1.6 Thematic Einstein Semester "Energy-Based Mathematical Methods for Reactive Multiphase Flows"

Matthias Liero, Alexander Mielke, Dirk Peschka, Marita Thomas, and Barbara Wagner

Research thrives on scientific exchange and discussion. To foster communication between different groups of mathematicians and to develop new ideas and topics, the Berlin Mathematics Research Center MATH$^+$ created *Thematic Einstein Semesters*, funded by the Einstein Foundation Berlin. This program usually runs for one semester and is organized by members of the MATH$^+$ faculty, Postdocs, Ph.D. students, as well as external colleagues from mathematics or other fields. The main goal of the Thematic Einstein Semesters is to initiate subsequent activities, such as new research collaborations between seemingly distant mathematical fields, the generation of novel research ideas that provide a basis for a potential new *Emerging Field* within MATH$^+$, or an external project proposal such as DFG *Research Training Groups* or projects with industry.

The Thematic Einstein Semester *Energy-Based Mathematical Methods for Reactive Multiphase Flows* in the winter term 2020/2021 is the fourth in the series and planning began with the proposal in February 2019. As the coronavirus pandemic worsened in 2020, the original concept was gradually transformed from an on-site event to a hybrid event, and finally to the following online events:

- Student Compact Course "Variational Methods for Fluids and Solids", October 12–23, 2020,
- Kick-Off Conference "Energy-Based Mathematical Methods for Reactive Multiphase Flows", October 26–30, 2020,
- Workshop "Mathematical Analysis for Mechanics (MA4M)", November 23–25, 2020,
- Weekly Seminar "Energy-Based Mathematical Methods and Thermodynamics",
- Final Conference "Structures in Evolution – Theory and Applications", February 23–25, 2021.

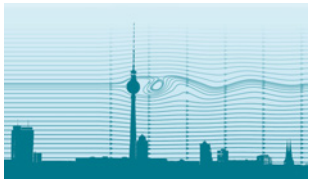


Fig. 1: *The Thematic Einstein Semester was jointly organized by Matthias Liero, Volker Mehrmann, Alexander Mielke, Dirk Peschka, Marita Thomas, and Barbara Wagner*

Since the early works of Lagrange and Hamilton for classical mechanics and Rayleigh and Helmholtz for dissipative processes, energetic variational methods for fluids and solids have been developed extensively. The relation to underlying microscopic stochastic models was pioneered by Onsager, leading to his celebrated reciprocal relations. However, most systematic developments concerned either purely conservative Hamiltonian systems or purely dissipative gradient systems. In the last two decades, a unification of these two extremes was addressed by developing frameworks for combining both conservative and dissipative dynamics. More recently, these topics evolved into mathematical theories such as GENERIC (*General Equations for Non-Equilibrium Reversible Irreversible Coupling*) and port-Hamiltonian structures.

Over the last decades, different communities have developed own languages and specific mathematical methods that are not always accessible to outsiders. Thus, the central aim of this Thematic Einstein Semester was to bring together scientists from different communities and to develop synergies between the different approaches and to contribute to the structural analysis of complex problems in materials science.

Topics and trends of the Thematic Einstein Semester

Applied mathematics in Berlin and especially at the Weierstrass Institute has a long tradition of linking application-oriented modeling with fundamental mathematical research. Mathematical modeling is a cornerstone of applied and interdisciplinary research with scientific and industrial partners and is prominent in the WIAS application areas *Flow and Transport*, *Materials Modeling*, *Nano- and Optoelectronics*, and *Quantitative Biomedicine*. In the Thematic Einstein Semester, we have seen contributions related to applications in thermohydrodynamics, magnetohydrodynamics, electrochemistry, hydrogels, suspensions, and granular media in the context of engineering, biological, physical, and geophysical applications. In particular, for complex coupled systems, the extension to interface thermodynamics was identified as an important research task. Variational modeling and the further development of corresponding mathematical analysis will also enable us in the future to build a bridge for mathematics to new scientific applications in these exciting topics.

The contributions and lectures in the Thematic Einstein Semester showed that the following topics will be most relevant in the context of energetic variational mathematical methods:

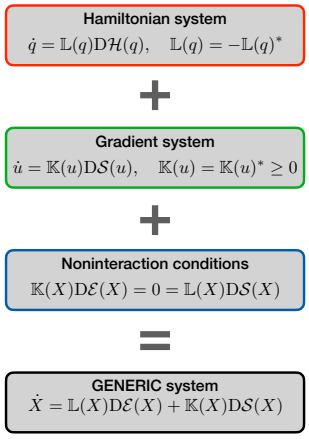
- Variational approaches are regarded as advantageous to investigate model hierarchies, scaling limits, and problems with different spatial or temporal scales. While the last point has been treated mathematically rigorously for gradient flows, corresponding results for Hamiltonian, damped Hamiltonian, port-Hamiltonian, and GENERIC systems have yet to be established.
- To put the formal beauty of variational structures into practice, many researchers investigate how to exploit them for rigorous mathematical analysis and how to develop structure-preserving space- and time-discretization schemes for the corresponding partial differential equations (see Figures 2 and 3).
- Control and optimization, inclusion of constraints, parameter identification, and aspects of Big Data are obviously relevant and hot topics in the context of materials modeling.
- While modeling often focuses on the important aspect of consistently coupling physical, chemical, or biological effects, the issue of bulk-interface coupling and the framework for considering open versus closed systems are usually neglected but imperative for realistic materials.

In the following, some WIAS specific aspects of the Einstein Semester are presented.

Energetic variational modeling approaches. The GENERIC framework was introduced by Grmela & Öttinger (1997) to combine reversible (Hamiltonian) dynamics, obtained via a skew-symmetric Poisson operator $\mathbb{L} = -\mathbb{L}^*$ and an energy functional $\mathcal{E}$, and irreversible (gradient) dynamics, obtained via a symmetric Onsager operator $\mathbb{K} = \mathbb{K}^* \geq 0$ and an entropy functional $\mathcal{S}$. Denoting by $X \in \mathcal{X}$ the state, the abstract evolution equation for the GENERIC system $(\mathcal{X}, \mathcal{E}, \mathcal{S}, \mathbb{L}, \mathbb{K})$ reads

$$\dot{X} = \mathbb{L}(X)\mathrm{D}\mathcal{E}(X) + \mathbb{K}(X)\mathrm{D}\mathcal{S}(X).$$

While the skew-symmetric operator induces a Poisson bracket $\{\cdot,\cdot\}_{\mathbb{L}}$, the symmetric and positive (semi-)definite operator induces a gradient structure with $\nabla_{\mathbb{K}}\mathcal{S} = \mathbb{K}\mathrm{D}\mathcal{S}$, defining the gradient of $\mathcal{S}$. The central additional assumptions of the GENERIC framework are the noninteraction conditions $\mathbb{L}\mathrm{D}\mathcal{S} \equiv 0$ and $\mathbb{K}\mathrm{D}\mathcal{E} \equiv 0$ that imply conservation of total energy and a nonnegative entropy



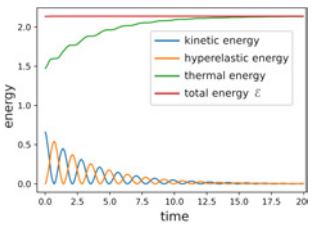


Fig. 2: *Evolution of energy $\mathcal{E} = \mathcal{E}_{kin} + \mathcal{E}_{elast} + \mathcal{E}_{therm}$ for a closed thermo-visco-elastic system shows energy conservation and increasing thermal energy over time*

production, i.e., $\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E}(X(t)) = 0$ and $\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{S}(X(t)) \geq 0$, as shown in Figure 2. Additional modeling concepts that were discussed during the Einstein Semester are port-Hamiltonian systems, gradient flows, Hamiltonian structures, Lagrangian approaches, and classical nonequilibrium thermodynamics.

Currently, at WIAS the research groups RG 1 *Partial Differential Equations*, RG 3 *Numerical Mathematics and Scientific Computing*, RG 4 *Nonlinear Optimization and Inverse Problems*, RG 7 *Thermodynamic Modeling and Analysis of Phase Transitions*, RG 8 *Nonsmooth Variational Problems and Operator Equations*, and WG 1 *Modeling, Analysis and Scaling Limits for for Bulk-Interface Processes* are actively working on coupling continuum mechanics of fluids and solids with the smooth and nonsmooth evolution of state variables such as entropy (thermal effects), concentrations (phase transitions), phase fields (damage or plasticity), and vectors or tensors (anisotropy, electromagnetism). Continuum models coupling thermal effects and elasticity with GENERIC are based on a description using the state $X = (\mathbf{u}, \mathbf{p}, s, z)$ representing displacement $\mathbf{u}$, linear momentum $\mathbf{p}$, entropy s, and further variables z to describe inelastic effects. For this one writes the Hamiltonian and entropy of the system as

$$\mathcal{E}(X) = \int_\Omega \frac{1}{2\varrho}|\mathbf{p}|^2 + U(\mathbf{u}, \nabla\mathbf{u}, s, z)\,\mathrm{d}x, \qquad \mathcal{S}(X) = \int_\Omega s\,\mathrm{d}x,$$

where the internal energy U features a thermal and a hyperelastic energy contribution, and additional coupling to the internal variable; see Figure 3. Depending on the material system, different choices of the internal energy are possible and can also be derived from the underlying statistical interpretation. In a Lagrangian description, for functionals $\mathcal{F}(X) = \int F\,\mathrm{d}x$ and $\mathcal{G}(X) = \int G\,\mathrm{d}x$ the corresponding Poisson structure can, not always, but often be considered to have the simple form

$$\{\mathcal{F}, \mathcal{G}\}_{\mathbb{L}}(X) = \langle \mathrm{D}\mathcal{F}(X), \mathbb{L}(X)\mathrm{D}\mathcal{G}(X)\rangle = \int_\Omega \sum_{i=1}^{d} \left(\frac{\delta F}{\delta \mathbf{u}_i}\frac{\delta G}{\delta \mathbf{p}_i} - \frac{\delta G}{\delta \mathbf{u}_i}\frac{\delta F}{\delta \mathbf{p}_i}\right)\mathrm{d}x$$

to satisfy the noninteraction condition. Thus, most of the nontrivial structure of coupled multiphysics descriptions for continuum mechanics is incorporated in the noninteraction conditions and in the irreversible operator $\mathbb{K}(X)$. While it is far from obvious how this can be done, in the past it has been well studied how different choices of $\mathbb{K}(X)$ generate mass-action-type reactions, diffusion, heat conduction, internal mechanical dissipation, and corresponding cross-coupling effects. More recent research has shown different ways to add further complexity to the range of GENERIC models studied at WIAS. For example, operators of the form

$$\langle \eta, \mathbb{K}(X)\eta\rangle = \int_\Omega a(X)\nabla\eta\cdot\nabla\eta\,\mathrm{d}x + \int_\Gamma b(X)|\eta|^2\,\mathrm{d}s$$

give rise to certain force balances on interfaces and similarly at contact lines. In order to explain normal pressures observed in mixtures of liquids with solid particles (suspensions), the Onsager operator $\mathbb{K}$ is replaced with the subdifferential of the nonsmooth dual dissipation potential

$$\mathcal{R}^*(X, \eta) = \int_\Omega W(X, \eta, \nabla\eta)\,\mathrm{d}x, \qquad W(X, y, \mathbf{z}) = \mu(X)\,|\mathbf{z}|^2 + \gamma(X)\,|\mathrm{tr}(\mathbf{z})|\,|\mathbf{z}| + M(X)|y|^2.$$

Similar ideas are currently extended to material systems spanning the whole range from soft matter to living materials, such as for models of hydrogels. The latter have been developed in RG 7

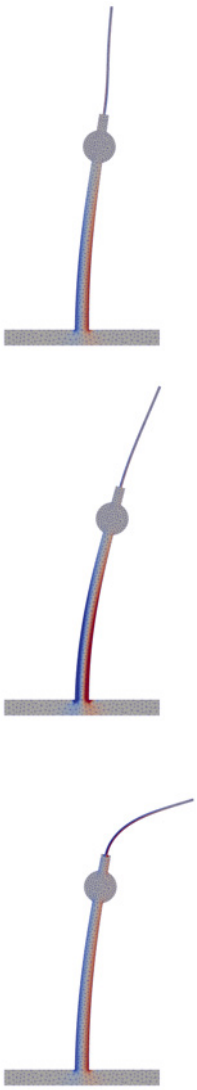


Fig. 3: *Evolution of deformation (mesh) and density (shading) using structure-preserving discretization of damped-Hamiltonian visco-elasto-dynamics. The numerical scheme was extended to GENERIC in a student project.*

and open the door to a multitude of biomedical applications such as tissue regeneration, or the development of biologically inspired materials. Furthermore, a central topic in cellular biology is mean-field material models that describe fundamental biological processes such as liquid-liquid phase separation to model the formation of subcellular structures, e.g., organelles. In the Einstein Semester, we saw many contributions related to variational modeling of complex material systems.

Multiscale problems and variational methods. Solutions of nonlinear partial differential equations often exhibit oscillations and concentration effects on multiple temporal or spatial scales; see, e.g., Figure 4. Let us consider a family of evolution equations $\dot{u}_\varepsilon = \mathcal{V}_\varepsilon(u_\varepsilon)$, where $\varepsilon > 0$ is a small parameter arising as the ratio between macro- and microscopic scales. A central question is the derivation of effective equations on the macroscale that fully take into account the effects on the microscale such that a limit u_0 of solutions u_ε satisfies the effective model $\dot{u}_0 = \mathcal{V}_0(u_0)$. If the evolution equations additionally have a geometric structure, e.g., via Hamiltonian, gradient, or GENERIC systems, it is natural to ask for a suitable notion of convergence of the systems to an effective limit system, thus providing additional information about the effective equation.

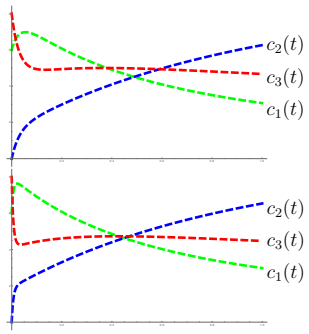


Fig. 4: *Solution behavior of a fast-slow reaction system* $\dot{\mathbf{c}} = \mathbf{R}_{slow} + \frac{1}{\varepsilon}\mathbf{R}_{fast}$ *for* $\varepsilon = 1$ *(top) and* $\varepsilon = 0.2$ *(bottom). Effective evolution is derived via EDP convergence.*

In particular, for generalized gradient systems the evolution is described in terms of two functionals, namely the energy functional $\mathcal{E}_\varepsilon$ and the dissipation potential $\mathcal{R}_\varepsilon$. Then, the evolution can be written in the doubly nonlinear form $\partial_{\dot{u}}\mathcal{R}_\varepsilon(u,\dot{u}) + \mathrm{D}\mathcal{E}_\varepsilon(u) \ni 0$. However, using the Legendre–Fenchel equivalences and the chain rule $\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E}_\varepsilon(u(t)) = \langle \mathrm{D}\mathcal{E}_\varepsilon(u(t)), \dot{u}(t)\rangle$, we arrive at an equivalent formulation of the evolution via the so-called *energy-dissipation principle* (EDP)

$$\forall\, t > 0: \qquad \mathcal{E}_\varepsilon(u_\varepsilon(t)) + \int_0^t \Big\{\mathcal{R}_\varepsilon(u_\varepsilon;\dot{u}_\varepsilon) + \mathcal{R}_\varepsilon^*\big(u;-\mathrm{D}\mathcal{E}_\varepsilon(u_\varepsilon)\big)\Big\}\mathrm{d}\tau = \mathcal{E}_\varepsilon(u_\varepsilon(0)).$$

Since this scalar equation is written entirely in terms of functionals, Γ-convergence can be used. Naively, one would hope that Γ-limits of the functionals give rise to an effective gradient system for the limit problem. While this is true in many examples, there are problems with nontrivial interaction between energy and dissipation. Indeed, Dondl, Frenzel, and Mielke (2019) showed that for wiggly energies of the form $\mathcal{E}_\varepsilon(u) = \Phi(u) + \varepsilon A\cos(u/\varepsilon)$, the microscopic fluctuations in $\mathcal{E}_\varepsilon$ "survive" in an effective dissipation potential $\mathcal{R}_{\mathrm{eff}}$ that satisfies $\mathcal{R}_{\mathrm{eff}} \neq \Gamma\text{-}\lim \mathcal{R}_\varepsilon$; see Figure 5.

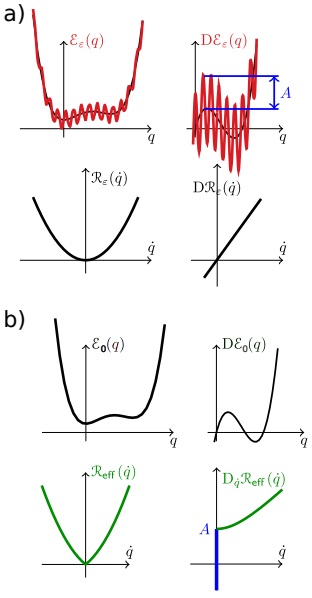


Fig. 5: *Derivation of an effective wiggly-energy model. Microscopic fluctuations from energy in a) survive in effective (nonsmooth) dissipation potential in b).*

Several notions of EDP convergence were introduced to better characterize this behavior: The *simple EDP convergence* demands Γ-convergence of $\mathcal{E}_\varepsilon$ and of the dissipation functionals $\mathcal{M}_\varepsilon(u) = \int_0^T \mathcal{R}_\varepsilon(u,\dot{u}) + \mathcal{R}_\varepsilon^*(u,-\mathrm{D}\mathcal{E}_\varepsilon(u))\,\mathrm{d}t$ to $\mathcal{E}_0$ and $\mathcal{M}_0$, where the latter must have the same form $\mathcal{M}_0(u) = \int_0^T \mathcal{R}_{\mathrm{eff}} \oplus \mathcal{R}_{\mathrm{eff}}^*\mathrm{d}t$. However, simple EDP convergence is often unsatisfactory as the effective limit $\mathcal{R}_{\mathrm{eff}}$ may depend on more than the microscopic behavior of the energy functionals $\mathcal{E}_\varepsilon$ that disappears in their macroscopic limit. Thus, the effective energy and dissipation functional are not truly independent of each other. To solve this problem, the notion of *tilted EDP convergence* was introduced, where modified energy functionals $\mathcal{E}_\varepsilon^\eta(u) = \mathcal{E}_\varepsilon(u) - \langle \eta, u\rangle$ and modified total dissipation functionals $\mathcal{M}_\varepsilon^\eta(u) = \int_0^T \mathcal{R}_\varepsilon(u,\dot{u}) + \mathcal{R}_\varepsilon(u,-\mathrm{D}\mathcal{E}_\varepsilon(u)+\eta)\,\mathrm{d}t$ with arbitrary "tilts" η are considered. The crucial condition is that the Γ-limit of $\mathcal{M}_\varepsilon^\eta(u)$ is independent of η with an integrand $\mathcal{N}_0(u,\dot{u},\eta)$, and an effective dual dissipation potential $\mathcal{R}_{\mathrm{eff}}^*(u,\xi) = \mathcal{N}_0(u,0,\xi+\mathrm{D}\mathcal{E}_0(u))$ can be found. However, it turns out that the notion of tilted EDP convergence is too strong and many interesting examples are excluded. This issue is resolved in *contact EDP convergence*, which

requires only that $\mathcal{R}_{\text{eff}}$ satisfies

$$\mathcal{R}_{\text{eff}}(u,v)+\mathcal{R}^*_{\text{eff}}(u,\xi)=\langle \xi, v\rangle \qquad \Leftrightarrow \qquad \mathcal{N}_0(u,v,\xi+\mathrm{D}\mathcal{E}_0(u))=\langle \xi, v\rangle.$$

The benefit of the intermediate concept of contact-EDP convergence lies in the combination of tilting, which allows the convergence of $\mathcal{M}_\varepsilon$ to roam over all of $(\dot{u},\xi)$ space, and the restriction to the contact set. Thus, the connection between $\mathcal{N}_0$ and $\mathcal{R}_{\text{eff}}$ is reduced to the case of contact, i.e., the kinetic relation $\xi \in \partial_{\dot{u}}\mathcal{R}_{\text{eff}}(u,\dot{u})$. Many interesting multiscale problems in connection to the various notions of EDP convergence were discussed during the Thematic Einstein Semester, ranging from slow-fast reactions to diffusion problems in thin structures to the discrete-to-continuous passage.

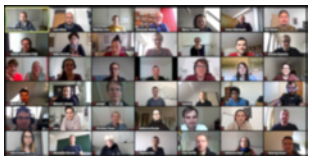


Fig. 6: *40–70 participants joined energetic interactive discussions during Zoom presentations, break-out sessions and round-table discussions*

Thematic Einstein Semester: Online. The activities of the Thematic Einstein Semester were organized with different goals and audiences in mind. The focus was on the involvement of students in the semester and the further development of energetic variational mathematical methods in the context of applications. All online events were designed to create plenty of opportunities for interaction. Before the semester, we looked into different platforms to support online conferencing: The key criteria were data protection, user-friendliness, reliability, and scalability. With these aspects in mind, we compared BigBlueButton, Zoom, Jitsi, Remo, and ultimately found Zoom with customized settings the best compromise. We also tested, but then decided against Zoom Webinars, so that participants could better interact with each other. In addition to the public website, we used the platform Zulip for registered participants to distribute up-to-date sensitive information (Zoom links, lecture notes, and recordings) and to initiate further discussions. The platform was used by 40–60 of about 140 registered users on a daily basis during the following main events:

The two-week course *Variational Methods for Fluids and Solids* (October 12–23) was organized in collaboration with the DFG Collaborative Research Center SFB 1114 *Scaling Cascades in Complex Systems* for undergraduate and graduate students interested in mathematical aspects of energetic approaches. These topics were covered in daily mini-courses given by invited external speakers and by the organizers of the program. Longer breaks between lectures allowed students to discuss with the lecturers in break-out rooms. All the lectures were recorded and made available together with lecture notes on Zulip. Of the 109 registered participants (mostly students) from 14 countries, 81 were from Germany, 52 were from Berlin, and 34 were female. About 40–70 people followed the lectures each day.

The *Kick-Off Conference* (October 26–30) targeted experienced researchers and students. Complementing the usual discussion after talks, there were extensive discussions in break-out rooms. As additional elements of an online conference, the program also included round-table discussions, online polls, and poster-style parallel discussions. While the round-table discussions turned out to be driven by experienced researchers, there were many insights to be gained for younger participants. The parallel poster session is a flexible format suited for technical discussions. Most talks of the conference were recorded and made available to participants during the time of the conference. The conference had 148 registered participants from 13 countries, with 40–70 people attending on a daily basis. From these, 96 participants were from Germany, 63 were from Berlin, 31 were female, 36 were students. Parts of the program were in cooperation with the DFG Collaborative Research Center SFB 910 *Control of Self-organizing Nonlinear Systems: Theoretical Methods and Concepts of Application*.

Conclusion and Outlook

The various events and the involvement of the Berlin Collaborative Research Centers, MATH$^+$, universities, and research institutes with over 320 local and international participants resulted in an inclusive event with the potential for many new collaborations in applied mathematics and interdisciplinary research. In particular, research on novel materials, scaling limits, bulk-interface coupling, and structure-preserving discretizations could be identified as hot topics. Despite all difficulties caused by the coronavirus, the Thematic Einstein Semester was a great success and contributed to the scientific discourse in these difficult times.