

Methods

Working group Wittkowski

See <https://www.uni-muenster.de/Physik.TP/wittkowski/methods.pdf> for an update.

The following list presents the methods applied or (further) developed in our research as well as our corresponding publications. All citations of publications in the following refer to the list of publications of R.W. that is available at <https://www.uni-muenster.de/Physik.TP/wittkowski/publications.pdf>.

M1. Analytical methods

M1.1. Classical density functional theory

M1.1.1. STATIC DENSITY FUNCTIONAL THEORY (DFT) [[Rp1](#), [Rr1](#), [Rr2](#), [Rr3](#), [A25](#), [A28](#), [A49](#), [A50](#)]

M1.1.2. DYNAMICAL DENSITY FUNCTIONAL THEORY (DDFT) [[Rp1](#), [A1](#), [Rr1](#), [Ri1](#), [Rr2](#), [Rr3](#), [A14](#), [A16](#), [A40](#), [A43](#), [A45](#), [A46](#)]

M1.2. Fokker-Planck equations [[E2](#), [A2](#), [A12](#), [A51](#)]

M1.3. Graph theory [[A6](#)]

M1.4. Hamiltonian twist maps [[A51](#)]

M1.5. Heuristic modeling [[A14](#), [A16](#), [A24](#), [A29](#), [A30](#)]

M1.6. Interaction-expansion method [[E2](#), [E5](#), [A6](#), [A18](#), [A21](#), [A26](#)]

M1.7. Langevin equations [[E2](#), [E5](#), [E7](#), [Rr1](#), [Rr2](#), [Rr3](#), [A2](#), [A5](#), [A6](#), [A11](#), [A12](#), [A18](#), [A19](#), [A21](#), [A22](#), [A26](#), [A27](#), [A29](#), [A30](#), [A32](#), [A33](#), [A34](#), [A35](#), [A36](#), [A42](#), [A44](#), [A47](#)]

M1.8. Liouville equation [[E2](#), [Rr1](#), [Ri1](#), [A12](#), [A23](#), [A40](#), [A43](#), [A51](#)]

M1.9. Machine learning

M1.10. Madelung transformation [[E2](#)]

M1.11. Master equations [[A12](#)]

M1.12. Mode-coupling theory (MCT) [[Rr1](#), [A43](#)]

- M1.13. Mori-Zwanzig projection operator formalism (MZF)** [[Rr1](#), [Ri1](#), [A11](#), [A13](#), [A23](#), [A40](#), [A43](#)]
- M1.14. Multiscale modeling** [[E2](#), [E5](#), [Rp1](#), [A1](#), [Rr1](#), [Ri1](#), [Rr3](#), [A6](#), [A11](#), [A18](#), [A21](#), [A23](#), [A26](#), [A40](#), [A43](#), [A46](#), [A49](#), [A50](#), [A51](#)]
- M1.15. Perturbation expansions** [[A51](#)]
- M1.16. Phase-field (PF) models** [[A37](#)]
- M1.17. Phase-field-crystal (PFC) models** [[Rp1](#), [A1](#), [Rr1](#), [Rr2](#), [Rr3](#), [A13](#), [A24](#), [A41](#), [A46](#), [A48](#), [A49](#), [A50](#)]
- M1.18. Phenomenological modeling** [[A13](#)]
- M1.19. Smoluchowski equations** [[E5](#), [Rp1](#), [Rr1](#), [Rr2](#), [Rr3](#), [A6](#), [A18](#), [A21](#), [A26](#), [A45](#)]
- M1.20. Stability analysis** [[E2](#), [E5](#), [A1](#), [Rr1](#), [A6](#), [A13](#), [A16](#), [A18](#), [A21](#), [A24](#), [A26](#)]
- M1.21. Symmetry-based modeling**
 - M1.21.1. EQUATIONS OF MOTION FROM SYMMETRY CONSIDERATIONS [[A39](#)]
 - M1.21.2. FAR-FROM-EQUILIBRIUM FIELD THEORIES FROM SYMMETRY CONSIDERATIONS [[A31](#), [A37](#)]
 - M1.21.3. GENERALIZED HYDRODYNAMICS [[A49](#), [A50](#)]
 - M1.21.4. GINZBURG-LANDAU APPROACH [[A46](#), [A49](#), [A50](#)]
- M1.22. Wigner functions and Stratonovich-Weyl mapping** [[A12](#), [A15](#)]

M2. Numerical methods

M2.1. Continuum simulations

- M2.1.1. FINITE-DIFFERENCE METHOD (FDM) [[A14](#), [A16](#), [A30](#), [A37](#), [S2](#)]
- M2.1.2. FINITE-ELEMENT METHOD (FEM) [[E3](#), [E4](#), [E6](#), [E7](#), [E8](#), [A3](#), [A7](#), [A8](#), [A10](#), [A17](#), [A24](#), [A41](#), [S4](#)]
- M2.1.3. FINITE-VOLUME METHOD (FVM) [[E3](#), [E4](#), [E6](#), [A3](#), [A7](#), [A8](#), [A10](#), [A17](#)]
- M2.1.4. FREE NUMERICAL MINIMIZATION [[A25](#), [A28](#), [A48](#)]

M2.2. Particle-based simulations

- M2.2.1. BROWNIAN-DYNAMICS (BD) SIMULATIONS [[E5](#), [Rr2](#), [A5](#), [A6](#), [A19](#), [A22](#), [A26](#), [A27](#), [A29](#), [A30](#), [A32](#), [A34](#), [A35](#), [A38](#), [A42](#), [A44](#), [A47](#)]
- M2.2.2. DETERMINISTIC OVERDAMPED DYNAMICS SIMULATIONS [[E7](#), [A9](#), [A39](#)]
- M2.2.3. LANGEVIN-DYNAMICS (LD) SIMULATIONS [[A2](#), [A12](#)]
- M2.2.4. MOLECULAR-DYNAMICS (MD) SIMULATIONS

M2.3. Other numerical methods

- M2.3.1. BEAD-MODEL CALCULATIONS WITHIN LOW-RE HYDRODYNAMICS [[E8](#), [A38](#), [A42](#)]
- M2.3.2. NUMERICAL PATH CONTINUATION [[E2](#), [A1](#)]