Energetic Variational Approach – Modeling, Analysis, and Computation

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Project Description

This project focuses on the *Energetic Variational Approach* (EnVarA) [1], a unified framework that combines the *Least Action Principle* (LAP) and the *Maximum Dissipation Principle* (MDP). By integrating conservative and dissipative forces under fundamental thermodynamic laws, EnVarA provides a robust methodology to derive governing equations for a wide range of physical systems, including complex fluids [2], solids, multi-phase flows, chemical reactions, and tumor growth.

Core Ideas. In EnVarA, the total energy—often composed of kinetic and free energy—is balanced by a dissipation functional. The approach derives forces through:

- *Least Action Principle (LAP)* for inertial and conservative forces.
- *Maximum Dissipation Principle (MDP)* for dissipative forces.

A concise form of these governing laws is:

$$\frac{d}{dt}(K+F) = -\mathcal{D}, \quad f_{\text{inertial}} = f_{\text{conservative}} + f_{\text{dissipative}},$$

where K is kinetic energy, F is the free energy, and $\mathcal{D}$ is the dissipation.

Chemical Reactions within EnVarA. An exciting new direction is the application of EnVarA to chemical reactions [3]. By introducing a *reaction trajectory* that tracks the progress of each reaction, one can construct a suitable free energy $\mathcal{F}$ and a dissipation functional $\mathcal{D}_{\text{chem}}$ associated with chemical transformations. This leads to an energy-dissipation law

$$\frac{d}{dt}\mathcal{F} \;=\; -\,\mathcal{D}_{\text{chem}},$$

where the reaction rate emerges naturally from a *force balance* condition, akin to mechanical systems. Importantly, this formulation recovers the classical *law of mass action* under near-equilibrium conditions, yet it also accommodates more general (non-quadratic) dissipation far from equilibrium. The same approach can be extended to *reaction-diffusion* equations, and in this project, we aim to explore how it can be further combined with other physical processes (e.g., ion transport, phase-field models) into one unified variational framework.

Modeling and Applications. Participants in this program will learn:

- How to derive governing equations consistent with thermodynamics for classical fluids, solids, and coupled chemo-mechanical systems.
- How EnVarA underpins multi-phase flow models, elasticity, reaction-diffusion systems, and more.
- Numerical methods and basic mathematical analysis to solve and investigate these systems.

Prerequisites. A strong background in Calculus, Linear Algebra, and Differential Equations, along with basic programming (e.g., MATLAB), is highly recommended. Familiarity with thermodynamics, variational principles, and numerical methods for differential equations will be beneficial.

Plan

- Introduction: Historical background, variational methods, LAP, and MDP.
- Modeling classical systems: Newtonian fluids, elastic solids, and viscoelasticity.
- Applications to complex systems: Diffusive interfaces and multi-phase dynamics.
- Extension to chemical reactions: Reaction-diffusion systems, coupling with ion transport and phase-field models.
- Numerical methods: Discretization and implementation of EnVarA-based models.
- Advanced topics: Real-world applications and computational challenges.

Teaching Assistant

A Teaching Assistant (TA) will be appointed to enhance student-mentor communication and support. The TA will assist with technical questions and computational tasks and lead discussion sessions. The appointment is to be announced before the program begins.

Objectives

By the end of this program, participants will:

- Understand the derivation of governing equations using EnVarA for fluids, solids, and chemical reactions.
- Gain computational and analytical skills to study reaction-diffusion problems under the EnVarA framework.
- Investigate chemo-mechanical coupling (e.g., ion transport, phase-field models) by extending EnVarA to multi-physics settings.
- Explore practical applications in multi-phase systems, complex fluids, and beyond.

Pre-program Reading Materials

Participants are encouraged to review the following materials before the program begins:

Continuum Mechanics and PDE Modeling
Harald Garcke et al., *Mathematical Modeling* [4], Ch. 5-7.
Focus: Basics of Continuum Mechanics, Reaction-diffusion and Cahn-Hilliard equations.

Analysis of Nonlinear PDEs
Juan Luis Vázquez, *The Porous Medium Equation: Mathematical Theory* [5], Ch. 1-4.
Focus: Analytical properties of PME solutions.

Computational PDEs
R.M.M. Mattheij et al., *Partial Differential Equations: Modeling, Analysis, Computation* [6], Ch. 10-11.
Focus: Numerical methods for parabolic PDEs.

Jie Shen, Tao Tang, Li-Lian Wang, *Spectral Methods: Algorithms, Analysis and Applications* [7], Ch. 1-2.
Focus: Theory of spectral methods.

Lloyd N. Trefethen, *Spectral Methods in MATLAB* [8], Ch. 1-4.
Focus: Implementation of spectral methods.

Participants should focus on understanding fundamental concepts rather than mastering all details.

References

[1] M.-H. Giga, A. Kirshtein, and C. Liu. Variational modeling and complex fluids. In Y. Giga and A. Novotny, editors, *Handbook of Mathematical Analysis in Mechanics of Viscous Fluids*, pages 73–113. Springer, 2017. URL: https://link.springer.com/referenceworkentry/10.1007/978-3-319-13344-7_2.

[2] J. Forster. Mathematical modeling of complex fluids. Master's thesis, Universität Würzburg, 2013. URL: https://d-nb.info/110280567X/34.

[3] Y. Wang and C. Liu. Some recent advances in energetic variational approaches. *Entropy*, 24(5):721, 2022. URL: https://www.mdpi.com/1099-4300/24/5/721, doi:10.3390/e24050721.

[4] Harald Garcke, Kei Fong Lam, and Emanuel Sitka. *Mathematical Modeling*. Springer, 2017. doi:10.1007/978-3-319-55942-3.

[5] Juan Luis Vázquez. *The Porous Medium Equation: Mathematical Theory*. Oxford Mathematical Monographs. Oxford University Press, 2007. doi:10.1093/acprof:oso/9780198569039.001.0001.

[6] Robert M. M. Mattheij, Sjoerd W. Rienstra, and Johannes H. M. ten Thije Boonkkamp. *Partial Differential Equations: Modeling, Analysis, Computation*. SIAM Monographs on Mathematical Modeling and Computation. SIAM: Society for Industrial and Applied Mathematics, 2005. doi:10.1137/1.9780898718270.

[7] Jie Shen, Tao Tang, and Li-Lian Wang. *Spectral Methods: Algorithms, Analysis and Applications*, volume 41 of *Springer Series in Computational Mathematics*. Springer, 2011. doi:10.1007/978-3-540-71041-7.

[8] Lloyd N. Trefethen. *Spectral Methods in MATLAB*, volume 10 of *Software, Environments, and Tools*. SIAM: Society for Industrial and Applied Mathematics, 2000. doi:10.1137/1.9780898719598.