernst–Planck-flux in terms of measurable quantities and provide an interpretation of the Kohlrausch law for electrolytes on the basis of cross-diffusion effects.

Robert Lasarzik (Weierstraß-Institut Berlin, Germany)

Energy-variational solutions for different viscoelastic fluid models

The concept of energy-variational solutions is introduced for a general class of evolution equations. Under certain convexity assumptions, the existence of such solutions can be shown constructively by an adapted minimizing movement scheme. Weak-strong uniqueness follows by a suitable relative energy inequality. Moreover, energy-variational solutions are compared to other generalized solution concepts for specific systems in fluid dynamics. Finally, the general result is applied to two different viscoelastic fluid models without stress diffusion, and a short comparison of different viscoelastic models hints at advantages and disadvantages of this energy-variational approach.

Yadong Liu (Universität Regensburg, Germany)

On a diffuse interface model for incompressible viscoelastic two-phase flows

This talk concerns a diffuse interface model for the flow of two incompressible viscoelastic fluids in a bounded domain. More specifically, the fluids are assumed to be macroscopically immiscible, but with a small transition region, where the two components are partially mixed. Considering the elasticity of both components, one ends up with a coupled Oldroyd-B/Cahn–Hilliard type system, which describes the behavior of two-phase viscoelastic fluids. Based on the total energy

$$\mathcal{E} = \underbrace{\int_\Omega \frac{\rho(\phi)}{2}\,|\mathbf{u}|^2\,\mathrm{d}x}_{\text{Kinetic energy}} + \underbrace{\int_\Omega \frac{\mu(\phi)}{2}\mathrm{Tr}(\mathbb{B}-\ln\mathbb{B}-\mathbb{I})\,\mathrm{d}x}_{\text{Elastic energy}} + \underbrace{\int_\Omega \tilde{\sigma}\Big(\frac{\epsilon}{2}\,|\nabla\phi|^2+\frac{1}{\epsilon}W(\phi)\Big)\,\mathrm{d}x}_{\text{Ginzburg–Landau free energy}},$$

we derive a thermodynamically consistent model for two-phase incompressible viscoelastic fluids of Oldroyd-B type [3], which in particular cases describe a fluid-structure interaction problem as in [4]. This model provides a viscoelastic fluid counterpart of the celebrated Abels–Garcke–Grün (AGG) model [1] for incompressible two-phase viscous flows. We prove the existence of weak solutions to the system in two dimensions for general (unmatched) mass densities, variable viscosities, different shear moduli, and a class of physically relevant and singular potentials that guarantee the order parameter stays in the physically reasonable interval. The proof is initiated by [2], which solved the AGG model by a time discretization scheme. We first introduce a novel spatial regularization of the original system, which preserves the energy-dissipation structure of the problem, as well as the uniform estimates. To address the regularized system, we propose a new *hybrid implicit time discretization* based on [2], which is solved by a Leray–Schauder argument, on noting the well-posedness of regularized Oldroyd-B equation for $\mathbb{B}$.

Acknowledgments: This work was partially supported by the Graduiertenkolleg 2339 *IntCom-Sin* of the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) – Project-ID 321821685. The support is gratefully acknowledged.

[1] H. Abels, H. Garcke, G. Grün, *Thermodynamically consistent, frame indifferent diffuse interface models for incompressible two-phase flows with different densities*, Math. Models Methods Appl. Sci. **22** (2012), no. 3, 1150013, 40 pp.

[2] H. Abels, D. Depner, H. Garcke, *Existence of weak solutions for a diffuse interface model for two-phase flows of incompressible fluids with different densities*, J. Math. Fluid Mech. **15** (2013), no. 3, 453–480.

[3] Y. Liu, D. Trautwein, *On a diffuse interface model for incompressible viscoelastic two-phase flows*. Preprint, 2022. arXiv:2212.13507.

[4] D. Mokbel, H. Abels, S. Aland, *A phase-field model for fluid-structure interaction*, J. Comput. Phys. **372** (2018), 823–840.

Annamaria Massimini (Technische Universität Wien, Austria)

Analysis of a Poisson–Nernst–Planck–Fermi system for charge transport in ion channels

In this talk, a modified Poisson–Nernst–Planck system in a bounded domain with mixed Dirichlet–Neumann boundary conditions is analyzed. It describes the concentrations of ions immersed in a polar solvent and the correlated electric potential due to the ion–solvent interaction. The considered mixture is saturated, meaning that the sum of the ion and solvent concentrations is constant. This assumption of finite ion sizes leads to cross-diffusion equations, which are thermodynamically consistent. The correlated electric potential depends nonlocally on the electric potential and solves the fourth-order Poisson–Fermi equation. The existence of global bounded weak solutions is presented by using the boundedness-by-entropy method. The novelty of the work is the proof of the weak–strong uniqueness property. In contrast to the existence proof, we include the solvent concentration in the cross-diffusion system, leading to a diffusion matrix with nontrivial kernel. Then the proof is based on the relative entropy method for the extended cross-diffusion system and the positive definiteness of a related diffusion matrix on a subspace.

Justyna Ogorzały (Military University of Technology, Warsaw, Poland)

The compressible Navier–Stokes equations with slip boundary conditions of friction type

We present, for the first time, the compressible Navier–Stokes equations with the slip boundary condition of friction type. We prove the existence of weak solutions in this setting. Since the slip boundary condition of friction type is particularly interesting for the modelling of fluids in moving domains or fluid-structure interaction, our result can be considered as a first stepping stone towards the study of these more sophisticated problems.

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[1] Š. Nečasová, J. Ogorzały, J. Scherz, *The compressible Navier–Stokes equations with slip boundary conditions of friction type*. Submitted, 2023. arxiv:2305.00822.

Benoît Perthame (Sorbonne Université, Paris, France)

Analysis of models of living tissues and free boundary problems

Tissue growth, as it occurs during solid tumors, can be described at a number of different scales from the cell to the organ. For a large number of cells, 'fluid mechanical' approaches have been advocated in mathematics, mechanics or biophysics. We will give an overview of the modeling aspects and focus on the links between those mathematical models. Then, we will focus on the 'compressible' description describing the cell population density based on systems of porous medium type equations with reaction terms. A more macroscopic 'incompressible' description is based on a free boundary problem close to the classical Hele–Shaw equation. In the stiff pressure limit, one can derive a weak formulation of the corresponding Hele–Shaw free boundary problem and one can make the connection with its geometric form. The mathematical tools related to these questions include multi-scale analysis, Aronson–Benilan estimate, uniform L^4 estimate on the pressure gradient, and emergence of instabilities.

Milan Pokorný (Mathematical Institute of Charles University, Prague, Czech Republic)

Existence analysis of a stationary compressible fluid model for heat-conducting and chemically reacting mixtures

The existence of large-data weak solutions to a steady compressible Navier–Stokes–Fourier system for chemically reacting fluid mixtures is proved. General free energies are considered satisfying some structural assumptions, with a pressure containing a γ-power law. The model is thermodynamically consistent and contains the Maxwell–Stefan cross-diffusion equations in the Fick–Onsager form as a special case. Compared to previous works, a very general model class is analyzed, including cross-diffusion effects, temperature gradients, compressible fluids, and different molar masses. A priori estimates are derived from the entropy balance and the total energy balance. The compactness for the total mass density follows from an estimate for the pressure in L^p with $p > 1$, the effective viscous flux identity, and uniform bounds related to Feireisl's oscillations defect measure. These bounds rely heavily on the convexity of the free energy and the strong convergence of the relative chemical potentials. The presentation follows the publication [1].

[1] M. Bulíček, A. Jüngel, M. Pokorný, N. Zamponi, *Existence analysis of a stationary compressible fluid model for heat-conducting and chemically reacting mixtures*, J. Math. Phys. **63** (2022), no. 5, Paper No. 051501, 48 pp.

Muhammad Uzair Qureshi (Technische Universität Berlin, Germany)

Reduced order model for catalyst characterization chambers by an asymptotic expansion for the small sample limit

In this work we present a reduced order approach based on the asymptotic expansion of the linear perturbations to tackle the stiff problem arising from the coupling of reaction rates and transport phenomena in a heterogeneous catalytic system.
Computational Fluid Dynamics (CFD) of reactive flows over heterogeneous catalysts is a challenging task even for simple laminar flows. This involves solving a system of Partial Differential Equations (PDEs) with highly non-linear boundary conditions imposed by the surface chemistry which leads to stiffness and bad conditioning of the overall system requiring extensive computational effort.
To ease the modelling of heterogeneous catalysis, catalyst characterization chambers are typically designed to obey certain reduced reactor models, e.g. stagnation point flows. However, during the last years, a number of experimental methods have been developed which can provide atomic scale information of the catalyst under operando conditions. These experiments are conducted on very general reactor geometries. To investigate these reaction chambers, we present a reduced order approach with a significant lower computational footprint than conventional CFD, which exploits the fact that many catalyst characterization experiments are conducted with rather small catalyst samples and is applicable to general reactor geometries. The approach is based on the observation that in many experiments the mixture density and the species transport coefficients are hardly affected by the surface chemistry. The velocity field then decouples from the chemistry and can be obtained from the non-reactive flow problem. This assumption becomes exact in the limit of low chemical reactivity and for excess of one or more species. Concentrating on this assumption, we exploit the fact that in the case of small sample limit, the lateral variation of the reactivity on the catalytic surface will be small. So, a leading order asymptotic series expansion for these species results in a problem, which can be solved by three simple steps. First, calculating the velocity field from the non-reactive solution. Second, obtaining the solution of a linear transport problem with constant reactivity. Finally, parametrically feeding this solution into a small non-linear algebraic problem, which has as many unknowns as species.
The approach has been implemented using VoronoiFVM Finite Volume package [1], which guarantees mass conservation. We will demonstrate the approach using the Methanol formation reaction from CO_2 and H_2 and for flow geometries where the zero-reactivity solution for the velocity field is known. Using these, we address the strengths and limitations of the approach. This approach is benchmarked against numerical simulations of the fully coupled problem using the CatalyticFoam solver [2].

Acknowledgments: We thank the Elsa Neumann Stipendium (Nachwuchsförderungsgesetz NaFöG) and Higher Education Comission Pakistan (ID 57589483) for the financial support for this project.

[1] J. Fuhrmann, D. Abdel, J. Weidner, A. Seiler, P. Farrell, M. Liero, *VoronoiFVM.jl - Finite volume solver for coupled nonlinear partial differential equations*, Zenodo. doi:10.5281/zenodo.3529808

[2] M. Maestri, A. Cuoci, *Coupling CFD with detailed microkinetic modeling in heterogeneous catalysis*, Chem. Eng. Sci. **96** (2013), 106–117. doi:10.1016/j.ces.2013.03.048

Alex Rossi (Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany)

Stability of stationary solutions to Allen–Cahn type opinion formation models

In this talk, after a short introduction to the kinetic theory, its methods and applications, we would like to introduce an Allen–Cahn type equation obtained from an integro-differential Boltzmann equation exposed in [3] for the description of opinion formation and perform a linear stability analysis with the help of some classical tools of spectral theory. Our analysis compares a nonlinear and a simplified linear model and their different microscopic interaction rules and such models are investigated from the numerical point of view as well. Moreover, a possible generalisation of the analysis to the continuous-opinion model presented in [5] is suggested.

Acknowledgments: The authors gratefully acknowledge the support by the RTG 2339 "Interfaces, Complex Structures and Singular Limits" of the German Research Foundation (DFG).

[1] M. Burger, N. Loy, A. Rossi, *Stability of stationary solutions to Allen-Cahn type opinion formation models*. In preparation.

[2] S. P. Eveson, *Compactness criteria for integral operators in L^1 and L^∞ spaces*, Proc. Amer. Math. Soc. **123** (1995), no. 12, 3709–3716.

[3] N. Loy, M. Raviola, A. Tosin, *Opinion polarization in social networks*, Philos. Trans. Roy. Soc. A **380** (2022), no. 2224, Paper No. 20210158, 15 pp.

[4] V. Nguyen, G. Xiao, X. Xu, Q. Wu, C. Xia, *Dynamics of opinion formation under majority rules on complex social networks*, Sci. Rep. **10** (2020), Paper no. 456, 9 pp.

[5] L. Pareschi, G. Toscani, *Interacting Multiagent Systems: Kinetic Equations and Monte Carlo Methods*, Oxford University Press, New York, 2014.

Lina Sophie Schmitz (Leibniz Universität Hannover, Germany)

Soap film bridge driven by an electrostatic force

We consider a tiny soap film spanned between two parallel metal rings subjected to an external electrostatic force changing the film's deflection. Assuming rotational symmetry, the deflection of the film can be described by a 1-dimensional degenerate parabolic equation with a non-local and singular source term. The equation is derived formally from an energy functional. We

present results on different behaviour of the film depending on the strength of the electrostatic force. One such result is concerned with local stability of stationary solutions in case that the force is not too strong. Its proof is based on the principle of linearised stability.

Agnieszka Świerczewska-Gwiazda (University of Warsaw, Poland)

Asymptotic analysis: from high friction gas dynamics to diffusion models

Several recent studies considered the high-friction limit for systems arising in fluid mechanics. Following this approach, we rigorously derive the nonlocal Cahn–Hilliard equation as a limit of the nonlocal Euler–Korteweg equation using the relative entropy method. Applying the recent result about relations between non-local and local Cahn–Hilliard, we also derive rigorously the large-friction nonlocal-to-local limit. The proof is formulated for dissipative measure-valued solutions of the nonlocal Euler–Korteweg equation which are known to exist on arbitrary intervals of time. This approach provides a new method to derive equations not enjoying classical solutions via relative entropy method by introducing the nonlocal effect in the fluid equation. During the talk I will also discuss the high-friction limit of the Euler–Korteweg system.

Bao Quoc Tang (Universität Graz, Austria)

Equilibration for chemically reacting flows with Maxwell–Stefan diffusion

The large-time asymptotics of weak solutions to Maxwell–Stefan diffusion systems for chemically reacting fluids with different molar masses and reversible reactions are investigated. More precisely, we consider the following reactions of N chemical species

$$\alpha_1^a A_1 + \cdots + \alpha_n^a A_n \underset{k_f^a}{\overset{k_b^a}{\rightleftharpoons}} \beta_1^a A_1 + \cdots + \beta_n^a A_n, \quad a = 1, \dots, N,$$

which results in the evolution system with Maxwell–Stefan diffusion

$$\partial_t \rho_i + \nabla \cdot \boldsymbol{j}_i = r_i(\boldsymbol{x}), \quad \nabla x_i = -\sum_{j=1}^{n} \frac{\rho_j \boldsymbol{j}_i - \rho_i \boldsymbol{j}_j}{c^2 M_i M_j D_{ij}}, \quad i = 1, \dots, n, \tag{1}$$

where ρ_i is partial mass density, M_i is the molar mass, $c_i = \rho_i / M_i$ is the partial concentration, $c = \sum_{i=1}^n c_i$ is the total concentration, and $x_i = c_i/c$ is the molar fraction, and

$$r_i(\boldsymbol{x}) = M_i \sum_{a=1}^{N} (\beta_i^a - \alpha_i^a) \left(k_f^a \boldsymbol{x}^{\boldsymbol{\alpha}^a} - k_b^a \boldsymbol{x}^{\boldsymbol{\beta}^a} \right), \quad \boldsymbol{x}^{\boldsymbol{\alpha}^a} = \prod_{i=1}^{n} x_i^{\alpha_i^a}.$$

The diffusion matrix of the system is generally neither symmetric nor positive definite, but the equations admit a formal gradient-flow structure which provides entropy (free energy) estimates. The main result is the exponential decay to the unique equilibrium with a rate that is constructive up to a finite-dimensional inequality.

Theorem 1 ([1]). *Assume detailed balance condition. Then there exists a non-negative global weak solution to (1). Moreover, if there are no boundary equilibria, then the solution converges exponentially to equilibrium with constructive rates, i.e.*

$$\sum_{i=1}^{n} \|x_i(t) - x_{i,\infty}\|_{L^p(\Omega)} \leq C_p e^{-\lambda_p t} \quad \forall t > 0, \forall p \geq 1.$$

The key elements of the proof are the existence of a unique detailed-balance equilibrium and the derivation of an inequality relating the entropy and the entropy production. The main difficulty comes from the fact that the reactions are represented by molar fractions while the conservation laws hold for the concentrations. The idea is to enlarge the space of n partial concentrations by adding the total concentration, viewed as an independent variable, thus working with $n + 1$ variables. Further results concern the existence of global bounded weak solutions to the parabolic system and an extension of the results to complex-balance systems.

[1] E. S. Daus, A. Jüngel, B. Q. Tang, *Exponential time decay of solutions to reaction-cross-diffusion systems of Maxwell-Stefan type*, Arch. Ration. Mech. Anal. **235** (2020), no. 2, 1059–1104.

Dennis Trautwein (Universität Regensburg, Germany)

Existence and approximation of a viscoelastic Cahn–Hilliard model for tumour growth

In this talk, we consider a macroscopic model for tumour growth in which cell-cell adhesion effects are taken into account with the help of a Ginzburg–Landau type energy. The resulting evolution is given by a Cahn–Hilliard equation with source and sink terms. Moreover, nutrient diffusion is included by a coupling to a reaction-diffusion equation. The system is coupled to an internal non-solenoidal velocity field which solves a viscoelastic system. It is well-known that the invasive potential of tumours can be enhanced by mechanical forces, as in particular the movement and growth of tumour cell aggregates can be directed by mechanical effects. Moreover, a lack of nutrients can favour chemotaxis which in general describes the movement along the gradient of a chemical species like nutrients. To include both phenomena in our model, we consider specific energy densities that are coupled to the phase-field variable, which results in cross-diffusion terms in the Cahn–Hilliard equation. For the full model, we present the numerical approximation with a fully-practical, stable and converging finite element scheme in two and three space dimensions, which preserves the physical properties of the model. Here, we introduce new approximations of some specific terms in the system with the goal to mimic an energy identity on the fully-discrete level. As the discretization parameters tend to zero, we pass to the limit in the numerical scheme and show (subsequence) convergence towards a global-in-time weak solution in two and three space dimensions. Finally, we illustrate the practicability of the discrete scheme with the help of numerical simulations.

Ewelina Zatorska (Imperial College London, United Kingdom)

Two-phase flows: challenges and insights

I will present two-phase flows, explaining their differences from mixtures and addressing the complexities they bring. I will then focus on analysis of the two-phase flow model under the algebraic pressure closure.

Throughout the talk, I will summarize key findings, including existence of global weak solutions, their regularity, uniqueness (or lack thereof), and conditional weak-strong uniqueness. I will also discuss the challenges we face in improving this conditional uniqueness result.

4 List of Participants

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	Wednesday, 13.09.2023	Thursday, 14.09.2023	Friday, 15.09.2023
08:30	Registration (35 min)		
09:05	Opening (10 min)		
09:15	Bulíček (45+5 min)	Christoforou (45+5 min)	Świerczewska-Gwiazda (45+5 min)
10:05	Pokorný (15+5 min)	Chiarello (15+5 min)	Rossi (15+5 min)
10:25	Coffee Break (35min)	Coffee Break (35min)	Coffee Break (35min)
11:00	Zatorska (45+5 min)	Giovangigli (45+5 min)	Lasarzik (45+5 min)
11:50	Ogorzały (15+5 min)	Liu (15+5 min)	Landstorfer (15+5 min)
12:10	Lunch Break (1,5h)	Lunch Break (1,5h)	Closing and Get Together
13:40	Fischer (45+5 min)	Perthame (45+5 min)	
14:30	Georgiadis (15+5 min)	Trautwein (15+5 min)	
14:50	Tang (15+5 min)	Hurm (15+5 min)	
15:10	Coffee Break (35min)	Coffee Break (35min)	
15:45	Ehrlacher (45+5 min)	Fellner (45+5 min)	
16:35	Cauvin-Vila (15+5 min)	Massimini (15+5 min)	
16:55			
17:00	Poster Session (60 min)	Coffee & Discussion (60 min)	
18:00			
18:30		Dinner (3,5 h)	