Hydrodynamics, Thermodynamics, and Mathematics

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Menu

1. structure of equations
2. example: hydrodynamics
3. solving vs. coarse graining
4. numerical solutions
5. boundary conditions

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1. structure of equations & geometry, implications for solutions
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Thermodynamic admissibility and mathematical well-posedness

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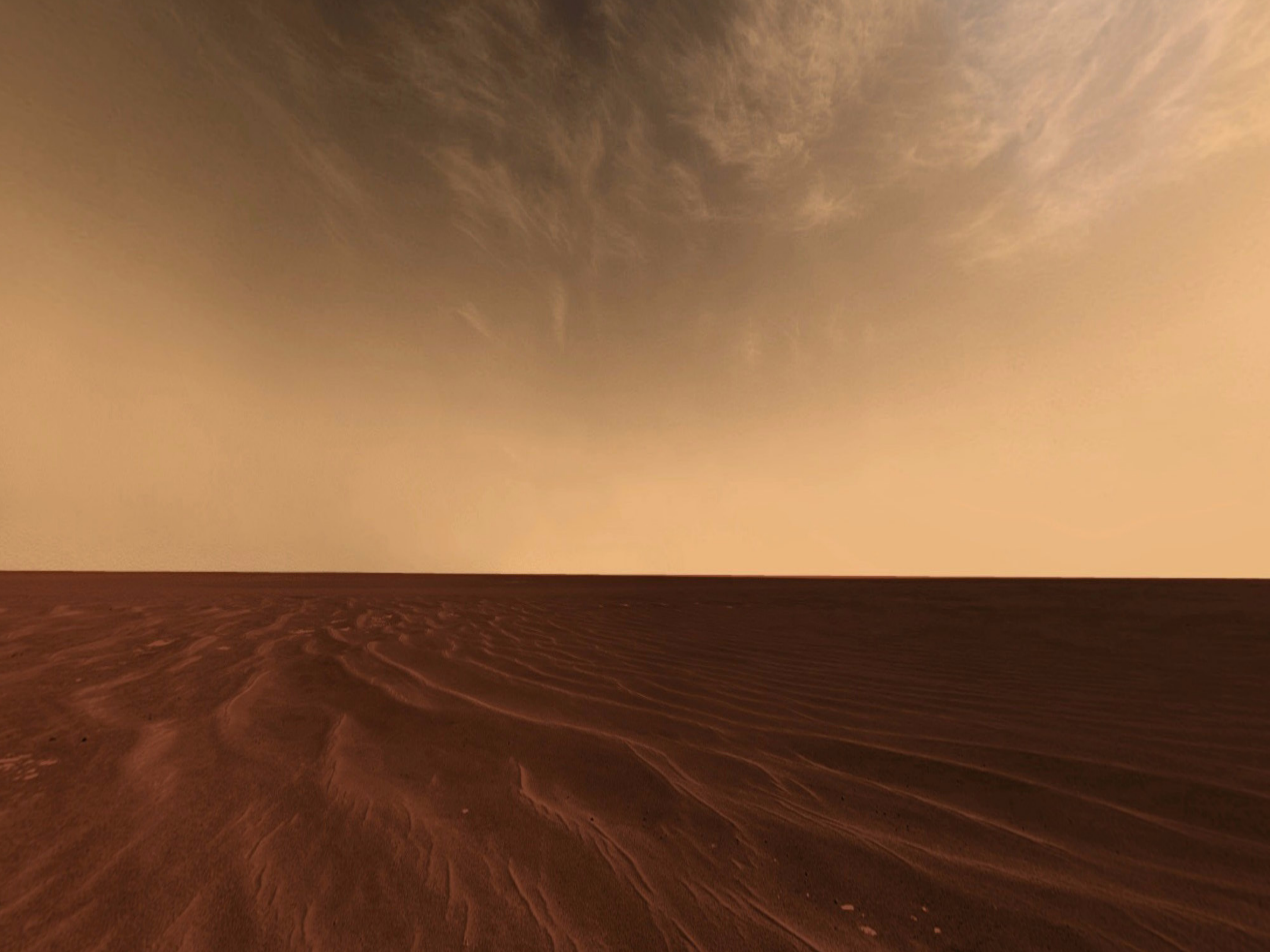

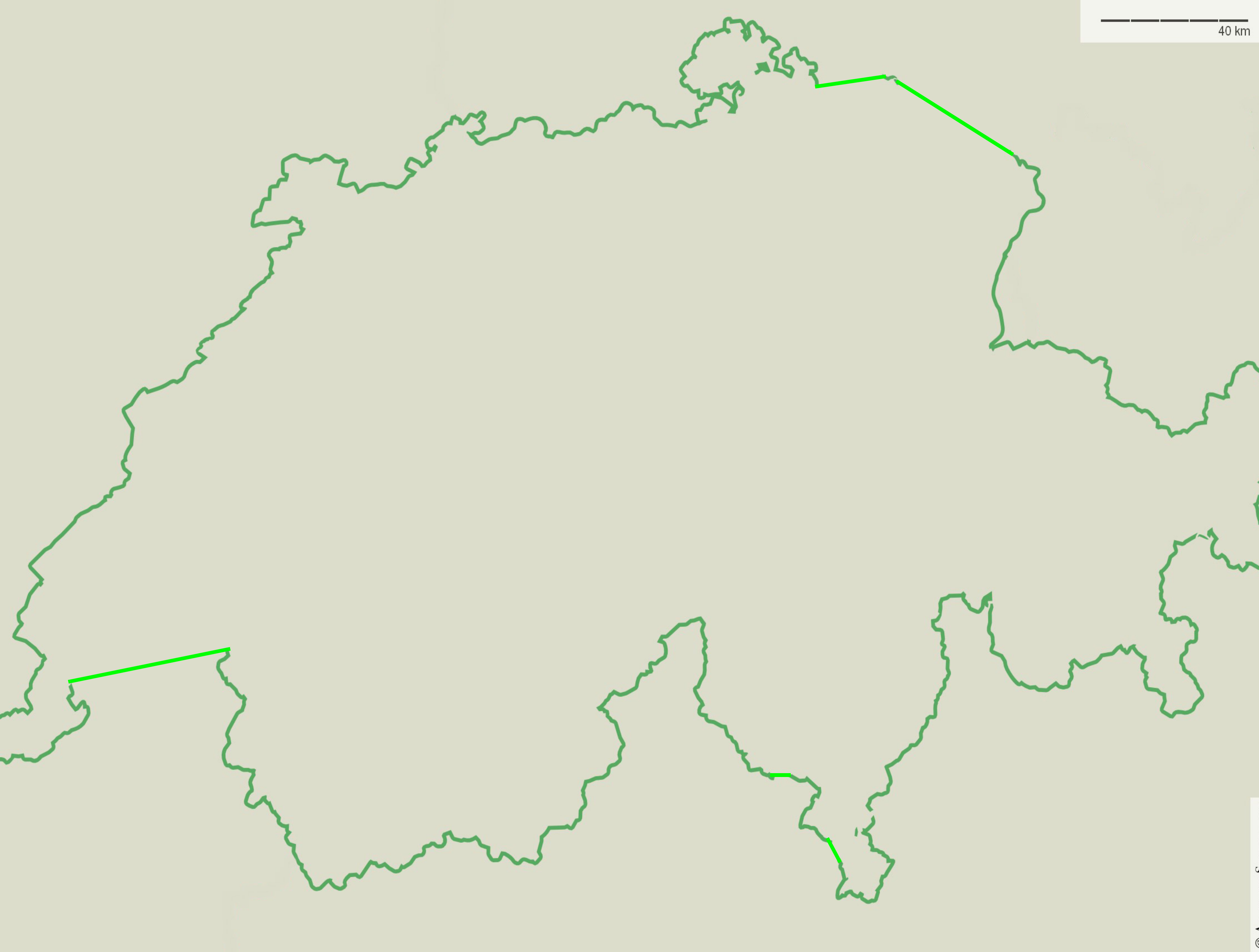
40 km


40 km
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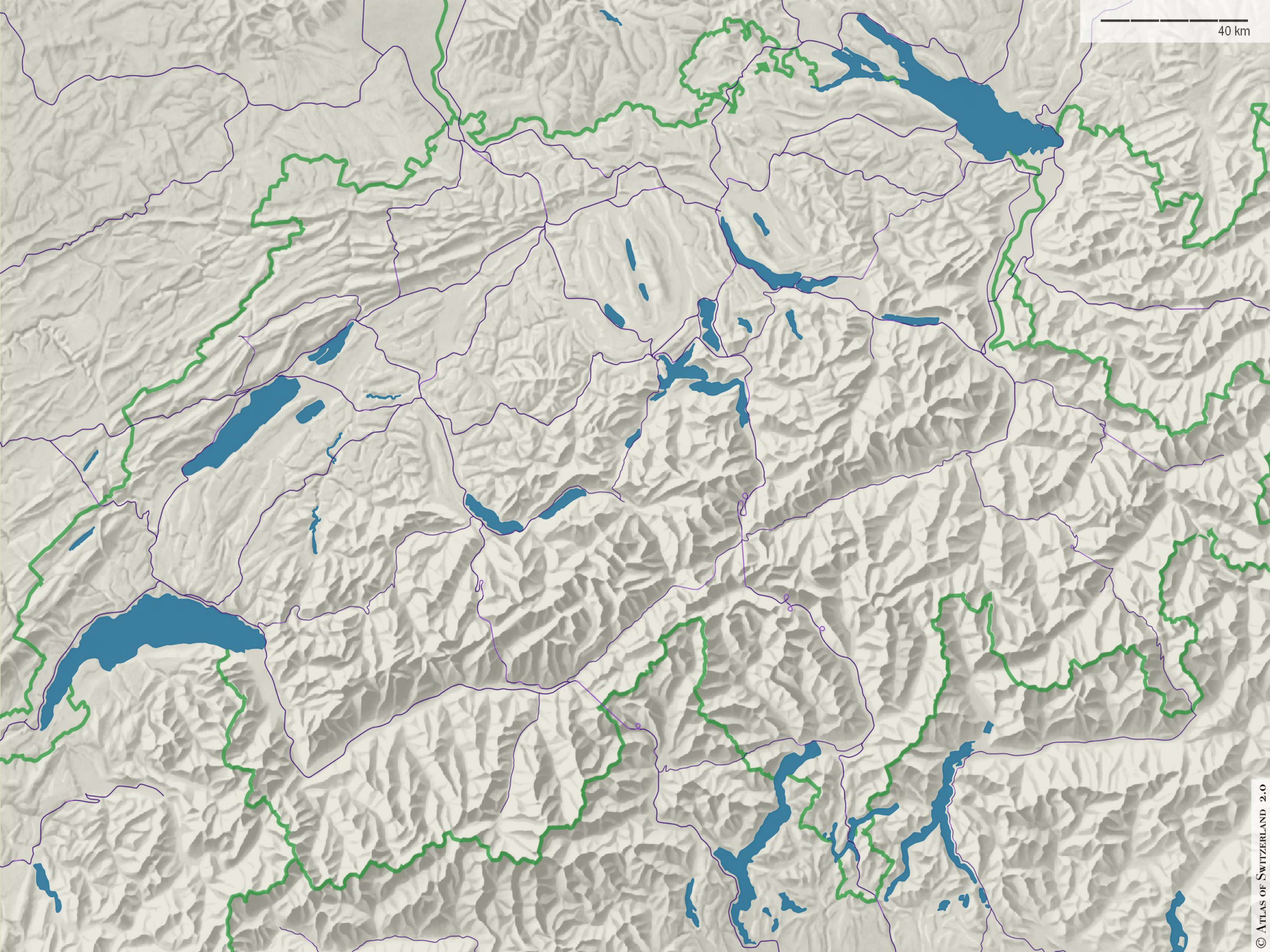
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BikeCam.ch

GENERIC Structure

General equation for the nonequilibrium reversible-irreversible coupling

metriplectic structure (P. J. Morrison, 1986)

$$\frac{dx}{dt} = L(x) \cdot \frac{\delta E(x)}{\delta x} + M(x) \cdot \frac{\delta S(x)}{\delta x}$$

$$L(x) \cdot \frac{\delta S(x)}{\delta x} = 0$$

L antisymmetric, Jacobi identity

$$M(x) \cdot \frac{\delta E(x)}{\delta x} = 0$$

M Onsager/Casimir symm., positive-semidefinite

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Nonequilibrium Thermodynamics

$$(\rho(\boldsymbol{r}),\ \boldsymbol{M}(\boldsymbol{r}),\ \varepsilon(\boldsymbol{r}),\ \text{structural variables})$$

- ρ: mass density
- $\boldsymbol{M}$: momentum density
- ε: internal energy density

balance equations

structured time-evolution equations (GENERIC)

Hydrodynamics

$$E = \int\left[\frac{1}{2}\frac{\boldsymbol{M}(\boldsymbol{r})^2}{\rho(\boldsymbol{r})} + \varepsilon(\boldsymbol{r})\right]d^3r$$

$$S = \int s(\rho(\boldsymbol{r}), \varepsilon(\boldsymbol{r}))d^3r$$

L is associated with the Lie group of space transformations: unique construction by following arguments:

- ρ, s are scalar densities
- $\boldsymbol{M}$ is a (contravariant) vector density

$$M = C \cdot D \cdot C^T$$

- separation of mechanical (C) and thermodynamic (D) effects
- C: well-known for relaxational and transport processes and given E
- D: viscosity, thermal conductivity, and diffusion coefficient

Diffusion in Hydrodynamics

$$C^T = \left[\frac{\partial}{\partial \boldsymbol{r}} \quad \left(\bar{\boldsymbol{v}}\frac{\partial}{\partial \boldsymbol{r}}\right)^T \quad \frac{\partial}{\partial \boldsymbol{r}}\frac{1}{2}\boldsymbol{v}^2 - \bar{\boldsymbol{v}} \cdot \left(\frac{\partial}{\partial \boldsymbol{r}}\boldsymbol{v}\right)^T + \left(\frac{1}{2}\bar{\boldsymbol{v}}^2 + \alpha\right)\frac{\partial}{\partial \boldsymbol{r}}\right]$$

$$\boldsymbol{v} = \frac{\boldsymbol{M}}{\rho}$$

$\bar{\boldsymbol{v}}$ reference velocity (constant)

α constant

Diffusion in Hydrodynamics

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$$\frac{\delta E}{\delta x} = \begin{bmatrix} -\frac{1}{2} \boldsymbol{v}^2 \\ \boldsymbol{v} \\ 1 \end{bmatrix}$$

Hydrodynamic Equations

$$\frac{\partial \rho}{\partial t} = -\frac{\partial}{\partial \boldsymbol{r}} \cdot (\boldsymbol{M} - \boldsymbol{j}\rho)$$

$$\frac{\partial \boldsymbol{M}}{\partial t} = -\frac{\partial}{\partial \boldsymbol{r}} \cdot \left(\frac{1}{\rho}\boldsymbol{M}\boldsymbol{M} - \boldsymbol{j}\rho\bar{\boldsymbol{v}} + p\mathbf{1} + \tau\right)$$

$$\frac{\partial s}{\partial t} = -\frac{\partial}{\partial \boldsymbol{r}} \cdot \left(\frac{1}{\rho}\boldsymbol{M}s + \boldsymbol{j}^s\right) + \text{dissipation}$$

$$\frac{\partial s}{\partial \rho} = -\frac{\mu}{T} \qquad \frac{\partial s}{\partial \varepsilon} = \frac{1}{T}$$

$$\tilde{\mu} = \mu - \frac{1}{2}(\boldsymbol{v} - \bar{\boldsymbol{v}})^2$$

$$\boldsymbol{j} = \frac{D'}{\rho}\left(\frac{\partial}{\partial \boldsymbol{r}}\frac{\tilde{\mu}}{T} - \alpha\frac{\partial}{\partial \boldsymbol{r}}\frac{1}{T}\right)$$

$$\boldsymbol{j}^s = \frac{1}{T}\boldsymbol{j}^q + (\tilde{\mu} - \alpha)\frac{\rho}{T}\boldsymbol{j}$$

Properties of Hydrodynamic Equations

- Momentum density and mass flux are two different quantities.
- Both momentum density and mass flux are conserved quantities.
- The conservation law for the mass flux is equivalent to the conservation law for the booster (expressing center-of-mass motion).
- Angular momentum is a conserved quantity.
- A rigidly rotating fluid is a solution of the hydrodynamic equations.
- Galilean invariance is satisfied.
- A new type of inertial forces occurs in the driving force for diffusion.

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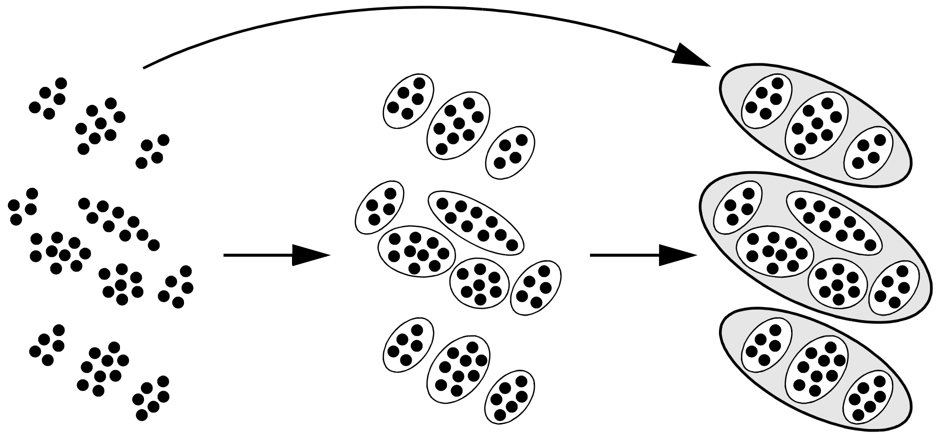
Statistical Mechanics: Entropy



relative entropy

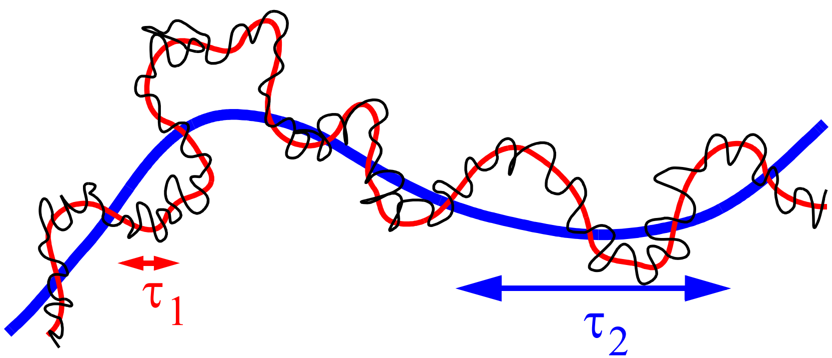
Statistical Mechanics: Friction Matrix

$$M_{jk} = \frac{1}{k_B}\int_0^{\tau} \langle \dot{\Pi}_k^{\mathrm{f}} e^{iL_0 \cancel{Q} t} \dot{\Pi}_j^{\mathrm{f}} \rangle_x \, dt$$ Green-Kubo

$$\langle \Pi_j \rangle_x = x_j$$

$$M_{jk} = \frac{1}{2 k_B \tau} \langle \Delta_\tau \Pi_j \, \Delta_\tau \Pi_k \rangle_x$$ Einstein

cf. $D = \frac{1}{2\Delta t} \langle (\Delta x)^2 \rangle$



Newton's (Hamilton's) equations of motion
or Liouville equation

birth of irreversibility!

Boltzmann's equation

Hilbert
Grad
Chapman-Enskog

more irreversibility?

Hydrodynamics

From Grad's 10-Moment Equations to Navier-Stokes

$$\frac{\partial \rho}{\partial t} = -\frac{\partial}{\partial \boldsymbol{r}} \cdot (\boldsymbol{v}\rho)$$

$$\frac{\partial \boldsymbol{v}}{\partial t} = -\boldsymbol{v} \cdot \frac{\partial}{\partial \boldsymbol{r}}\boldsymbol{v} - \frac{1}{\rho}\frac{\partial}{\partial \boldsymbol{r}} \cdot \pi$$

$$\frac{\partial T}{\partial t} = -\boldsymbol{v} \cdot \frac{\partial}{\partial \boldsymbol{r}} T - \frac{2m}{3\rho k}\pi : \kappa$$

$$\frac{\partial \sigma}{\partial t} = -\frac{\partial}{\partial \boldsymbol{r}} \cdot (\boldsymbol{v}\sigma) - \kappa \cdot \pi - \pi \cdot \kappa^T + \frac{2}{3}\mathbf{1}(\pi : \kappa) - \frac{1}{\tau}\sigma$$

$$\pi = p\mathbf{1} + \sigma$$

$$\kappa = \left(\frac{\partial}{\partial \boldsymbol{r}}\boldsymbol{v}\right)^T$$

Singular perturbation theory:

$$\sigma = -\eta\left[\kappa + \kappa^T - \frac{2}{3}(\mathbf{1} : \kappa)\mathbf{1}\right] \qquad \eta = p\tau$$

MULTISCALE MODEL. SIMUL.
Vol. 6, No. 1, pp. 53–69

THE MATHEMATICAL PROCEDURE OF COARSE GRAINING: FROM GRAD'S TEN-MOMENT EQUATIONS TO HYDRODYNAMICS*

HANS CHRISTIAN ÖTTINGER† AND HENNING STRUCHTRUP‡

Abstract. We employ systematic coarse graining techniques to derive hydrodynamic equations from Grad's ten-moment equations. The coarse graining procedure is designed such that it manifestly preserves the thermodynamic structure of the equations. The relevant thermodynamic structure and the coarse graining recipes suggested by statistical mechanics are described in detail and are illustrated by the example of hydrodynamics. A number of mathematical challenges associated with structure-preserving coarse graining of evolution equations for thermodynamic systems as a generalization of Hamiltonian dynamic systems are presented. Coarse graining is a key step that should always be considered before attempting to solve an equation.

Functional Integrals

For a systematic calculation of the coarse grained hydrodynamic entropy:

$$\Omega(\rho, T) = \int \exp\left\{ \int \frac{\rho}{2m} \ln\det\left(\mathbf{1} + \frac{\sigma}{p} \right) d^3 r \right\} \mathcal{D}\sigma$$

Functional integrals occur most naturally in systematic coarse graining!

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Symplectic Integrators

J. Moser (1968):

$$\frac{dx}{dt} = L \cdot \frac{\delta E_{\Delta t}}{\delta x}$$

reproduces values of integration scheme at times $n\Delta t$

Alternatives:

- canonical transformations in each time step
- Lagrangian formulation (variational principle instead of symplectic structure)

GENERIC Integrators

$$\frac{dx}{dt} = L \cdot \frac{\delta E_{\Delta t}}{\delta x} + M_{\Delta t} \cdot \frac{\delta S}{\delta x}$$

$$L \cdot \frac{\delta S}{\delta x} = 0$$

L antisymmetric, Jacobi identity

$$M_{\Delta t} \cdot \frac{\delta E_{\Delta t}}{\delta x} = 0$$

$M_{\Delta t}$ Onsager/Casimir symm., positive-semidefinite

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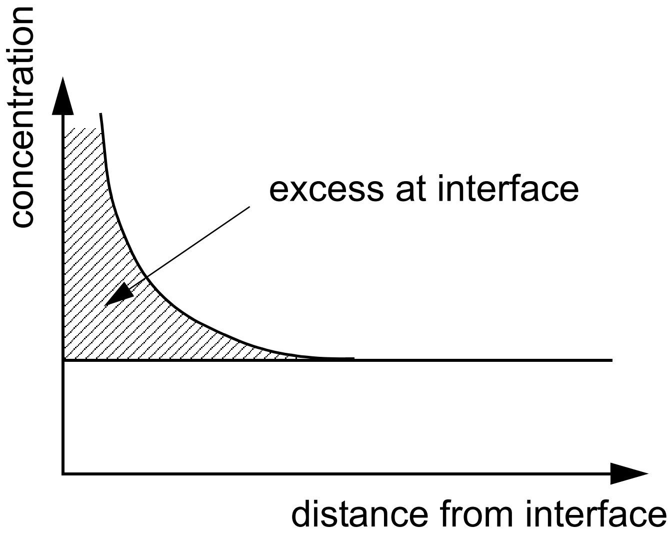
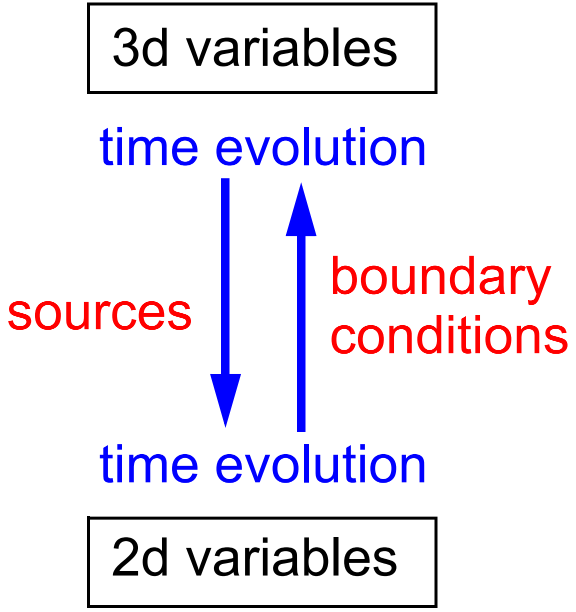
Boundary Thermodynamics





GENERIC Structure

General equation for the nonequilibrium reversible-irreversible coupling

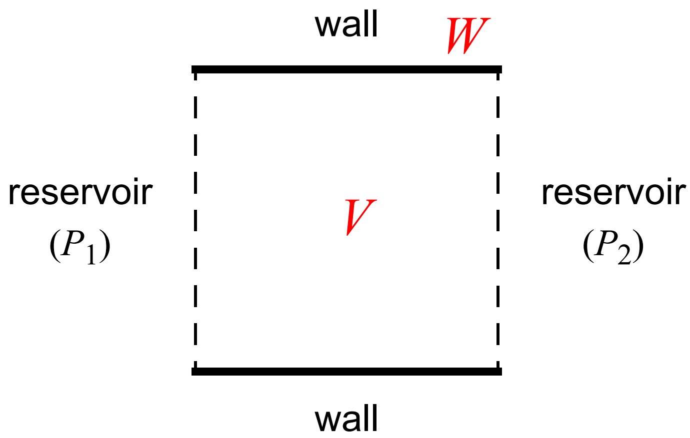
$$\frac{dx}{dt} = L(x) \cdot \frac{\delta E(x)}{\delta x} + M(x) \cdot \frac{\delta S(x)}{\delta x}$$

$$\frac{dA}{dt} = \frac{\delta A}{\delta x} \cdot \frac{dx}{dt} = \frac{\delta A}{\delta x} \cdot L \cdot \frac{\delta E}{\delta x} + \frac{\delta A}{\delta x} \cdot M \cdot \frac{\delta S}{\delta x}$$

$$= \{A, E\} + [A, S]$$

Poisson & dissipative brackets

Example: Diffusion Cell



System: Solute particle number densities

- P in the bulk
- p at the wall

$$\frac{\delta S}{\delta P} = -k_B \ln \frac{P}{P_0}, \qquad \frac{\delta S}{\delta p} = -k_B \ln \frac{p}{p_0}$$

Brenner & Ganesan, Phys. Rev. E 61 (2000) 6879
hco, Phys. Rev. E 73 (2006) 036126

$$k_B[A, B] = \int_V D_b \left[\frac{\partial}{\partial \boldsymbol{r}} \frac{\delta A}{\delta P}\right] \cdot \left[\frac{\partial}{\partial \boldsymbol{r}} \frac{\delta B}{\delta P}\right] P d^3 r + \int_W D_s \left[\frac{\partial}{\partial \boldsymbol{r}} \frac{\delta A}{\delta p}\right] \cdot \left[\frac{\partial}{\partial \boldsymbol{r}} \frac{\delta B}{\delta p}\right] p d^2 r$$

$$+ \int_W \nu_s \left[\frac{\delta A}{\delta p} - \Omega \frac{\delta A}{\delta P}\right]\left[\frac{\delta B}{\delta p} - \Omega \frac{\delta B}{\delta P}\right] p d^2 r$$

$\Omega = 1$

ν_s: ad/desorption rate

Diffusion Cell: Results

$$[A, S] = \int_V \frac{\delta A}{\delta P} \cdot \left[\frac{\mathrm{d}P}{\mathrm{d}t}\right]_{\mathrm{irr}} d^3r + \int_W \frac{\delta A}{\delta p} \cdot \left[\frac{\mathrm{d}p}{\mathrm{d}t}\right]_{\mathrm{irr}} d^2r + \int_{\partial V} J^A_{\mathrm{irr}} d^2r$$

open boundaries: $J^A_{\mathrm{irr}} = -\frac{\delta A}{\delta P}\boldsymbol{n} \cdot D_{\mathrm{b}} \frac{\partial P}{\partial \boldsymbol{r}}$ wall: $J^A_{\mathrm{irr}} = 0$

evolution equations:

$$\frac{\mathrm{d}P}{\mathrm{d}t} = \frac{\partial}{\partial \boldsymbol{r}} \cdot D_{\mathrm{b}} \frac{\partial P}{\partial \boldsymbol{r}}$$

$$\frac{\mathrm{d}p}{\mathrm{d}t} = \frac{\partial}{\partial \boldsymbol{r}} \cdot D_{\mathrm{s}} \frac{\partial p}{\partial \boldsymbol{r}} - \boldsymbol{n} \cdot D_{\mathrm{b}} \frac{\partial P}{\partial \boldsymbol{r}}$$

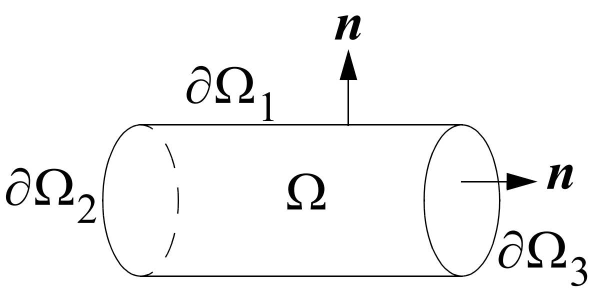
boundary condition on wall:

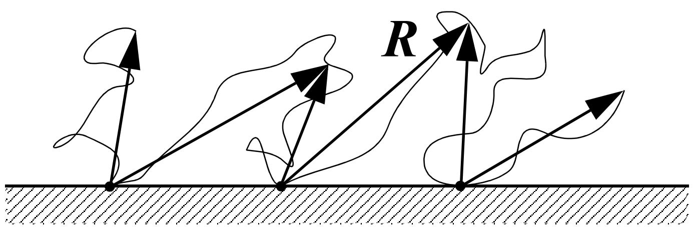
$$-\boldsymbol{n} \cdot D_{\mathrm{b}} \frac{\partial P}{\partial \boldsymbol{r}} = \nu_{\mathrm{s}} p \ln \frac{HP}{p}$$

$$H = p_0 / P_0$$

characteristic length scale

Example: Wall Slip





tethered subchains
(semiloops and tails)

System

bulk variables

$\rho, \boldsymbol{M}, s$ ← tangential on wall

$\Psi(\boldsymbol{Q})$ ← segment cdf

temporary network model

boundary variables

c, s ← entropy density

$\psi(\boldsymbol{R})$ ← subchain cdf

Wall Slip: Building Blocks

Entropy: trivially available

Energy: internal energies depend on

$$s - \rho \int \hat{s}_{\rm net}(\Psi) d^3Q$$

$$\bar{s} - \int s_{\rm teth}(c, \psi) d^3R$$

Poisson bracket: from a natural action of space transformations that leave the wall invariant

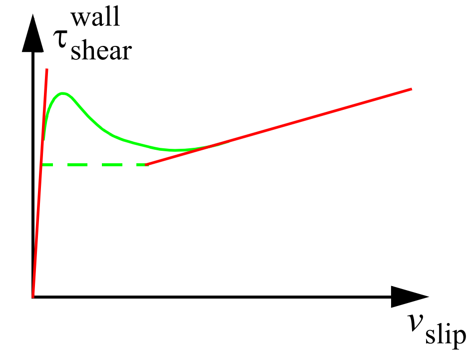
Dissipative bracket:

$$[A, B] = \text{heat conduction (bulk, wall)} + \text{polymer relaxation (bulk, wall)}$$

$$+ \int_{\partial\Omega_1} \frac{T\bar{T}}{R_{\rm K}} \left[\frac{1}{T}\frac{\delta A}{\delta s} - \frac{1}{\bar{T}}\frac{\delta A}{\delta \bar{s}}\right]\left[\frac{1}{T}\frac{\delta B}{\delta s} - \frac{1}{\bar{T}}\frac{\delta B}{\delta \bar{s}}\right] d^2r$$

Kapitza resistance

Wall Slip: Results



$$\boldsymbol{n} \cdot (\tau + p\mathbf{1}) = -T\int \psi \frac{\partial}{\partial \boldsymbol{R}} \frac{\partial s_{\text{teth}}}{\partial \psi} d^3R + s\frac{\partial T}{\partial \boldsymbol{r}_{\parallel}}$$

$$\frac{\partial c}{\partial t} = \frac{c_{\text{eq}}}{\tau_{\text{s}}^{\text{av,eq}}} - \frac{c}{\tau_{\text{s}}^{\text{av}}} + r\frac{c_{\text{eq}} - c}{\tau_{\text{s}}^{\text{av}}}$$

Yarin & Graham, JoR (1998)

requires ψ (or *ansatz*!)

strength of binding

$$\frac{1}{\tau_{\text{s}}^{\text{av}}} = \int \frac{1}{\tau_{\text{s}}(\boldsymbol{R})} \psi(\boldsymbol{R}) d^3R$$

$$\tau_{\text{shear}}^{\text{wall}} = v_{\text{slip}} c k_{\text{B}} T \int \tau_{\text{s}} \left(\frac{\partial \ln \psi}{\partial \boldsymbol{R}_{\parallel}}\right)^2 \psi d^3R$$

Wall-slip law:
Giesekus-type

$$\tau_{\text{shear}}^{\text{wall}} = c_{\text{eq}} k_{\text{B}} T \int \psi_{\text{eq}} \frac{\partial}{\partial \boldsymbol{R}_{\parallel}} \ln\left(\frac{\psi}{\psi_{\text{eq}}}\right) d^3R \Rightarrow$$

$$\tau_{\text{shear}}^{\text{wall}} = v_{\text{slip}} \frac{c_{\text{eq}} k_{\text{B}} T \tau_{\text{s}}^{\text{av}}}{R_{\text{eq}}^2}$$

$$\ln\left(\frac{\psi}{\psi_{\text{eq}}}\right) = \frac{\boldsymbol{R} \cdot \langle \boldsymbol{R} \rangle}{R_{\text{eq}}^2} \qquad \langle \boldsymbol{R} \rangle = v_{\text{slip}} \tau_{\text{s}}^{\text{av}}$$

Next Steps

- Free boundaries
- Moving interfaces
- Viscoelastic interfaces
- More general relations between bulk and boundary variables
- Variables characterizing the geometry of interfaces
- Functional calculus
- Statistical mechanics

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Thanks to Miroslav Grmela, Howard Brenner, Henning Struchtrup, Mario Liu

GENERIC with Fluctuations

$$\frac{dx}{dt} = L(x) \cdot \frac{\delta E(x)}{\delta x} + M(x) \cdot \frac{\delta S(x)}{\delta x} + B(x) \cdot \frac{dW_t}{dt} + k_B \frac{\delta}{\delta x} \cdot M(x)$$

Itô

$$B(x) \cdot B(x)^T = 2 k_B M(x)$$

fluctuation-dissipation theorem

$$\langle \frac{dW_t}{dt} \rangle = 0 \qquad \langle \frac{dW_t}{dt} \frac{dW_{t'}}{dt'} \rangle = \delta(t - t')\mathbf{1}$$

Wiener process

GENERIC with Fluctuations

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Wiener process

Some important issues:

- Partial stochastic differential equations
- Fluctuation renormalization (long-time tails, mode-coupling)