# Remarks on Evolutionary Multiscale Systems Driven by Functionals

**Alexander Mielke**

Weierstraß-Institut für Angewandte Analysis und Stochastik, Berlin
www.wias-berlin.de/people/mielke/


Workshop on Intellectual Challenges in
Multiscale Modelling of Solids
Oxford, 4–5 July 2011

# Overview

# 1. Introduction

We are interested in phenomena described by nonlinear PDEs exhibiting oscillations or concentrations on multiple temporal or spatial scales.

**AIM: Understanding of the interplay of effects on different scales**

- Develop a mathematical framework for analyzing and modeling coupled systems with multiple scales
- Combine Hamiltonian systems and dissipative dynamics (like gradient flows or rate-independent systems)

# 1. Introduction

We are interested in phenomena described by nonlinear PDEs exhibiting oscillations or concentrations on multiple temporal or spatial scales.

**AIM: Understanding of the interplay of effects on different scales**

- Develop a mathematical framework for analyzing and modeling coupled systems with multiple scales
- Combine Hamiltonian systems and dissipative dynamics (like gradient flows or rate-independent systems)

**Applications involve**

- elastoplasticity, phase-field systems, dislocation models
- reaction-diffusion systems, Fokker-Planck equations and Markov processes
- optoelectronics (pulse interaction, Maxwell-Bloch systems, semiconductors)
- quantum mechanical systems coupled to heat baths

# 1. Introduction

Systems driven by **functionals** :

Typically a triple:

- $\mathcal{X}$ state space with states $u$
- $\Phi : [0,T] \times \mathcal{X} \to \mathbb{R}$ a (possibly time-dependent) functional
- a geometric structure (symplectic, dissipative=Riemann)

**Hamiltonian systems** $(\mathcal{X}, \mathcal{H}, \mathcal{L} = \Omega^{-1})$

$$\Omega(u)\dot{u} = \mathrm{D}\mathcal{H}(u) \qquad \Leftrightarrow \qquad \dot{u} = \mathcal{L}(u)\mathrm{D}\mathcal{H}(u)$$

Poisson bracket $\{\mathcal{F}, \mathcal{G}\}(u) = \langle \mathrm{D}\mathcal{F}(u), \mathcal{L}(u)\mathrm{D}\mathcal{G}(u) \rangle$

**Gradient systems** $(\mathcal{X}, \Phi, \mathcal{K} = \mathcal{G}^{-1})$

$$\mathcal{G}(u)\dot{u} = -\mathrm{D}\Phi(u) \qquad \Leftrightarrow \qquad \dot{u} = -\mathcal{K}(u)\mathrm{D}\Phi(u) = -\boldsymbol{\nabla}_{\mathcal{G}}\Phi(u)$$

$\mathcal{G}$ Riemannian metric tensor , $\mathcal{K} = \mathcal{K}^{\mathsf{T}} \geq 0$ Onsager operator

$\Phi$ = free energy $\mathcal{F}$ or negentropy $-\mathcal{S}$

# 1. Introduction

**GENERIC systems**

$$\dot{u} = \underset{\text{reversible}}{\mathcal{L}(u)\mathrm{D}\mathcal{E}(u)} + \underset{\text{irreversible}}{\mathcal{K}(u)\mathrm{D}\mathcal{S}(u)}$$

**G**eneral **E**quations for **N**on-**E**quilibrium **R**eversible **I**rreversible **C**oupling

Quintuple $(\mathcal{X}, \mathcal{E}, \mathcal{S}, \mathcal{L}, \mathcal{K})$:

- state space $\mathcal{X}$ (Banach/Hilbert space, manifold)
- energy $\mathcal{E} : \mathcal{X} \to \mathbb{R}$ (conserved)
- entropy $\mathcal{S} : \mathcal{X} \to \mathbb{R}$ (increasing)
- co-symplectic structure $\mathcal{L} = -\mathcal{L}^{\mathsf{T}}$ (Poisson bracket)
- Onsager structure $\mathcal{K} = \mathcal{K}^{\mathsf{T}} \geq 0$ (dissipative structure)

# 1. Introduction

**GENERIC systems**

$$\dot{u} = \underset{\text{reversible}}{\mathcal{L}(u)\mathrm{D}\mathcal{E}(u)} + \underset{\text{irreversible}}{\mathcal{K}(u)\mathrm{D}\mathcal{S}(u)}$$

**G**eneral **E**quations for **N**on-**E**quilibrium **R**eversible **I**rreversible **C**oupling

**Multiscale system** with small parameter $\varepsilon > 0$

For family of systems $((\mathcal{X}, \mathcal{E}_\varepsilon, \mathcal{S}_\varepsilon, \mathcal{L}_\varepsilon, \mathcal{K}_\varepsilon))_{\varepsilon>0}$ giving $\dot{u}_\varepsilon = \boldsymbol{G}_\varepsilon(u_\varepsilon)$

find a limit system $(\mathcal{Y}, \mathcal{E}_0, \mathcal{S}_0, \mathcal{L}_0, \mathcal{K}_0)$ giving $\dot{y} = \boldsymbol{G}_0(y)$

| | microsc. system | | macrosc. system |
|---|---|---|---|
| | $\dot{u}_\varepsilon = \boldsymbol{G}_\varepsilon(u_\varepsilon)$ | | $\dot{y} = \boldsymbol{G}_0(y)$ |
| initial state | $u_\varepsilon^0$ | $\xrightarrow[\boldsymbol{M}_\varepsilon]{\text{upscaling}}$ | $y^0$ |
| time evolution | $\downarrow$ | | $\downarrow$ |
| | $u_\varepsilon(t) = \boldsymbol{S}_\varepsilon(t, u_\varepsilon^0)$ | $\xrightarrow[\boldsymbol{M}_\varepsilon]{\text{upscaling}}$ | $y(t) = \boldsymbol{S}_0(t, y^0)$ |

Mathematical task: Prove $\lim_{\varepsilon\to 0} \boldsymbol{M}_\varepsilon \circ \boldsymbol{S}_\varepsilon(t, \cdot) = \boldsymbol{S}_0(t, \lim_{\varepsilon\to 0} \boldsymbol{M}_\varepsilon(\cdot))$

# 1. Introduction

What type of convergence do we need for $(\mathcal{X}, \mathcal{E}_\varepsilon, \mathcal{S}_\varepsilon, \mathcal{L}_\varepsilon, \mathcal{K}_\varepsilon) \rightsquigarrow (\mathcal{Y}, \mathcal{E}_0, \mathcal{S}_0, \mathcal{L}_0, \mathcal{K}_0)$ to conclude "$u_\varepsilon^0 \to y^0 \implies u_\varepsilon(t) \to y(t)$ for $t \in [0,T]$" ???

**Different levels of problems:**

- **Simplest case: individual convergence** (& mutual recovery condition)
  (applies to homogenization, dimension reduction, discrete-to-continuum, ....)
  $\mathcal{E}_\varepsilon \to \mathcal{E}_0$, $\mathcal{S}_\varepsilon \to \mathcal{S}_0$, $\mathcal{L}_\varepsilon \to \mathcal{L}_0$, $\mathcal{K}_\varepsilon \to \mathcal{K}_0$

# 1. Introduction

What type of convergence do we need for $(\mathcal{X}, \mathcal{E}_\varepsilon, \mathcal{S}_\varepsilon, \mathcal{L}_\varepsilon, \mathcal{K}_\varepsilon) \rightsquigarrow (\mathcal{Y}, \mathcal{E}_0, \mathcal{S}_0, \mathcal{L}_0, \mathcal{K}_0)$
to conclude "$u_\varepsilon^0 \to y^0 \implies u_\varepsilon(t) \to y(t)$ for $t \in [0,T]$" ???

**Different levels of problems:**

- **Simplest case: individual convergence** (& mutual recovery condition)
  (applies to homogenization, dimension reduction, discrete-to-continuum, ....)
  $\mathcal{E}_\varepsilon \to \mathcal{E}_0$, $\mathcal{S}_\varepsilon \to \mathcal{S}_0$, $\mathcal{L}_\varepsilon \to \mathcal{L}_0$, $\mathcal{K}_\varepsilon \to \mathcal{K}_0$
- **Type of dissipation changes**
  (e.g. viscous friction in wiggly energies gives dry friction)
  $\mathcal{K}_\varepsilon^{-1} \to 0$, $\mathcal{F}_\varepsilon = \mathcal{F}_0 + \mathcal{W}_\varepsilon$ where $\mathcal{W}_\varepsilon \rightsquigarrow \mathcal{K}_0^{\text{dry friction}}$
- **Coarse graining = thermodynamic limit**
  Fast-slow Hamiltonian dynamics leads to dissipative dynamics
  $\mathcal{S}_\varepsilon = 0$, $u_\varepsilon \in \mathbb{R}^{N_\varepsilon}$ rapidly fluctuating $\rightsquigarrow$ distribution $\rho_y(u)\mathrm{d}u$
  $y \in \mathcal{Y}$ slow macroscopic variable $\mathcal{S}_0(y) = -k_\mathrm{B} \int_\mathcal{X} \rho_y(u) \log \rho_y(u) \, \mathrm{d}u$
  $\mathcal{K}_0(y) =$???? fluctuations

# Overview

# 2. Convergence of functionals and forces

**Desired Theorem.** Given $((\mathcal{X},\mathcal{F}_\varepsilon,\mathcal{V}_\varepsilon))_{\varepsilon>0}$ and $u_\varepsilon : [0,T] \to \mathcal{X}$ solves $\dot u = \mathcal{V}_\varepsilon(u)\mathrm{D}\mathcal{F}_\varepsilon(u)$. Moreover, $\mathcal{F}_\varepsilon \rightsquigarrow \mathcal{F}_0$ and $\mathcal{V}_\varepsilon \rightsquigarrow \mathcal{V}_0$. Then,

$$\left.\begin{array}{c} u_\varepsilon(0) \rightharpoonup y(0) \text{ and} \\ \text{additional conditions} \end{array}\right\} \implies \left\{\begin{array}{c} \text{for all } t \in [0,T]\text{: } u_\varepsilon(t) \rightharpoonup y(t) \\ \text{and } y \text{ solves } (\mathcal{Y},\mathcal{F}_0,\mathcal{V}_0) \end{array}\right.$$

For static multiscale systems $\Gamma$-convergence is appropriate:

# 2. Convergence of functionals and forces

**Desired Theorem.** Given $((\mathcal{X},\mathcal{F}_\varepsilon,\mathcal{V}_\varepsilon))_{\varepsilon>0}$ and $u_\varepsilon : [0,T] \to \mathcal{X}$ solves $\dot u = \mathcal{V}_\varepsilon(u)\mathrm{D}\mathcal{F}_\varepsilon(u)$. Moreover, $\mathcal{F}_\varepsilon \rightsquigarrow \mathcal{F}_0$ and $\mathcal{V}_\varepsilon \rightsquigarrow \mathcal{V}_0$. Then,

$$\left.\begin{array}{c} u_\varepsilon(0) \rightharpoonup y(0) \text{ and} \\ \text{additional conditions} \end{array}\right\} \implies \left\{\begin{array}{c} \text{for all } t\in[0,T]\colon u_\varepsilon(t) \rightharpoonup y(t) \\ \text{and } y \text{ solves } (\mathcal{Y},\mathcal{F}_0,\mathcal{V}_0) \end{array}\right.$$

For static multiscale systems $\Gamma$-convergence is appropriate:

$$\mathcal{F}_\varepsilon \overset{\Gamma}{\to} \mathcal{F}_0 \quad \text{or} \quad \mathcal{F}_0 = \Gamma\text{-}\lim_{\varepsilon\to 0}\mathcal{F}_\varepsilon \qquad \text{if}$$

(G1) $u_\varepsilon \rightharpoonup u_0 \implies \mathcal{F}_0(u_0) \le \liminf_\varepsilon \mathcal{F}_\varepsilon(u_\varepsilon)$

(G2) For all $u_0$ there exists a recovery sequence $u_\varepsilon$ such that
(i) $u_\varepsilon \rightharpoonup u_0$ (ii) $\mathcal{F}_\varepsilon(u_\varepsilon) \to \mathcal{F}_0(u_0)$

**Static theorem** (De Giorgi'74): If $\mathcal{F}_\varepsilon \overset{\Gamma}{\to} \mathcal{F}_0$, then
$u_\varepsilon$ minimizes $\mathcal{F}_\varepsilon$ and $u_\varepsilon \rightharpoonup y \implies y$ minimizes $\mathcal{F}_0$

# 2. Convergence of functionals and forces

**Desired evolutionary theorem:** Given $((\mathcal{X},\mathcal{F}_\varepsilon,\mathcal{V}_\varepsilon))_{\varepsilon>0}$ and $u_\varepsilon : [0,T] \to \mathcal{X}$ solves $\dot u = \mathcal{V}_\varepsilon(u)\mathrm{D}\mathcal{F}_\varepsilon(u)$. Moreover, $\mathcal{F}_\varepsilon \rightsquigarrow \mathcal{F}_0$ and $\mathcal{V}_\varepsilon \rightsquigarrow \mathcal{V}_0$. Then,

$$\left.\begin{array}{c} u_\varepsilon(0) \rightharpoonup y(0) \text{ and} \\ \text{additional conditions} \end{array}\right\} \quad \Longrightarrow \quad \left\{\begin{array}{c} \text{for all } t \in [0,T]\text{: } u_\varepsilon(t) \rightharpoonup y(t) \\ \text{and } y \text{ solves } (\mathcal{Y},\mathcal{F}_0,\mathcal{V}_0) \end{array}\right.$$

$\rightsquigarrow$ for evolution driven by $\mathcal{F}_\varepsilon$ we need control of the driving force $\mathrm{D}\mathcal{F}_\varepsilon$.

# 2. Convergence of functionals and forces

**Desired evolutionary theorem:** Given $((\mathcal{X},\mathcal{F}_\varepsilon,\mathcal{V}_\varepsilon))_{\varepsilon>0}$ and $u_\varepsilon : [0,T] \to \mathcal{X}$ solves $\dot u = \mathcal{V}_\varepsilon(u)\mathrm{D}\mathcal{F}_\varepsilon(u)$. Moreover, $\mathcal{F}_\varepsilon \rightsquigarrow \mathcal{F}_0$ and $\mathcal{V}_\varepsilon \rightsquigarrow \mathcal{V}_0$. Then,

$$\left.\begin{array}{c} u_\varepsilon(0) \rightharpoonup y(0) \text{ and} \\ \text{additional conditions} \end{array}\right\} \quad \Longrightarrow \quad \left\{\begin{array}{c} \text{for all } t \in [0,T]\text{: } u_\varepsilon(t) \rightharpoonup y(t) \\ \text{and } y \text{ solves } (\mathcal{Y},\mathcal{F}_0,\mathcal{V}_0) \end{array}\right.$$

$\rightsquigarrow$ for evolution driven by $\mathcal{F}_\varepsilon$ we need control of the driving force $\mathrm{D}\mathcal{F}_\varepsilon$.

**Guiding theme** througout this talk:

**Convergence of functionals** and **convergence of driving forces**

Question: What type of convergence $\mathcal{F}_\varepsilon \to \mathcal{F}_0$ do we need to have that

$u^\varepsilon \rightharpoonup y \quad \Longrightarrow \quad \mathrm{D}\mathcal{F}_\varepsilon(u_\varepsilon) \rightharpoonup \mathrm{D}\mathcal{F}_0(y)$ ???

# 2. Convergence of functionals and forces

**Desired evolutionary theorem:** Given $((\mathcal{X},\mathcal{F}_\varepsilon,\mathcal{V}_\varepsilon))_{\varepsilon>0}$ and $u_\varepsilon : [0,T] \to \mathcal{X}$ solves $\dot u = \mathcal{V}_\varepsilon(u)\mathrm{D}\mathcal{F}_\varepsilon(u)$. Moreover, $\mathcal{F}_\varepsilon \rightsquigarrow \mathcal{F}_0$ and $\mathcal{V}_\varepsilon \rightsquigarrow \mathcal{V}_0$. Then,

$$\left.\begin{array}{c} u_\varepsilon(0) \rightharpoonup y(0) \text{ and} \\ \text{additional conditions} \end{array}\right\} \quad \Longrightarrow \quad \left\{\begin{array}{c} \text{for all } t\in[0,T]\text{: } u_\varepsilon(t) \rightharpoonup y(t) \\ \text{and } y \text{ solves } (\mathcal{Y},\mathcal{F}_0,\mathcal{V}_0) \end{array}\right.$$

$\rightsquigarrow$ for evolution driven by $\mathcal{F}_\varepsilon$ we need control of the driving force $\mathrm{D}\mathcal{F}_\varepsilon$.

**Main message today:**

Assume $\mathcal{F}_\varepsilon \xrightarrow{\Gamma} \mathcal{F}_0$ and *suitable conditions*, then

$$\left.\begin{array}{c} u_\varepsilon \rightharpoonup y \\ \mathcal{F}_\varepsilon(u_\varepsilon) \to \mathcal{F}_0(y) \end{array}\right\} \quad \Longrightarrow \quad \mathrm{D}\mathcal{F}_\varepsilon(u_\varepsilon) \rightharpoonup \mathrm{D}\mathcal{F}_0(y).$$

Functional convergence should imply

force convergence = vector-field convergence

which then MAY imply convergence of solutions

# 2. Convergence of functionals and forces

A simply prototype result:

**Proposition (Convergence of forces)**

Assume $\mathcal{F}_\varepsilon \in \mathsf{C}^1(\mathcal{X};\mathbb{R})$, $\mathcal{F}_\varepsilon \xrightarrow{\Gamma} \mathcal{F}_0$ and the additional conditions

(i) $\mathcal{F}_\varepsilon(u+w) \le \mathcal{F}_\varepsilon(u) + \langle \mathsf{D}\mathcal{F}_\varepsilon(u), w\rangle + C\|w\|^2$
uniformly in $\varepsilon$, $u$, and $w$.

(ii) $\forall\, E\ \exists C\ \forall \varepsilon > 0: \quad \mathcal{F}_\varepsilon(u) \le E \ \Rightarrow\ \|\mathsf{D}\mathcal{F}_\varepsilon(u)\| \le C.$

Then,

$$\Big(u_\varepsilon \rightharpoonup y \ \&\ \mathcal{F}_\varepsilon(u_\varepsilon) \to \mathcal{F}_0(y)\Big) \quad \Longrightarrow \quad \mathsf{D}\mathcal{F}_\varepsilon(u_\varepsilon) \rightharpoonup \mathsf{D}\mathcal{F}_0(y).$$

# 2. Convergence of functionals and forces

A simply prototype result:

**Proposition (Convergence of forces)**

Assume $\mathcal{F}_\varepsilon \in \mathsf{C}^1(\mathcal{X};\mathbb{R})$, $\mathcal{F}_\varepsilon \xrightarrow{\Gamma} \mathcal{F}_0$ and the additional conditions

(i) $\mathcal{F}_\varepsilon(u+w) \le \mathcal{F}_\varepsilon(u) + \langle \mathsf{D}\mathcal{F}_\varepsilon(u), w\rangle + C\|w\|^2$
uniformly in $\varepsilon$, $u$, and $w$.

(ii) $\forall\, E\ \exists C\ \forall \varepsilon > 0: \quad \mathcal{F}_\varepsilon(u) \le E \ \Rightarrow\ \|\mathsf{D}\mathcal{F}_\varepsilon(u)\| \le C.$

Then,

$$\Big(u_\varepsilon \rightharpoonup y \ \&\ \mathcal{F}_\varepsilon(u_\varepsilon) \to \mathcal{F}_0(y)\Big) \quad \Longrightarrow \quad \mathsf{D}\mathcal{F}_\varepsilon(u_\varepsilon) \rightharpoonup \mathsf{D}\mathcal{F}_0(y).$$

Proof:

By (ii) $\mathsf{D}\mathcal{F}_{\varepsilon_j}(u_{\varepsilon_j}) \rightharpoonup \sigma$. Inserting $u = u_{\varepsilon_j}$ into (i) and taking $\varepsilon_j \to 0$ yield

$$\begin{aligned}\mathcal{F}_0(y_0+w) &\le_{\text{(G1)}} \liminf \mathcal{F}_{\varepsilon_j}(u_{\varepsilon_j}+w)\\ &\le \liminf \mathcal{F}_{\varepsilon_j}(u_{\varepsilon_j}) + \langle \mathsf{D}\mathcal{F}_{\varepsilon_j}(u_{\varepsilon_j}), w\rangle + C\|w\|^2 = \mathcal{F}_0(y) + \langle \sigma, w\rangle + C\|w\|^2\end{aligned}$$

We conclude $\sigma = \mathsf{D}\mathcal{F}_0(y)$ and hence $\mathsf{D}\mathcal{F}_\varepsilon(u_\varepsilon) \rightharpoonup \mathsf{D}\mathcal{F}_0(y)$. $\square$

# 2. Convergence of functionals and forces

**Similar results:**

- **Functional analysis:** $X = \mathsf{L}^p(\Omega)$

$u_n \rightharpoonup u$ and $\mathcal{F}(u_n) = \|u_n\|_p^p \to \mathcal{F}(u) = \|u\|_p^p$

$$\Longrightarrow \quad u_n \to u \quad \Longrightarrow \quad \mathsf{D}\mathcal{F}(u) = pu_n^{p-1} \to \mathsf{D}\mathcal{F}(u) = pu^{p-1} \in \mathsf{L}^{p^*}$$

(More general: Visintin's argument 1984)

# 2. Convergence of functionals and forces

**Similar results:**

- **Functional analysis:** $X = \mathsf{L}^p(\Omega)$

$u_n \rightharpoonup u$ and $\mathcal{F}(u_n) = \|u_n\|_p^p \to \mathcal{F}(u) = \|u\|_p^p$

$$\Longrightarrow \quad u_n \to u \quad \Longrightarrow \quad \mathsf{D}\mathcal{F}(u) = pu_n^{p-1} \to \mathsf{D}\mathcal{F}(u) = pu^{p-1} \in \mathsf{L}^{p^*}$$

(More general: Visintin's argument 1984)

- **Gradient Young measures:** (Ball, Kirchheim, Kristensen 2000):

$W^{\mathsf{qc}}(F) = \int_{\mathbb{R}^{m\times d}} W(\widetilde{F})\nu(\mathrm{d}\widetilde{F})$

$$\Longrightarrow \quad \text{stress } \mathsf{D}W^{\mathsf{qc}}(F) = \int_{\mathbb{R}^{m\times d}} \mathsf{D}_{\widetilde{F}} W(\widetilde{F})\nu(\mathrm{d}\widetilde{F})$$

In our context this means for $u_\varepsilon \rightharpoonup y$ in $\mathsf{W}^{1,p}(\Omega)$ that

$$\left.\begin{array}{c} \nabla u_\varepsilon \xrightarrow{\mathsf{YM}} \nu \\ \int_\Omega W(\nabla u_\varepsilon)\,\mathrm{d}x \to \int_\Omega W^{\mathsf{qc}}(\nabla y)\,\mathrm{d}x \end{array}\right\} \quad \Longrightarrow \quad \mathsf{D}W(\nabla u_\varepsilon) \rightharpoonup \mathsf{D}W^{\mathsf{qc}}(\nabla y)$$

# 2. Convergence of functionals and forces

**Similar results:**

- **Functional analysis:** $X = \mathsf{L}^p(\Omega)$

$u_n \rightharpoonup u$ and $\mathcal{F}(u_n) = \|u_n\|_p^p \to \mathcal{F}(u) = \|u\|_p^p$

$$\implies \quad u_n \to u \quad \implies \quad \mathsf{D}\mathcal{F}(u) = pu_n^{p-1} \to \mathsf{D}\mathcal{F}(u) = pu^{p-1} \in \mathsf{L}^{p^*}$$

(More general: Visintin's argument 1984)

- **Gradient Young measures:** (Ball, Kirchheim, Kristensen 2000):

$W^{\mathsf{qc}}(F) = \int_{\mathbb{R}^{m\times d}} W(\widetilde{F})\nu(\mathrm{d}\widetilde{F})$

$$\implies \quad \text{stress } \mathsf{D}W^{\mathsf{qc}}(F) = \int_{\mathbb{R}^{m\times d}} \mathsf{D}_{\widetilde{F}} W(\widetilde{F})\nu(\mathrm{d}\widetilde{F})$$

- **Weakly lower semicontinuous, differentiable functional $\mathcal{F}$:**

(Dal Maso, Franfort, Toader 2005):

$$u_n \rightharpoonup u,\ \mathcal{F}(u_n) \to \mathcal{F}(u) \quad \implies \quad \mathsf{D}\mathcal{F}(u_n) \rightharpoonup \mathsf{D}\mathcal{F}(u)$$

# Overview

# 3. GENERIC and coarse graining

**G**eneral **E**quations for **N**on-**E**quilibrium **R**eversible **I**rreversible **C**oupling

... was developed by Öttinger/Grmela '97 (mainly for polymeric fluids)

... also works for solids with internal variables (M'11 Cont.Mech.Thermodyn.2011)

# 3. GENERIC and coarse graining

**G**eneral **E**quations for **N**on-**E**quilibrium **R**eversible **I**rreversible **C**oupling

... was developed by Öttinger/Grmela '97 (mainly for polymeric fluids)

... also works for solids with internal variables (M'11 Cont.Mech.Thermodyn.2011)

Here, we discuss parts of Öttinger: *Beyond Equilibrium Thermodynamics* 2005

# 3. GENERIC and coarse graining

**G**eneral **E**quations for **N**on-**E**quilibrium **R**eversible **I**rreversible **C**oupling

... was developed by Öttinger/Grmela '97 (mainly for polymeric fluids)

... also works for solids with internal variables (M'11 Cont.Mech.Thermodyn.2011)

Here, we discuss parts of Öttinger: *Beyond Equilibrium Thermodynamics* 2005

**G** eneral
**E** quations for
**N** on-
**E** quilibrium
**R** eversible
**I** rreversible
**C** oupling

Quintuple $(\mathcal{X}, \mathcal{E}, \mathcal{S}, \mathcal{L}, \mathcal{K})$

$$\boxed{\dot{u} = \mathcal{L}(u)\mathrm{D}\mathcal{E}(u) + \mathcal{K}(u)\mathrm{D}\mathcal{S}(u)}$$

$\mathcal{E}$ energy, $\mathcal{S}$ entropy

$\mathcal{L} = -\mathcal{L}^*$ Poisson structure

$\mathcal{K} = \mathcal{K}^* \geq 0$ dissipative structure (Onsager)

**Noninteraction conditions** $\mathcal{L}\mathrm{D}\mathcal{S} \equiv 0 \equiv \mathcal{K}\mathrm{D}\mathcal{E}$

# 3. GENERIC and coarse graining

**G**eneral **E**quations for **N**on-**E**quilibrium **R**eversible **I**rreversible **C**oupling

... was developed by Öttinger/Grmela '97 (mainly for polymeric fluids)

... also works for solids with internal variables (M'11 Cont.Mech.Thermodyn.2011)

Here, we discuss parts of Öttinger: *Beyond Equilibrium Thermodynamics* 2005

**G** eneral
**E** quations for
**N** on-
**E** quilibrium
**R** eversible
**I** rreversible
**C** oupling

Quintuple $(\mathcal{X}, \mathcal{E}, \mathcal{S}, \mathcal{L}, \mathcal{K})$

$$\boxed{\dot{u} = \mathcal{L}(u)\mathrm{D}\mathcal{E}(u) + \mathcal{K}(u)\mathrm{D}\mathcal{S}(u)}$$

$\mathcal{E}$ energy, $\mathcal{S}$ entropy

$\mathcal{L} = -\mathcal{L}^*$ Poisson structure

$\mathcal{K} = \mathcal{K}^* \geq 0$ dissipative structure (Onsager)

**Noninteraction conditions** $\mathcal{L}\mathrm{D}\mathcal{S} \equiv 0 \equiv \mathcal{K}\mathrm{D}\mathcal{E}$

For solids with internal variables, we set $u = (\boldsymbol{\varphi}, \rho\dot{\boldsymbol{\varphi}}, z, \theta)$ and

$\mathcal{E}(u) = \int_\Omega \frac{\rho}{2}|\dot{\boldsymbol{\varphi}}|^2 + \widehat{e}(\nabla\boldsymbol{\varphi}, z, \theta) - f_{\text{ext}}\cdot\boldsymbol{\varphi}\,\mathrm{d}x$

$\mathcal{S}(u) = \int_\Omega \widehat{s}(\nabla\boldsymbol{\varphi}, z, \theta)\,\mathrm{d}x$

# 3. GENERIC and coarse graining

**G**eneral **E**quations for **N**on-**E**quilibrium **R**eversible **I**rreversible **C**oupling

... was developed by Öttinger/Grmela '97 (mainly for polymeric fluids)

... also works for solids with internal variables (M'11 Cont.Mech.Thermodyn.2011)

Here, we discuss parts of Öttinger: *Beyond Equilibrium Thermodynamics* 2005

**G** eneral
**E** quations for
**N** on-
**E** quilibrium
**R** eversible
**I** rreversible
**C** oupling

Quintuple $(\mathcal{X}, \mathcal{E}, \mathcal{S}, \mathcal{L}, \mathcal{K})$

$$\boxed{\dot{u} = \mathcal{L}(u)\mathrm{D}\mathcal{E}(u) + \mathcal{K}(u)\mathrm{D}\mathcal{S}(u)}$$

$\mathcal{E}$ energy, $\mathcal{S}$ entropy

$\mathcal{L} = -\mathcal{L}^*$ Poisson structure

$\mathcal{K} = \mathcal{K}^* \geq 0$ dissipative structure (Onsager)

**Noninteraction conditions** $\mathcal{L}\mathrm{D}\mathcal{S} \equiv 0 \equiv \mathcal{K}\mathrm{D}\mathcal{E}$

For time-independent CLOSED systems we have :

- Energy conservation: $\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E}(u(t)) = \langle \mathrm{D}\mathcal{E}, \mathcal{L}\mathrm{D}\mathcal{E}\rangle + \langle \mathrm{D}\mathcal{E}, \mathcal{K}\mathrm{D}\mathcal{S}\rangle = 0$
- Entropy production: $\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{S}(u(t)) = \langle \mathrm{D}\mathcal{S}, \mathcal{L}\mathrm{D}\mathcal{E}\rangle + \langle \mathrm{D}\mathcal{S}, \mathcal{K}\mathrm{D}\mathcal{S}\rangle \geq 0$

# 3. GENERIC and coarse graining

**Why GENERIC $\dot{u} = \mathcal{L}(u)\mathrm{D}\mathcal{E}(u) + \mathcal{K}(u)\mathrm{D}\mathcal{S}(u)$ ??**

- **geometric structure of mechanics and physics**
  - additional structure on top of thermodynamics (TD)
  - automatic correctness of $1^{\text{st}}$ and $2^{\text{nd}}$ law of TD
  - additional information on thermodynamic driving forces
  - easy coupling of effects (optics & electronics, quantum & heat)

# 3. GENERIC and coarse graining

## Why GENERIC $\dot{u} = \mathcal{L}(u)\mathrm{D}\mathcal{E}(u) + \mathcal{K}(u)\mathrm{D}\mathcal{S}(u)$ ??

- **geometric structure of mechanics and physics**
  - additional structure on top of thermodynamics (TD)
  - automatic correctness of 1st and 2nd law of TD
  - additional information on thermodynamic driving forces
  - easy coupling of effects (optics & electronics, quantum & heat)
- **additional mathematical structures**
  - Liapunov functions $\mathcal{E}$ and $-\mathcal{S}$
  - $L, K$ define function spaces
  - natural splitting method $\dot{X} = \underbrace{L(X)\mathrm{D}\mathcal{E}(X)}_{\text{Hamiltonian flow}} \leftrightarrow \dot{X} = \underbrace{K(X)\mathrm{D}\mathcal{S}(X)}_{\text{gradient flow}}$

# 3. GENERIC and coarse graining

## Why GENERIC $\dot{u} = \mathcal{L}(u)\mathrm{D}\mathcal{E}(u) + \mathcal{K}(u)\mathrm{D}\mathcal{S}(u)$ ??

- **geometric structure of mechanics and physics**
  - additional structure on top of thermodynamics (TD)
  - automatic correctness of 1st and 2nd law of TD
  - additional information on thermodynamic driving forces
  - easy coupling of effects (optics & electronics, quantum & heat)
- **additional mathematical structures**
  - Liapunov functions $\mathcal{E}$ and $-\mathcal{S}$
  - $L, K$ define function spaces
  - natural splitting method $\dot{X} = \underbrace{L(X)\mathrm{D}\mathcal{E}(X)}_{\text{Hamiltonian flow}} \leftrightarrow \dot{X} = \underbrace{K(X)\mathrm{D}\mathcal{S}(X)}_{\text{gradient flow}}$
- **Öttinger 2005: Systematic coarse graining**
  - atomistic Hamiltonian systems $\rightsquigarrow$ continuum thermodynamics
  - discrete dislocation dynamics $\rightsquigarrow$ continuum plasticity

# 3. GENERIC and coarse graining

**Coarse graining** of microsystem $(\mathcal{X}, \mathcal{E}_\varepsilon, \mathcal{S}_\varepsilon \equiv 0, \mathcal{L}_\varepsilon, \mathcal{K}_\varepsilon \equiv 0)$

according to **Öttinger: *Beyond equilibrium Thermodynamics* 2005**
(Section 6 Projection methods, projection operators, statistical approach)

# 3. GENERIC and coarse graining

**Coarse graining** of microsystem $(\mathcal{X}, \mathcal{E}_\varepsilon, \mathcal{S}_\varepsilon \equiv 0, \mathcal{L}_\varepsilon, \mathcal{K}_\varepsilon \equiv 0)$

according to **Öttinger: *Beyond equilibrium Thermodynamics* 2005**
(Section 6 Projection methods, projection operators, statistical approach)

$$\dot{u}_\varepsilon = \mathcal{L}_\varepsilon(u_\varepsilon)\mathsf{D}\mathcal{E}_\varepsilon(u_\varepsilon) \quad \xrightarrow{y=\Pi_\varepsilon(u_\varepsilon)} \quad \dot{y} = \mathbb{L}(y)\mathsf{D}\mathbb{E}(y) + \mathbb{K}(y)\mathsf{D}\mathbb{S}(y)$$

Typically $u_\varepsilon = (u_{\mathsf{slow}}, u_{\mathsf{fast}})$ (e.g. (action,angle) variables)

$y = u_{\mathsf{slow}}$ with $\dot{u}_{\mathsf{slow}} = O(1)$ and $\dot{u}_{\mathsf{fast}} = O(1/\varepsilon)$.

# 3. GENERIC and coarse graining

**Coarse graining** of microsystem $(\mathcal{X}, \mathcal{E}_\varepsilon, \mathcal{S}_\varepsilon \equiv 0, \mathcal{L}_\varepsilon, \mathcal{K}_\varepsilon \equiv 0)$

according to **Öttinger: *Beyond equilibrium Thermodynamics* 2005**

(Section 6 Projection methods, projection operators, statistical approach)

$$\dot{u}_\varepsilon = \mathcal{L}_\varepsilon(u_\varepsilon)\mathrm{D}\mathcal{E}_\varepsilon(u_\varepsilon) \quad \xrightarrow{y=\Pi_\varepsilon(u_\varepsilon)} \quad \dot{y} = \mathbb{L}(y)\mathrm{D}\mathbb{E}(y) + \mathbb{K}(y)\mathrm{D}\mathbb{S}(y)$$

Typically $u_\varepsilon = (u_{\mathsf{slow}}, u_{\mathsf{fast}})$ (e.g. (action,angle) variables)

$y = u_{\mathsf{slow}}$ with $\dot{u}_{\mathsf{slow}} = O(1)$ and $\dot{u}_{\mathsf{fast}} = O(1/\varepsilon)$.

Fluctuating fast variables give rise to a probability distribution

$\rho_y(u)\,\mathrm{d}u$ (e.g. a Young measure $\lim_{\varepsilon\to 0} \int_{\tau=0}^{\sqrt{\varepsilon}} \Phi(u_\varepsilon(t+\tau))\,\mathrm{d}\tau \to \int_{\mathcal{X}} \Phi(u)\rho_{y(t)}(u)\,\mathrm{d}u$

where $\Pi_\varepsilon(u_\varepsilon(t)) \to y(t)$

## Macroscopic functionals

$$\mathbb{E}(y) = \int_{\mathcal{X}} \mathcal{E}(u)\rho_y(u)\,\mathrm{d}u \qquad \text{(statics!)}$$

$$\mathbb{S}(y) = -k_{\mathsf{B}} \int_{\mathcal{X}} \rho_y(u)\log\rho_y(u)\,\mathrm{d}u \qquad \text{(statics!)}$$

$$\mathbb{L}(y) = \int_{\mathcal{X}} \mathrm{D}\Pi(u)\mathcal{L}(u)\mathrm{D}\Pi(u)^{\mathsf{T}}\rho_y(u)\,\mathrm{d}u \qquad \text{(statics!)}$$

$\mathbb{K}(y) = \mathbb{K}_{\mathsf{fluctuation}}$ **from dynamics !!**

# 3. GENERIC and coarse graining

To show: $\dot{u}_\varepsilon = \boldsymbol{G}_\varepsilon(u_\varepsilon) = \mathcal{L}_\varepsilon(u_\varepsilon)\mathsf{D}\mathcal{E}_\varepsilon(u_\varepsilon) \xrightarrow{y=\Pi_\varepsilon(u_\varepsilon)} \dot{y} = \mathbb{L}(y)\mathsf{D}\mathbb{E}(y) + \mathbb{K}(y)\mathsf{D}\mathbb{S}(y)$

$y = \Pi_\varepsilon(u), \quad \mathbb{E}(y) = \int_{\mathcal{X}} \mathcal{E}(u)\rho_y(u)\,\mathsf{d}u, \quad \mathbb{S}(y) = -k_{\mathsf{B}} \int_{\mathcal{X}} \rho_y(u) \log \rho_y(u)\,\mathsf{d}u$

$\mathbb{L}(y) = \int_{\mathcal{X}} \mathsf{D}\Pi(u)\mathcal{L}(u)\mathsf{D}\Pi(u)^{\mathsf{T}}\rho_y(u)\,\mathsf{d}u, \quad \mathbb{K}(y) = ???$

---

$\mathbb{K}(y) : \mathsf{T}^*_y\mathcal{Y} \to \mathsf{T}_y\mathcal{Y}$ needs dynamics (for well separated time scales)!!

For an observable (testfunction) $F : \mathcal{Y} \to \mathbb{R}$ we obtain correlations via

$\langle \mathsf{D}F(y), \mathbb{K}(y)\mathsf{D}F(y)\rangle =$

$$\lim_{\varepsilon\to 0} \frac{1}{k_{\mathsf{B}}} \int_{\tau=0}^{\sqrt{\varepsilon}} \mathcal{Q}_\varepsilon[\underbrace{\langle \mathsf{D}F, \mathsf{D}\Pi_\varepsilon \boldsymbol{G}_\varepsilon\rangle}_{=\frac{\mathsf{d}}{\mathsf{d}t}F(\Pi_\varepsilon(u_\varepsilon(t)))}](u_\varepsilon(t))\; \mathcal{Q}_\varepsilon[\underbrace{\langle \mathsf{D}F, \mathsf{D}\Pi_\varepsilon \boldsymbol{G}_\varepsilon\rangle}_{=\frac{\mathsf{d}}{\mathsf{d}t}F(\Pi_\varepsilon(u_\varepsilon(t+\tau)))}](u_\varepsilon(t+\tau))\,\mathsf{d}\tau$$

# 3. GENERIC and coarse graining

To show: $\dot{u}_\varepsilon = \boldsymbol{G}_\varepsilon(u_\varepsilon) = \mathcal{L}_\varepsilon(u_\varepsilon)\mathsf{D}\mathcal{E}_\varepsilon(u_\varepsilon) \xrightarrow{y=\Pi_\varepsilon(u_\varepsilon)} \dot{y} = \mathbb{L}(y)\mathsf{D}\mathbb{E}(y) + \mathbb{K}(y)\mathsf{D}\mathbb{S}(y)$

$y = \Pi_\varepsilon(u), \quad \mathbb{E}(y) = \int_{\mathcal{X}} \mathcal{E}(u)\rho_y(u)\,\mathsf{d}u, \quad \mathbb{S}(y) = -k_\mathsf{B}\int_{\mathcal{X}} \rho_y(u)\log\rho_y(u)\,\mathsf{d}u$

$\mathbb{L}(y) = \int_{\mathcal{X}} \mathsf{D}\Pi(u)\mathcal{L}(u)\mathsf{D}\Pi(u)^\mathsf{T}\rho_y(u)\,\mathsf{d}u, \quad \mathbb{K}(y) = ???$

---

$\mathbb{K}(y) : \mathsf{T}^*_y\mathcal{Y} \to \mathsf{T}_y\mathcal{Y}$ needs dynamics (for well separated time scales)!!

For an observable (testfunction) $F : \mathcal{Y} \to \mathbb{R}$ we obtain correlations via

$\langle \mathsf{D}F(y), \mathbb{K}(y)\mathsf{D}F(y)\rangle =$

$$\lim_{\varepsilon\to 0} \frac{1}{k_\mathsf{B}} \int_{\tau=0}^{\sqrt{\varepsilon}} \mathcal{Q}_\varepsilon[\underbrace{\langle \mathsf{D}F, \mathsf{D}\Pi_\varepsilon \boldsymbol{G}_\varepsilon\rangle}_{=\frac{\mathsf{d}}{\mathsf{d}t}F(\Pi_\varepsilon(u_\varepsilon(t)))}](u_\varepsilon(t))\; \mathcal{Q}_\varepsilon[\underbrace{\langle \mathsf{D}F, \mathsf{D}\Pi_\varepsilon \boldsymbol{G}_\varepsilon\rangle}_{=\frac{\mathsf{d}}{\mathsf{d}t}F(\Pi_\varepsilon(u_\varepsilon(t+\tau)))}](u_\varepsilon(t+\tau))\,\mathsf{d}\tau$$

projection operators $\mathcal{P}_\varepsilon : \mathsf{C}(\mathcal{X}) \to \mathsf{C}(\mathcal{X})$ and $\mathcal{Q}_\varepsilon = \mathsf{id} - \mathcal{P}_\varepsilon$

with $\mathcal{P}_\varepsilon[\mathcal{F}](u) = \int_{\mathcal{X}} \mathcal{F}(\widehat{u})\rho_{\Pi_\varepsilon(u)}(\widehat{u})\,\mathsf{d}\widehat{u}$ $\qquad$ $\mathcal{Q}_\varepsilon$ keeps only fluctuations!

Hence, we have $\quad \mathcal{G} = \mathcal{P}_\varepsilon[\mathcal{F}] \quad \Longleftrightarrow \quad \exists\, \mathbb{G}\colon \mathcal{Y} \to \mathbb{R} : \quad \mathcal{G}(u) = \mathbb{G}(\Pi_\varepsilon(u))$

# 3. GENERIC and coarse graining

To show: $\dot{u}_\varepsilon = \boldsymbol{G}_\varepsilon(u_\varepsilon) = \mathcal{L}_\varepsilon(u_\varepsilon)\mathsf{D}\mathcal{E}_\varepsilon(u_\varepsilon) \xrightarrow{y=\Pi_\varepsilon(u_\varepsilon)} \dot{y} = \mathbb{L}(y)\mathsf{D}\mathbb{E}(y) + \mathbb{K}(y)\mathsf{D}\mathbb{S}(y)$

$y = \Pi_\varepsilon(u), \quad \mathbb{E}(y) = \int_{\mathcal{X}} \mathcal{E}(u)\rho_y(u)\,\mathsf{d}u, \quad \mathbb{S}(y) = -k_{\mathsf{B}} \int_{\mathcal{X}} \rho_y(u) \log \rho_y(u)\,\mathsf{d}u$

$\mathbb{L}(y) = \int_{\mathcal{X}} \mathsf{D}\Pi(u)\mathcal{L}(u)\mathsf{D}\Pi(u)^{\mathsf{T}}\rho_y(u)\,\mathsf{d}u, \quad \mathbb{K}(y) = ???$

---

$\mathbb{K}(y) : \mathsf{T}_y^*\mathcal{Y} \to \mathsf{T}_y\mathcal{Y}$ needs dynamics (for well separated time scales)!!

For an observable (testfunction) $F : \mathcal{Y} \to \mathbb{R}$ we obtain correlations via

$\langle \mathsf{D}F(y), \mathbb{K}(y)\mathsf{D}F(y)\rangle =$

$$\lim_{\varepsilon\to 0} \frac{1}{k_{\mathsf{B}}} \int_{\tau=0}^{\sqrt{\varepsilon}} \mathcal{Q}_\varepsilon[\underbrace{\langle \mathsf{D}F, \mathsf{D}\Pi_\varepsilon \boldsymbol{G}_\varepsilon\rangle}_{=\frac{\mathsf{d}}{\mathsf{d}t}F(\Pi_\varepsilon(u_\varepsilon(t)))}](u_\varepsilon(t))\; \mathcal{Q}_\varepsilon[\underbrace{\langle \mathsf{D}F, \mathsf{D}\Pi_\varepsilon \boldsymbol{G}_\varepsilon\rangle}_{=\frac{\mathsf{d}}{\mathsf{d}t}F(\Pi_\varepsilon(u_\varepsilon(t+\tau)))}](u_\varepsilon(t+\tau))\,\mathsf{d}\tau$$

projection operators $\mathcal{P}_\varepsilon : \mathsf{C}(\mathcal{X}) \to \mathsf{C}(\mathcal{X})$ and $\mathcal{Q}_\varepsilon = \mathsf{id} - \mathcal{P}_\varepsilon$

with $\mathcal{P}_\varepsilon[\mathcal{F}](u) = \int_{\mathcal{X}} \mathcal{F}(\widehat{u})\rho_{\Pi_\varepsilon(u)}(\widehat{u})\,\mathsf{d}\widehat{u}$ $\quad$ $\mathcal{Q}_\varepsilon$ keeps only fluctuations!

**Green-Kubo formula 1966** for "macroscopic friction matrices"

# 3. GENERIC and coarse graining

To show: $\dot{u}_\varepsilon = \boldsymbol{G}_\varepsilon(u_\varepsilon) = \mathcal{L}_\varepsilon(u_\varepsilon)\mathsf{D}\mathcal{E}_\varepsilon(u_\varepsilon) \xrightarrow{y=\Pi_\varepsilon(u_\varepsilon)} \dot{y} = \mathbb{L}(y)\mathsf{D}\mathbb{E}(y) + \mathbb{K}(y)\mathsf{D}\mathbb{S}(y)$

$y = \Pi_\varepsilon(u), \quad \mathbb{E}(y) = \int_{\mathcal{X}} \mathcal{E}(u)\rho_y(u)\,\mathsf{d}u, \quad \mathbb{S}(y) = -k_\mathsf{B}\int_{\mathcal{X}} \rho_y(u)\log\rho_y(u)\,\mathsf{d}u$

$\mathbb{L}(y) = \int_{\mathcal{X}} \mathsf{D}\Pi(u)\mathcal{L}(u)\mathsf{D}\Pi(u)^\mathsf{T}\rho_y(u)\,\mathsf{d}u, \quad \mathbb{K}(y) = ???$

---

$\mathbb{K}(y) : \mathsf{T}^*_y\mathcal{Y} \to \mathsf{T}_y\mathcal{Y}$ needs dynamics (for well separated time scales)!!

For an observable (testfunction) $F : \mathcal{Y} \to \mathbb{R}$ we obtain correlations via

$\langle \mathsf{D}F(y), \mathbb{K}(y)\mathsf{D}F(y)\rangle =$

$$\lim_{\varepsilon\to 0} \frac{1}{k_\mathsf{B}} \int_{\tau=0}^{\sqrt{\varepsilon}} \mathcal{Q}_\varepsilon[\underbrace{\langle \mathsf{D}F, \mathsf{D}\Pi_\varepsilon \boldsymbol{G}_\varepsilon\rangle}_{=\frac{\mathsf{d}}{\mathsf{d}t}F(\Pi_\varepsilon(u_\varepsilon(t)))}](u_\varepsilon(t))\; \mathcal{Q}_\varepsilon[\underbrace{\langle \mathsf{D}F, \mathsf{D}\Pi_\varepsilon \boldsymbol{G}_\varepsilon\rangle}_{=\frac{\mathsf{d}}{\mathsf{d}t}F(\Pi_\varepsilon(u_\varepsilon(t+\tau)))}](u_\varepsilon(t+\tau))\,\mathsf{d}\tau$$

projection operators $\mathcal{P}_\varepsilon : \mathsf{C}(\mathcal{X}) \to \mathsf{C}(\mathcal{X})$ and $\mathcal{Q}_\varepsilon = \mathsf{id} - \mathcal{P}_\varepsilon$

with $\mathcal{P}_\varepsilon[\mathcal{F}](u) = \int_{\mathcal{X}} \mathcal{F}(\widehat{u})\rho_{\Pi_\varepsilon(u)}(\widehat{u})\,\mathsf{d}\widehat{u}$ $\qquad$ $\mathcal{Q}_\varepsilon$ keeps only fluctuations!

**Claim in BET'05:** Under *natural assumptions* (???) one has

- $(\mathcal{Y}, \mathbb{E}, \mathbb{S}, \mathbb{L}, \mathbb{K})$ is a GENERIC system
- $\Pi_\varepsilon(u_\varepsilon(t)) \longrightarrow y(t)$ solving $(\mathcal{Y}, \mathbb{E}, \mathbb{S}, \mathbb{L}, \mathbb{K})$

# 3. GENERIC and coarse graining

**Mathematical challenge: Prove this for one nontrivial case:**

1. $\mathbb{L}$ Poisson structure  ($\mathbb{L} = -\mathbb{L}^{\mathsf{T}}$ obvious, but Jacobi identity ?)
2. $\mathbb{K} = \mathbb{K}^{\mathsf{T}} \geq 0$  (classical fluctuation theory)
3. (a) $\mathbb{L}(y)\mathrm{D}\mathbb{S}(y) = 0$ and (b) $\mathbb{K}(y)\mathrm{D}\mathbb{E}(y) = 0$ on $\mathcal{Y}$
4. $\left.\begin{array}{l} u_\varepsilon \text{ solves } (\mathcal{X}, \mathcal{E}_\varepsilon, \mathbb{L}_\varepsilon) \\ \text{and } \Pi(u_\varepsilon(t)) \to y(t) \end{array}\right\} \implies y \text{ solves } (\mathcal{Y}, \mathbb{E}, \mathbb{S}, \mathbb{L}, \mathbb{K})$

# 3. GENERIC and coarse graining

**Mathematical challenge: Prove this for one nontrivial case:**

1. $\mathbb{L}$ Poisson structure  ($\mathbb{L} = -\mathbb{L}^{\mathsf{T}}$ obvious, but Jacobi identity ?)
2. $\mathbb{K} = \mathbb{K}^{\mathsf{T}} \geq 0$  (classical fluctuation theory)
3. (a) $\mathbb{L}(y)\mathrm{D}\mathbb{S}(y) = 0$ and (b) $\mathbb{K}(y)\mathrm{D}\mathbb{E}(y) = 0$ on $\mathcal{Y}$
4. $\left.\begin{array}{l} u_\varepsilon \text{ solves } (\mathcal{X}, \mathcal{E}_\varepsilon, \mathbb{L}_\varepsilon) \\ \text{and } \Pi(u_\varepsilon(t)) \to y(t) \end{array}\right\} \implies y \text{ solves } (\mathcal{Y}, \mathbb{E}, \mathbb{S}, \mathbb{L}, \mathbb{K})$

General intuition: (for well-separated time scales, i.e. $\varepsilon \to 0$)

- sppt $\rho_y(\cdot) \subset N_\varepsilon(\Pi_\varepsilon^{-1}(y)) \ \Rightarrow\ \int_{\mathcal{X}} F(\Pi_\varepsilon(u))\rho_y(u)\,\mathrm{d}u \approx F(y) \ \Rightarrow\ \mathcal{P}_\varepsilon^2 \approx \mathcal{P}_\varepsilon$
- Energy should be accessible, i.e. $\mathcal{E}_\varepsilon(u) \approx \mathbb{E}(\Pi_\varepsilon(u)) \iff \mathcal{P}_\varepsilon\mathcal{E}_\varepsilon \approx \mathcal{E}_\varepsilon$

# 3. GENERIC and coarse graining

**Mathematical challenge: Prove this for one nontrivial case:**

1. $\mathbb{L}$ Poisson structure ($\mathbb{L} = -\mathbb{L}^{\mathsf{T}}$ obvious, but Jacobi identity ?)
2. $\mathbb{K} = \mathbb{K}^{\mathsf{T}} \geq 0$ (classical fluctuation theory)
3. (a) $\mathbb{L}(y)\mathrm{D}\mathbb{S}(y) = 0$ and (b) $\mathbb{K}(y)\mathrm{D}\mathbb{E}(y) = 0$ on $\mathcal{Y}$
4. $\left.\begin{array}{l} u_\varepsilon \text{ solves } (\mathcal{X}, \mathcal{E}_\varepsilon, \mathbb{L}_\varepsilon) \\ \text{and } \Pi(u_\varepsilon(t)) \to y(t) \end{array}\right\} \implies y \text{ solves } (\mathcal{Y}, \mathbb{E}, \mathbb{S}, \mathbb{L}, \mathbb{K})$

General intuition: (for well-separated time scales, i.e. $\varepsilon \to 0$)

- sppt $\rho_y(\cdot) \subset N_\varepsilon(\Pi_\varepsilon^{-1}(y)) \ \Rightarrow \ \int_{\mathcal{X}} F(\Pi_\varepsilon(u))\rho_y(u)\,\mathrm{d}u \approx F(y) \ \Rightarrow \ \mathcal{P}_\varepsilon^2 \approx \mathcal{P}_\varepsilon$
- Energy should be accessible, i.e. $\mathcal{E}_\varepsilon(u) \approx \mathbb{E}(\Pi_\varepsilon(u)) \iff \mathcal{P}_\varepsilon\mathcal{E}_\varepsilon \approx \mathcal{E}_\varepsilon$

**Ad 3(a):**

- energy converge $\Pi_\varepsilon(u_\varepsilon) \to y \ \Rightarrow \ \mathcal{E}(u_\varepsilon) = \mathbb{E}(\Pi_\varepsilon(u_\varepsilon)) \to \mathbb{E}(y)$
- $\mathrm{D}\mathbb{E}(y) \approx \mathrm{D}\Pi_\varepsilon(u_\varepsilon)\mathrm{D}\mathcal{E}(\varepsilon)$ for all $u_\varepsilon \in \Pi^{-1}(y) \approx \text{sppt}\,\rho_y \subset \mathcal{X}$
- $\mathcal{Q}_\varepsilon[\langle \mathrm{D}\mathbb{E}, \mathrm{D}\Pi_\varepsilon\mathcal{L}_\varepsilon\mathrm{D}\mathcal{E}_\varepsilon\rangle] \approx \mathcal{Q}_\varepsilon[\langle \mathrm{D}\mathcal{E}_\varepsilon, \mathcal{L}_\varepsilon\mathrm{D}\mathcal{E}_\varepsilon] \equiv 0 \implies \mathbb{K}(y)\mathbb{E}(y) = 0$

# 3. GENERIC and coarse graining

**Mathematical challenge: Prove this for one nontrivial case:**

1. $\mathbb{L}$ Poisson structure ($\mathbb{L} = -\mathbb{L}^{\mathsf{T}}$ obvious, but Jacobi identity ?)
2. $\mathbb{K} = \mathbb{K}^{\mathsf{T}} \geq 0$ (classical fluctuation theory)
3. (a) $\mathbb{L}(y)\mathrm{D}\mathbb{S}(y) = 0$ and (b) $\mathbb{K}(y)\mathrm{D}\mathbb{E}(y) = 0$ on $\mathcal{Y}$
4. $\left.\begin{array}{l} u_\varepsilon \text{ solves } (\mathcal{X}, \mathcal{E}_\varepsilon, \mathbb{L}_\varepsilon) \\ \text{and } \Pi(u_\varepsilon(t)) \to y(t) \end{array}\right\} \implies y \text{ solves } (\mathcal{Y}, \mathbb{E}, \mathbb{S}, \mathbb{L}, \mathbb{K})$

General intuition: (for well-separated time scales, i.e. $\varepsilon \to 0$)

- sppt $\rho_y(\cdot) \subset N_\varepsilon(\Pi_\varepsilon^{-1}(y)) \ \Rightarrow \ \int_{\mathcal{X}} F(\Pi_\varepsilon(u))\rho_y(u)\,\mathrm{d}u \approx F(y) \ \Rightarrow \ \mathcal{P}_\varepsilon^2 \approx \mathcal{P}_\varepsilon$
- Energy should be accessible, i.e. $\mathcal{E}_\varepsilon(u) \approx \mathbb{E}(\Pi_\varepsilon(u)) \iff \mathcal{P}_\varepsilon\mathcal{E}_\varepsilon \approx \mathcal{E}_\varepsilon$

**Ad 4(rev):**

$\mathrm{D}\mathbb{E}(y) \approx \mathrm{D}\Pi_\varepsilon(u_\varepsilon)\mathrm{D}\mathcal{E}(\varepsilon)$ for all $u_\varepsilon \in \Pi^{-1}(y) \approx \text{sppt}\,\rho_y \subset \mathcal{X}$

$$(\dot{y})_{\text{rev}} = \int_{\mathcal{X}} \left(\tfrac{\mathrm{d}}{\mathrm{d}t}\Pi_\varepsilon(u)\right)_{\text{rev}} \rho_y(u)\,\mathrm{d}u = \int_{\mathcal{X}} \mathrm{D}\Pi_\varepsilon(u)\mathcal{L}(u)\mathrm{D}\mathcal{E}(u)\rho_y(u)\,\mathrm{d}u$$

$$\approx \int_{\mathcal{X}} \mathrm{D}\Pi_\varepsilon(u)\mathcal{L}(u)\mathrm{D}\Pi_\varepsilon(u)^{\mathsf{T}}\mathrm{D}\mathbb{E}(\Pi_\varepsilon(u))\rho_y(u)\,\mathrm{d}u = \mathbb{L}(y)\mathrm{D}\mathbb{E}(y)$$

# Overview

# 4. Nonlinear Schrödinger equation

## Multiscale limit inside the class of Hamiltonian systems

$$(\mathcal{X}, \mathcal{H}_\varepsilon, \mathcal{L}_\varepsilon) \quad \rightsquigarrow \quad (\mathcal{Y}, \mathcal{H}_0, \mathcal{L}_0)$$

Partially confined nonlinear Schrödinger equation

$$-\mathrm{i}z_\tau = -\Delta_{\xi,y} z + V(y)z + |z|^2 z, \quad (\xi, y) \in \mathbb{R}^2, \ \tau \in \mathbb{R}$$

Confinement operator $\mathcal{C}z := -z_{yy} + V(y)z$ with compact resolvent
discrete spectrum $\mathcal{C}\Phi_n = E_n \Phi_n$.

Small parameter $\varepsilon$ only in init. cond.: $z_\varepsilon(0, \xi, y) = \varepsilon \mathrm{e}^{\mathrm{i}\theta_* \xi} A(\varepsilon\xi)\Phi_1(y)$.

## Multiscale limit inside the class of Hamiltonian systems

$$(\mathcal{X}, \mathcal{H}_\varepsilon, \mathcal{L}_\varepsilon) \quad \rightsquigarrow \quad (\mathcal{Y}, \mathcal{H}_0, \mathcal{L}_0)$$

Partially confined nonlinear Schrödinger equation

$$-\mathrm{i}z_\tau = -\Delta_{\xi,y} z + V(y)z + |z|^2 z, \quad (\xi, y) \in \mathbb{R}^2,\ \tau \in \mathbb{R}$$

Confinement operator $\mathcal{C}z := -z_{yy} + V(y)z$ with compact resolvent
discrete spectrum $\mathcal{C}\Phi_n = E_n \Phi_n$.

Small parameter $\varepsilon$ only in init. cond.: $z_\varepsilon(0, \xi, y) = \varepsilon \mathrm{e}^{\mathrm{i}\theta_* \xi} A(\varepsilon\xi)\Phi_1(y)$.

Expected traveling modulated waves:

$$z(\tau, \xi, y) = Z_A^\varepsilon(\tau, \xi, y) := \varepsilon \mathrm{e}^{\mathrm{i}(\theta_* \xi + \omega_* \tau)} A(\underbrace{\varepsilon^2 \tau}_{=:t}, \underbrace{\varepsilon(\xi + c_* \tau)}_{=:x}) \Phi_1(y) + \text{h.o.t.}$$

# 4. Nonlinear Schrödinger equation

## Multiscale limit inside the class of Hamiltonian systems

$$(\mathcal{X}, \mathcal{H}_\varepsilon, \mathcal{L}_\varepsilon) \quad \rightsquigarrow \quad (\mathcal{Y}, \mathcal{H}_0, \mathcal{L}_0)$$

Partially confined nonlinear Schrödinger equation

$$-\mathrm{i}z_\tau = -\Delta_{\xi,y} z + V(y)z + |z|^2 z, \quad (\xi, y) \in \mathbb{R}^2,\ \tau \in \mathbb{R}$$

Confinement operator $\mathcal{C}z := -z_{yy} + V(y)z$ with compact resolvent
discrete spectrum $\mathcal{C}\Phi_n = E_n \Phi_n$.

Small parameter $\varepsilon$ only in init. cond.: $z_\varepsilon(0, \xi, y) = \varepsilon \mathrm{e}^{\mathrm{i}\theta_* \xi} A(\varepsilon\xi)\Phi_1(y)$.

Expected traveling modulated waves:

$$z(\tau, \xi, y) = Z_A^\varepsilon(\tau, \xi, y) := \varepsilon \mathrm{e}^{\mathrm{i}(\theta_* \xi + \omega_* \tau)} A(\underbrace{\varepsilon^2 \tau}_{=:t}, \underbrace{\varepsilon(\xi + c_* \tau)}_{=:x}) \Phi_1(y) + \text{h.o.t.}$$

Slow time $t = \varepsilon^2 \tau$, macroscopic space $x = \varepsilon(\xi + c_* \tau)$.

Dispersion relations $\omega_* = \Omega_1(\theta_*) = \theta_*^2 + E_1$

group velocity $c_* = \Omega_1'(\theta_*) = 2\theta_*$

# 4. Nonlinear Schrödinger equation

## Multiscale limit inside the class of Hamiltonian systems

$$(\mathcal{X}, \mathcal{H}_\varepsilon, \mathcal{L}_\varepsilon) \quad \rightsquigarrow \quad (\mathcal{Y}, \mathcal{H}_0, \mathcal{L}_0)$$

Partially confined nonlinear Schrödinger equation

$$-\mathrm{i}z_\tau = -\Delta_{\xi,y} z + V(y)z + |z|^2 z, \quad (\xi, y) \in \mathbb{R}^2,\ \tau \in \mathbb{R}$$

Confinement operator $\mathcal{C}z := -z_{yy} + V(y)z$ with compact resolvent
discrete spectrum $\mathcal{C}\Phi_n = E_n \Phi_n$.

Small parameter $\varepsilon$ only in init. cond.: $z_\varepsilon(0, \xi, y) = \varepsilon \mathrm{e}^{\mathrm{i}\theta_* \xi} A(\varepsilon\xi)\Phi_1(y)$.

Expected traveling modulated waves:

$$z(\tau, \xi, y) = Z_A^\varepsilon(\tau, \xi, y) := \varepsilon \mathrm{e}^{\mathrm{i}(\theta_* \xi + \omega_* \tau)} A(\underbrace{\varepsilon^2 \tau}_{=:t}, \underbrace{\varepsilon(\xi + c_* \tau)}_{=:x}) \Phi_1(y) + \text{h.o.t.}$$

Aim: reprove under weaker assumptions

**Theorem (Schneider'95–10, Giannoulis-Herrmann-M.'06)**
$A \in \mathsf{C}^0([0,T]; \mathsf{H}^3(\mathbb{R};\mathbb{C}))$ solves $-\mathrm{i}A_t = -A_{xx} + c|A|^2 A$ $\quad (c = \int_{\mathbb{R}} \Phi_1^4 \,\mathrm{d}y)$
$z(0) = Z_A^\varepsilon(0) \implies \|z^\varepsilon(\tau) - Z_A^\varepsilon(\tau)\|_{\mathsf{H}^1} \le C_A \varepsilon^{3/2}$ for $\tau \in [0, T/\varepsilon^2]$.

# 4. Nonlinear Schrödinger equation

$-\mathrm{i}z_\tau = \mathrm{D}\mathcal{H}(z)$ with $\mathcal{H}(z) = \int_{\mathbb{R}^2} \frac{1}{2}|\nabla z|^2 + \frac{V(y)}{2}|z|^2 + \frac{1}{4}|z|^4 \,\mathrm{d}\xi\,\mathrm{d}y$.

By symmetry, there are two additionals integrals :

$\mathcal{I}_1(z) = \int_{\mathbb{R}^2} \frac{1}{2}|z|^2 \,\mathrm{d}\xi\,\mathrm{d}y$ phase invariance $z \mapsto \mathrm{e}^{\mathrm{i}\alpha} z$

$\mathcal{I}_2(z) = \int_{\mathbb{R}^2} \mathrm{Im}(z_\xi \overline{z})\,\mathrm{d}\xi\,\mathrm{d}y$ translation invariance $\xi \mapsto \xi + \beta$

# 4. Nonlinear Schrödinger equation

$-\mathrm{i}z_\tau = \mathrm{D}\mathcal{H}(z)$ with $\mathcal{H}(z) = \int_{\mathbb{R}^2} \frac{1}{2}|\nabla z|^2 + \frac{V(y)}{2}|z|^2 + \frac{1}{4}|z|^4 \,\mathrm{d}\xi\,\mathrm{d}y$.

By symmetry, there are two additionals integrals :

$\mathcal{I}_1(z) = \int_{\mathbb{R}^2} \frac{1}{2}|z|^2 \,\mathrm{d}\xi\,\mathrm{d}y$ phase invariance $z \mapsto \mathrm{e}^{\mathrm{i}\alpha} z$

$\mathcal{I}_2(z) = \int_{\mathbb{R}^2} \mathrm{Im}(z_\xi \overline{z})\,\mathrm{d}\xi\,\mathrm{d}y$ translation invariance $\xi \mapsto \xi + \beta$

**Preparation of system** (GHM'08)

**= transformation to see the "good" observables**

$u(t,x,y) = \mathcal{T}_\varepsilon z(t,x,y) = \frac{1}{\varepsilon}\mathrm{e}^{\mathrm{i}((\omega_* - \theta_* c_*)t/\varepsilon^2 + \theta_* x/\varepsilon)} z(\frac{t}{\varepsilon}, \frac{x}{\varepsilon} - \frac{c_* t}{\varepsilon^2})$.

Augmented Hamiltonian $\mathcal{H}_* = \mathcal{H} + (\omega_* - \theta_* c_*)\mathcal{I} + \theta_* \mathcal{I}_2$.

# 4. Nonlinear Schrödinger equation

$-\mathrm{i}z_\tau = \mathrm{D}\mathcal{H}(z)$ with $\mathcal{H}(z) = \int_{\mathbb{R}^2} \frac{1}{2}|\nabla z|^2 + \frac{V(y)}{2}|z|^2 + \frac{1}{4}|z|^4 \,\mathrm{d}\xi\,\mathrm{d}y.$

By symmetry, there are two additionals integrals :

$\mathcal{I}_1(z) = \int_{\mathbb{R}^2} \frac{1}{2}|z|^2 \,\mathrm{d}\xi\,\mathrm{d}y$ phase invariance $z \mapsto \mathrm{e}^{\mathrm{i}\alpha} z$

$\mathcal{I}_2(z) = \int_{\mathbb{R}^2} \mathrm{Im}(z_\xi \overline{z})\,\mathrm{d}\xi\,\mathrm{d}y$ translation invariance $\xi \mapsto \xi + \beta$

**Preparation of system** (GHM'08)

**= transformation to see the "good" observables**

$u(t,x,y) = \mathcal{T}_\varepsilon z(t,x,y) = \frac{1}{\varepsilon}\mathrm{e}^{\mathrm{i}((\omega_* - \theta_* c_*)t/\varepsilon^2 + \theta_* x/\varepsilon)} z(\frac{t}{\varepsilon}, \frac{x}{\varepsilon} - \frac{c_* t}{\varepsilon^2}).$

Augmented Hamiltonian $\mathcal{H}_* = \mathcal{H} + (\omega_* - \theta_* c_*)\mathcal{I} + \theta_* \mathcal{I}_2.$

We find after some calculations (see GHM08 for general setup)

$-\mathrm{i}u_t = \boldsymbol{H}_\varepsilon(u)$ where $\boldsymbol{H}_\varepsilon(u) = \underbrace{\frac{1}{\varepsilon^2}\frac{1}{\varepsilon}}_{\text{rescalings}} \mathcal{H}_*(\mathcal{T}_\varepsilon^{-1} u)$

with

$\boldsymbol{H}_\varepsilon(u) = \int_{\mathbb{R}^2} \frac{1}{2}|u_x|^2 + \frac{1}{2\varepsilon^2}\big(|u_y|^2 + V(y)|u|^2 - E_1|u|^2\big) + \frac{1}{4}|u|^4 \,\mathrm{d}x\,\mathrm{d}y$

# 4. Nonlinear Schrödinger equation

$$U_0 = \{\, u : (x,y) \mapsto A(x)\Phi_1(y) \mid A \in \mathsf{L}^2(\mathbb{R}) \,\} \subset U := \mathsf{L}^2(\mathbb{R}^2)$$
$$U_1 = U_0 \cap H^1(\mathbb{R}^2), \quad U_2 = U_0^\perp \cap H^1(\mathbb{R}^2)$$
$$\widetilde{\boldsymbol{H}} : U_1 \to \mathbb{R}; u = A\Phi_1 \mapsto \textstyle\int_{\mathbb{R}} \frac{1}{2}|A_x|^2 + \frac{c}{4}|A|^4 \,\mathsf{d}x.$$

**Proposition on $\Gamma$-limit.**

(A) $$\boldsymbol{H}_\varepsilon \xrightarrow{\Gamma} \boldsymbol{H}_0 : u \mapsto \begin{cases} \widetilde{\boldsymbol{H}}(u) & \text{for } u \in U_1, \\ \infty & \text{otherwise.} \end{cases}$$

(B) $$\left.\begin{array}{c} u_\varepsilon \rightharpoonup u_0 \\ \boldsymbol{H}_\varepsilon(u_\varepsilon) \to \boldsymbol{H}_0(u_0) < \infty \end{array}\right\} \implies \mathsf{D}\boldsymbol{H}_\varepsilon(u_\varepsilon)|_{U_1} \rightharpoonup \mathsf{D}\widetilde{\boldsymbol{H}}(u_0)$$

# 4. Nonlinear Schrödinger equation

$$U_0 = \{\, u : (x,y) \mapsto A(x)\Phi_1(y) \mid A \in \mathsf{L}^2(\mathbb{R}) \,\} \subset U := \mathsf{L}^2(\mathbb{R}^2)$$
$$U_1 = U_0 \cap H^1(\mathbb{R}^2), \quad U_2 = U_0^\perp \cap H^1(\mathbb{R}^2)$$
$$\widetilde{\boldsymbol{H}} : U_1 \to \mathbb{R}; u = A\Phi_1 \mapsto \textstyle\int_{\mathbb{R}} \frac{1}{2}|A_x|^2 + \frac{c}{4}|A|^4 \,\mathsf{d}x.$$

**Proposition on $\Gamma$-limit.**

(A) $\boldsymbol{H}_\varepsilon \xrightarrow{\Gamma} \boldsymbol{H}_0 : u \mapsto \begin{cases} \widetilde{\boldsymbol{H}}(u) & \text{for } u \in U_1, \\ \infty & \text{otherwise.} \end{cases}$

(B) $\left.\begin{array}{c} u_\varepsilon \rightharpoonup u_0 \\ \boldsymbol{H}_\varepsilon(u_\varepsilon) \to \boldsymbol{H}_0(u_0) < \infty \end{array}\right\} \implies \mathsf{D}\boldsymbol{H}_\varepsilon(u_\varepsilon)|_{U_1} \rightharpoonup \mathsf{D}\widetilde{\boldsymbol{H}}(u_0)$

Remarks:

1. In (B) $\mathsf{D}\boldsymbol{H}_\varepsilon(u_\varepsilon)|_{U_2}$ is in general unbounded.
2. To obtain $-\mathrm{i}\dot{u}_0 = \mathsf{D}\widetilde{\boldsymbol{H}}(u_0)$ is suffices to test $-\mathrm{i}\dot{u}_\varepsilon = \mathsf{D}\boldsymbol{H}_\varepsilon(u_\varepsilon)$ with $w_0 \in \mathsf{C}^1_{\mathsf{c}}(\mathbb{R}; U_1)$.

# 4. Nonlinear Schrödinger equation

$$U_0 = \{\, u : (x,y) \mapsto A(x)\Phi_1(y) \mid A \in \mathsf{L}^2(\mathbb{R}) \,\} \subset U := \mathsf{L}^2(\mathbb{R}^2)$$
$$U_1 = U_0 \cap H^1(\mathbb{R}^2), \quad U_2 = U_0^\perp \cap H^1(\mathbb{R}^2)$$
$$\widetilde{\boldsymbol{H}} : U_1 \to \mathbb{R}; u = A\Phi_1 \mapsto \textstyle\int_{\mathbb{R}} \frac{1}{2}|A_x|^2 + \frac{c}{4}|A|^4 \,\mathrm{d}x.$$

**Proposition on $\Gamma$-limit.**

(A) $\boldsymbol{H}_\varepsilon \xrightarrow{\Gamma} \boldsymbol{H}_0 : u \mapsto \begin{cases} \widetilde{\boldsymbol{H}}(u) & \text{for } u \in U_1, \\ \infty & \text{otherwise.} \end{cases}$

(B) $\left.\begin{array}{c} u_\varepsilon \rightharpoonup u_0 \\ \boldsymbol{H}_\varepsilon(u_\varepsilon) \to \boldsymbol{H}_0(u_0) < \infty \end{array}\right\} \implies \mathsf{D}\boldsymbol{H}_\varepsilon(u_\varepsilon)|_{U_1} \rightharpoonup \mathsf{D}\widetilde{\boldsymbol{H}}(u_0)$

**Theorem.** If $u_\varepsilon$ solves $-\mathrm{i}\dot{u} = \mathsf{D}\boldsymbol{H}_\varepsilon(u)$ and $u_\varepsilon(0) \rightharpoonup u_0(0)$ in $\mathsf{H}^1$ and $\boldsymbol{H}_\varepsilon(u_\varepsilon(0)) \to \boldsymbol{H}_0(u_0(0)) < \infty$, then

$$u_\varepsilon(t) \rightharpoonup u_0(t) \text{ in } \mathsf{H}^1(\mathbb{R}^2) \text{ for all } t \in \mathbb{R},$$

where $u_0$ solves $-\mathrm{i}\dot{u}_0 = \mathsf{D}\widetilde{\boldsymbol{H}}(u_0)$.

# Overview

# 5. From viscous to dry friction

For purely dissipative systems (i.e. $\mathcal{L}_\varepsilon \equiv 0$) we prefer the **dissipation potential** $\mathcal{R}_\varepsilon$ against the Onsager operator $\mathcal{K}_\varepsilon$:

$\mathcal{R}_\varepsilon(u,\dot u) = \frac{1}{2}\langle K_\varepsilon(u)^{-1}\dot u, \dot u\rangle$

$$0 = \mathsf{D}_{\dot u}\mathcal{R}_\varepsilon(u,\dot u) + \mathsf{D}\mathcal{F}_\varepsilon(u) \quad \Longleftrightarrow \quad \dot u = -\mathcal{K}_\varepsilon(u)\mathsf{D}\mathcal{F}_\varepsilon(u)$$

(internal) force balance versus rate equation

# 5. From viscous to dry friction

For purely dissipative systems (i.e. $\mathcal{L}_\varepsilon \equiv 0$) we prefer the **dissipation potential** $\mathcal{R}_\varepsilon$ against the Onsager operator $\mathcal{K}_\varepsilon$:

$\mathcal{R}_\varepsilon(u,\dot u) = \frac{1}{2}\langle K_\varepsilon(u)^{-1}\dot u, \dot u\rangle$

$$0 = \mathrm{D}_{\dot u}\mathcal{R}_\varepsilon(u,\dot u) + \mathrm{D}\mathcal{F}_\varepsilon(u) \qquad \Longleftrightarrow \qquad \dot u = -\mathcal{K}_\varepsilon(u)\mathrm{D}\mathcal{F}_\varepsilon(u)$$

(internal) force balance versus rate equation

We call the energy-driven system $(\mathcal{X},\mathcal{F}_\varepsilon,\mathcal{R}_\varepsilon)$ a viscous system or a generalized gradient system.

**Same question as before:**

If $\mathcal{F}_\varepsilon \rightsquigarrow \mathcal{F}_0$ and $\mathcal{R}_\varepsilon \rightsquigarrow \mathcal{R}_0$, do we have

$u_\varepsilon(0) \rightharpoonup y(0) \quad \Longrightarrow \quad u_\varepsilon(t) \rightharpoonup y(t)$ which solves $(\mathcal{Y},\mathcal{F}_0,\mathcal{R}_0)$?

# 5. From viscous to dry friction

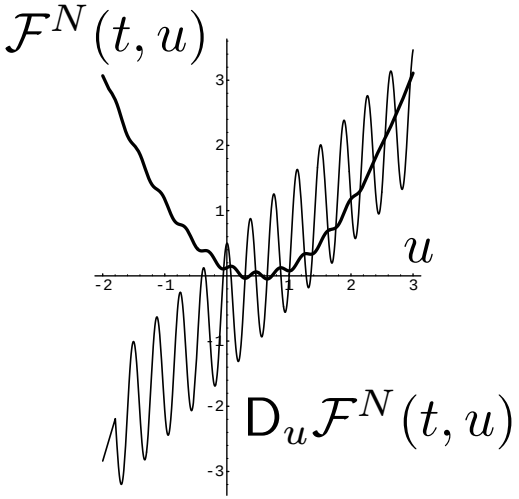
**Scalar model with *wiggly energy landscape***

**James '96, Menon '02** ($N = 1/\varepsilon \to \infty$)
Puglisi&Truskinovsky '02,'05 ($N \to \infty,\ \nu \to 0$)

***wiggly energy*** on $\mathcal{X} = \mathbb{R}$:
$\mathcal{F}^N(t,u) = \frac{1}{2}u^2 - \ell(t)u + \frac{1}{N}w(u,Nu)$

macroscopic part of energy

wiggly part $w(u,r)$
is 1-periodic in $r = Nu$




$$\boxed{\nu\dot{u} = -\mathsf{D}_u\mathcal{F}^N(t,u) = -\big(u-\ell(t)\big) - \big(\tfrac{1}{N}w_u(u,Nu) + w_r(u,Nu)\big)}$$

$u_{N,\nu}(t) \to y(t) = ???$ for $N \to \infty$ and $\nu \to 0$ $\quad (\nu = \frac{\text{loading rate}}{\text{viscosity}})$

# 5. From viscous to dry friction

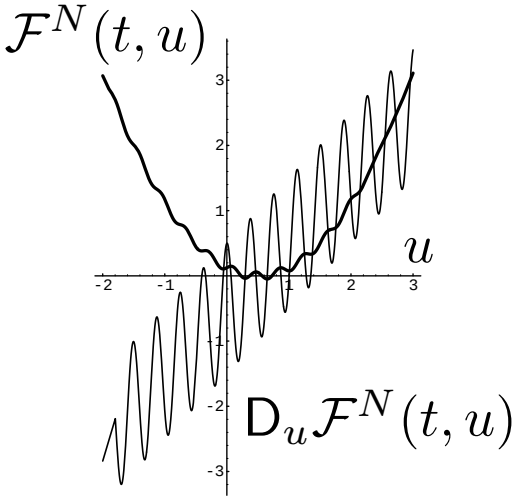
**Scalar model with *wiggly energy landscape***

**James '96, Menon '02** ($N = 1/\varepsilon \to \infty$)
Puglisi&Truskinovsky '02,'05 ($N \to \infty,\ \nu \to 0$)

***wiggly energy*** on $\mathcal{X} = \mathbb{R}$:
$\mathcal{F}^N(t,u) = \frac{1}{2}u^2 - \ell(t)u + \frac{1}{N}w(u,Nu)$

macroscopic part of energy

wiggly part $w(u,r)$
is 1-periodic in $r = Nu$




$$\boxed{\nu\dot{u} = -\mathsf{D}_u\mathcal{F}^N(t,u) = -\big(u-\ell(t)\big) - \big(\tfrac{1}{N}w_u(u,Nu) + w_r(u,Nu)\big)}$$

$u_{N,\nu}(t) \to y(t) = ???$ for $N \to \infty$ and $\nu \to 0$ $\quad (\nu = \frac{\text{loading rate}}{\text{viscosity}})$

$\mathcal{F}^N(t,u^N) \to \mathcal{F}^\infty(t,y) = \frac{1}{2}y^2 - \ell(t)y + 0$

Of course: $y$ does **not** solve $0 = -\mathsf{D}_y\mathcal{F}^\infty(t,y(t))$

# 5. From viscous to dry friction

Simulation: $\mathcal{F}^N(t,u) = \frac{1}{2}u^2 - \ell(t)u - \frac{1}{N}\cos(Nu)$,

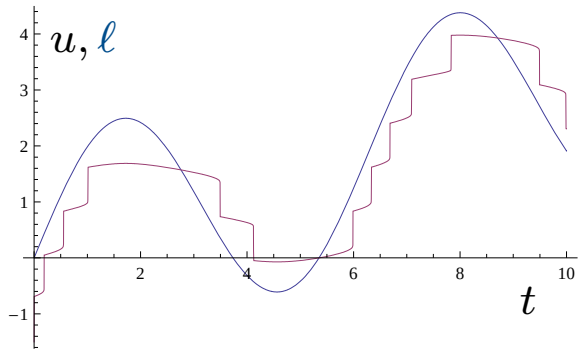
$\ell(t) = 2\sin t + 0.3\,t, \quad u(0) = -1.0, \quad \nu = 10^{-3}$

# 5. From viscous to dry friction

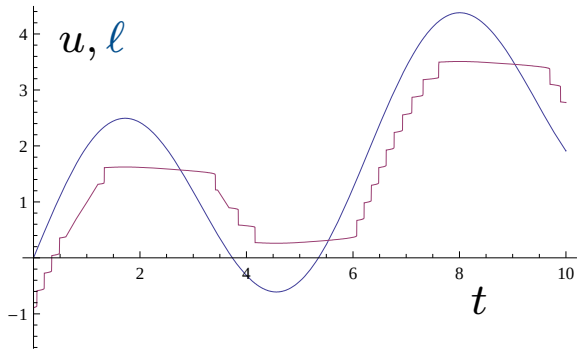
Simulation: $\mathcal{F}^N(t,u) = \frac{1}{2}u^2 - \ell(t)u - \frac{1}{N}\cos(Nu)$,

$\ell(t) = 2\sin t + 0.3\,t, \quad u(0) = -1.0, \quad \nu = 10^{-3}$

$N = 8$




$N = 20$

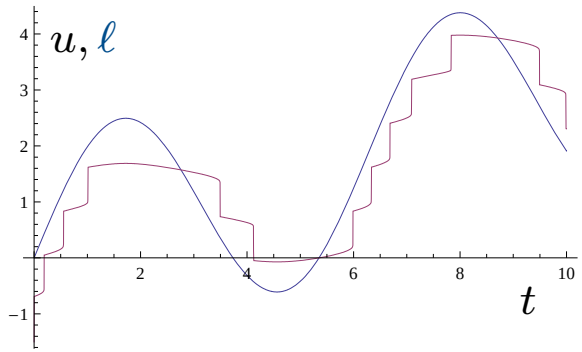


# 5. From viscous to dry friction

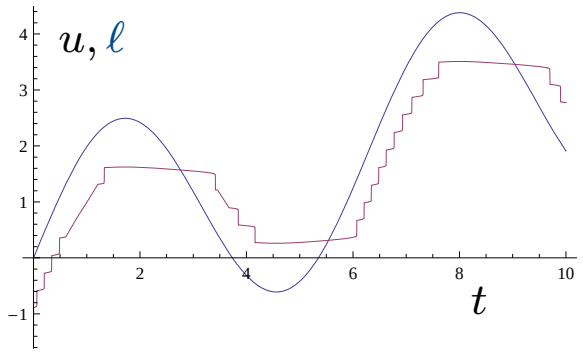
Simulation: $\mathcal{F}^N(t,u) = \frac{1}{2}u^2 - \ell(t)u - \frac{1}{N}\cos(Nu)$,

$\ell(t) = 2\sin t + 0.3\,t, \quad u(0) = -1.0, \quad \nu = 10^{-3}$

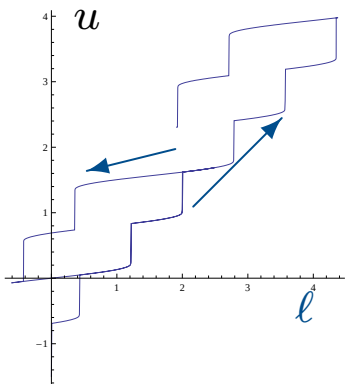
$N = 8$



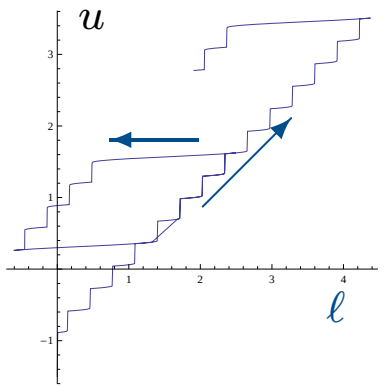

$N = 20$




$N = 8$




$N = 20$




For $N \to \infty$ and $\nu \to 0$ (vanishing-viscosity limit):
Convergence to a rate-independent hysteresis operator: play operator

# 5. From viscous to dry friction

Rate-independent limit exists and displays hysteresis

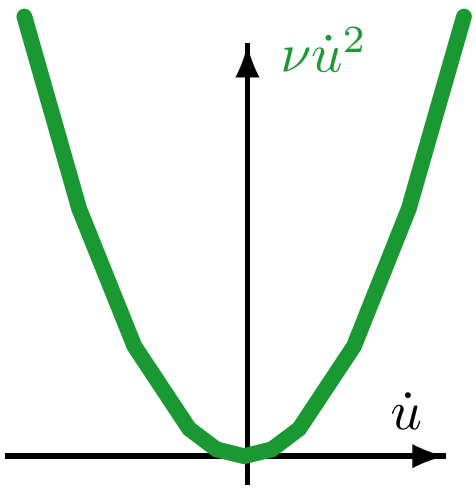
Limits for $N \to \infty$ and $\nu \to 0$:

Dissipation potential $\mathcal{R}^\infty(y,\dot y) = \begin{cases} \rho_+(y)\dot y & \text{for } \dot y \geq 0, \\ \rho_-(y)|\dot y| & \text{for } \dot y \leq 0, \end{cases}$

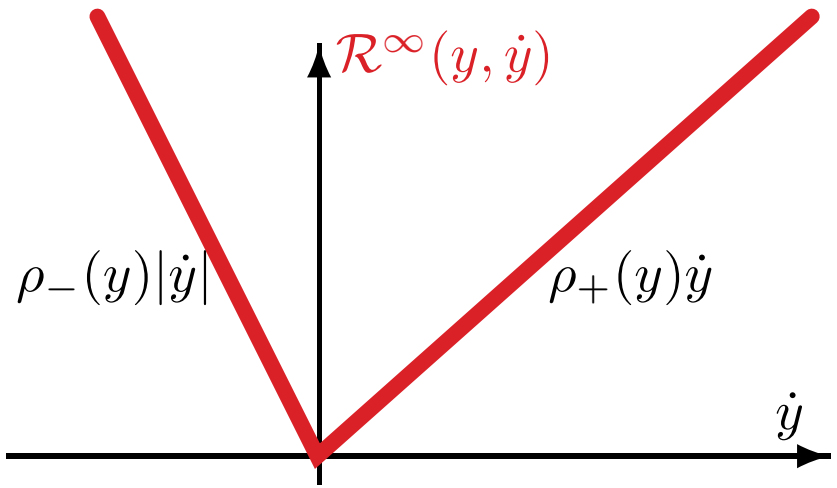
$$\rho_+(y) = \max\{\, w_r(y,r) \mid r \in \mathbb{R}\,\} > 0, \quad \rho_-(y) = -\min\{\, w_r(y,r) \mid r \in \mathbb{R}\,\} > 0$$

(maximal slopes of the wiggles)

viscous dissipation




rate-independent dissipation



# 5. From viscous to dry friction

Rate-independent limit exists and displays hysteresis

Limits for $N \to \infty$ and $\nu \to 0$:

Dissipation potential $\mathcal{R}^\infty(y,\dot y) = \begin{cases} \rho_+(y)\dot y & \text{for } \dot y \geq 0, \\ \rho_-(y)|\dot y| & \text{for } \dot y \leq 0, \end{cases}$

$$\rho_+(y) = \max\{\, w_r(y,r) \mid r \in \mathbb{R}\,\} > 0, \quad \rho_-(y) = -\min\{\, w_r(y,r) \mid r \in \mathbb{R}\,\} > 0$$

(maximal slopes of the wiggles)

**Theorem** (Puglisi & Truskinovsky 2002/05)
If $N \to \infty$ and $\nu \to 0$ (in any order),
then $u^N(t) \to y(t)$ and $y$ is the unique solution of

$$0 \in \partial^{\mathsf{sub}}_{\dot q}\mathcal{R}^\infty(y,\dot y) + \mathsf{D}_y\mathcal{F}^\infty(t,y)$$

Hence, we have $(\mathbb{R}, \mathcal{F}^N, \mathcal{R}^N) \rightsquigarrow (\mathbb{R}, \mathcal{F}^\infty, \mathcal{R}^\infty)$ !!

Rate-independent dissipation $\mathcal{R}^\infty$ arises from wiggly part of energy landscape!

- Stochastic wiggles give the same result, cf. T. Sullivan, PhD Thesis 2009
- Spatially distributed bi-stable chain leads to elastoplasticity, cf. M-Truskinovsky'10

# 5. From viscous to dry friction

Rate-independent limit exists and displays hysteresis

Limits for $N \to \infty$ and $\nu \to 0$:

Dissipation potential $\mathcal{R}^\infty(y,\dot y) = \begin{cases} \rho_+(y)\dot y & \text{for } \dot y \geq 0, \\ \rho_-(y)|\dot y| & \text{for } \dot y \leq 0, \end{cases}$

$$\rho_+(y) = \max\{\, w_r(y,r) \mid r \in \mathbb{R}\,\} > 0, \qquad \rho_-(y) = -\min\{\, w_r(y,r) \mid r \in \mathbb{R}\,\} > 0$$

(maximal slopes of the wiggles)

**Major challenge:**

**Provide a rigorous derivation of rate-independent plasticity from viscous (or even dynamic) models for dislocations.**

# Overview

# 6. Rate-independent systems and a dislocation model

**Rate-independent systems** have a dissipation potential
$\mathcal{R}(q,\cdot) : \mathsf{T}_q\mathcal{Q} \to [0,\infty]$ that is positively homogeneqous of degree 1,
viz. $\mathcal{R}(q,\gamma\dot{q}) = \gamma^1\,\mathcal{R}(q,\dot{q})$ for $\gamma > 0$.

The dissipative force is **rate-independent**: $\quad \mathsf{D}_{\dot{q}}\mathcal{R}(q,\gamma\dot{q}) = \gamma^0\,\mathsf{D}_{\dot{q}}\mathcal{R}(q,\dot{q})$

# 6. Rate-independent systems and a dislocation model

**Rate-independent systems** have a dissipation potential $\mathcal{R}(q,\cdot) : \mathsf{T}_q\mathcal{Q} \to [0,\infty]$ that is positively homogeneqous of degree 1, viz. $\mathcal{R}(q,\gamma\dot{q}) = \gamma^1\,\mathcal{R}(q,\dot{q})$ for $\gamma > 0$.

The dissipative force is **rate-independent**: $\mathsf{D}_{\dot{q}}\mathcal{R}(q,\gamma\dot{q}) = \gamma^0\,\mathsf{D}_{\dot{q}}\mathcal{R}(q,\dot{q})$

We define the **dissipation distance** $\mathcal{D} : \mathcal{Q}\times\mathcal{Q} \to [0,\infty]$ via

$$\mathcal{D}(q_1,q_2) \stackrel{\text{def}}{=} \inf\{\, \int_0^1 \mathcal{R}(\widetilde{q}(s),\dot{\widetilde{q}}(s))\,\mathsf{d}s \mid q_1 \xrightarrow{\widetilde{q}\in\mathsf{C}^1} q_2 \,\}$$

The force balance $0 = \mathsf{D}_{\dot{q}}\mathcal{R}(q,\dot{q}) + \mathsf{D}\mathcal{E}(t,q)$ can be reformulated in **energetic form** as follows.

Triples $(\mathcal{Q},\mathcal{E},\mathcal{D})$ are called **rate-independent systems (RIS)**.

# 6. Rate-independent systems and a dislocation model

**Definition:** $q = [0,T] \to \mathcal{Q}$ is an ***energetic solution*** of the RIS $(\mathcal{Q}, \mathcal{E}, \mathcal{D})$, if for all $t \in [0,T]$ **global stability (S)** and **energy balance (E)** hold:

**(S)** $\mathcal{E}(t, q(t)) \le \mathcal{E}(t, \widehat{q}) + \mathcal{D}(q(t), \widehat{q})$ for all $\widehat{q} \in \mathcal{Q}$;

**(E)** $\mathcal{E}(t, q(t)) + \mathrm{Diss}_{\mathcal{D}}(q, [0,t]) = \mathcal{E}(0, q(0)) + \int_0^t \partial_s \mathcal{E}(s, q(s)) \, \mathrm{d}s$

where

$\mathrm{Diss}_{\mathcal{D}}(q, [0,t]) \stackrel{\text{def}}{=} \sup\{ \sum_{j=1}^{N} \mathcal{D}(q(r_{j-1}), q(r_j)) \,|\, 0 = r_0 < r_1 < \cdots r_N = t \}$

# 6. Rate-independent systems and a dislocation model

**Definition:** $q = [0,T] \to \mathcal{Q}$ is an ***energetic solution*** of the RIS $(\mathcal{Q}, \mathcal{E}, \mathcal{D})$, if for all $t \in [0,T]$ **global stability (S)** and **energy balance (E)** hold:

**(S)** $\mathcal{E}(t, q(t)) \le \mathcal{E}(t, \widehat{q}) + \mathcal{D}(q(t), \widehat{q})$ for all $\widehat{q} \in \mathcal{Q}$;

**(E)** $\mathcal{E}(t, q(t)) + \mathrm{Diss}_{\mathcal{D}}(q, [0,t]) = \mathcal{E}(0, q(0)) + \int_0^t \partial_s \mathcal{E}(s, q(s)) \, \mathrm{d}s$

Energetic formulation **(S)&(E)**

- is totally rate independent,
- is derivative-free, as no linear structure needed !!
  (works in topological spaces)
- can be used for very general state spaces:
  applications with finite-strain elasticity (i.e. $\det \nabla \varphi > 0$)
  ... multiplicative elastoplasticity $\nabla \varphi = \boldsymbol{F}_{\mathsf{elast}} \boldsymbol{F}_{\mathsf{plast}}$ with $\det \boldsymbol{F}_{\mathsf{plast}} \equiv 1$
  ... microstructures (gradient Young measures), discrete indicators

# 6. Rate-independent systems and a dislocation model

**Definition:** $q = [0,T] \to \mathcal{Q}$ is an ***energetic solution*** of the RIS $(\mathcal{Q}, \mathcal{E}, \mathcal{D})$, if for all $t \in [0,T]$ **global stability (S)** and **energy balance (E)** hold:

**(S)** $\mathcal{E}(t, q(t)) \le \mathcal{E}(t, \widehat{q}) + \mathcal{D}(q(t), \widehat{q})$ for all $\widehat{q} \in \mathcal{Q}$;

**(E)** $\mathcal{E}(t, q(t)) + \mathrm{Diss}_{\mathcal{D}}(q, [0,t]) = \mathcal{E}(0, q(0)) + \int_0^t \partial_s \mathcal{E}(s, q(s)) \, \mathrm{d}s$

Energetic formulation **(S)&(E)**

- is equivalent to evolution equation, if $\mathcal{E}$ convex and $q \in \mathrm{C}^1$,
- admits a nice and very general existence theory for many material models:
  - hysteresis in shape-memory alloys (M-Theil-Levitas'99/'02),
  - brittle fracture, damage, crack evolution, delamination (e.g. Francfort-Dal Maso et al'98..'05, Roubicek-Thomas, ....),
  - strain-gradient elastoplasticity at finite strain (Mainik-M'09)
- is optimally suited for **evolutionary $\Gamma$-limits**

# 6. Rate-independent systems and a dislocation model

**$\Gamma$-convergence for RIS** (M-Roubíček-Stefanelli 2008 Calc Var PDE)

## Standard assumptions

- $\mathcal{E}_\varepsilon$ uniformly compact sublevels
- $\mathcal{E}_\varepsilon \overset{\Gamma}{\to} \mathcal{E}_0$ and $\mathcal{D}_\varepsilon \overset{\Gamma}{\to} \mathcal{D}_0$
- convergence of stresses/power $\partial_t \mathcal{E}_\varepsilon(t, q_\varepsilon) \to \partial_t \mathcal{E}_0(t, q_0)$ if $q_\varepsilon \rightharpoonup q_0$ and $q_\varepsilon$ is stable (i.e. (S) for $(\mathcal{Q}, \mathcal{E}_\varepsilon, \mathcal{D}_\varepsilon)$)

# 6. Rate-independent systems and a dislocation model

**$\Gamma$-convergence for RIS** (M-Roubíček-Stefanelli 2008 Calc Var PDE)

**Standard assumptions**

- $\mathcal{E}_\varepsilon$ uniformly compact sublevels
- $\mathcal{E}_\varepsilon \overset{\Gamma}{\to} \mathcal{E}_0$ and $\mathcal{D}_\varepsilon \overset{\Gamma}{\to} \mathcal{D}_0$
- convergence of stresses/power $\partial_t \mathcal{E}_\varepsilon(t, q_\varepsilon) \to \partial_t \mathcal{E}_0(t, q_0)$ if $q_\varepsilon \rightharpoonup q_0$ and $q_\varepsilon$ is stable (i.e. (S) for $(\mathcal{Q}, \mathcal{E}_\varepsilon, \mathcal{D}_\varepsilon)$)

**Dynamic interaction condition = exist. of mutual recovery sequences**

$$\limsup_{\varepsilon\to 0} \mathcal{E}_\varepsilon(t, \widehat{q}_\varepsilon) + \mathcal{D}_\varepsilon(q_\varepsilon, \widehat{q}_\varepsilon) - \mathcal{E}_\varepsilon(t, q_\varepsilon) \le \mathcal{E}_0(t, \widehat{q}) + \mathcal{D}_0(q_0, \widehat{q}_0) - \mathcal{E}_0(t, q_0)$$

**Theorem.** Under the above and additional technical conditions we have:

**If** $q_\varepsilon : [0,T] \to \mathcal{Q}$ are energetic solutions for $(\mathcal{Q}, \mathcal{E}_\varepsilon, \mathcal{D}_\varepsilon)$ for $\varepsilon > 0$ and
$q_\varepsilon(0) \rightharpoonup q_0^0$ and $\mathcal{E}_\varepsilon(0, q_\varepsilon(0)) \to \mathcal{E}_0(0, q_0^0)$,

**then**, $q_\varepsilon(t) \rightharpoonup q_0(t)$ (for a subsequence),
$q_0 : [0,T] \to \mathcal{Q}$ is energetic solution of $(\mathcal{Q}, \mathcal{E}_0, \mathcal{D}_0)$, and
$\mathcal{E}_\varepsilon(t, q_\varepsilon(t)) \to \mathcal{E}_0(t, q_0(t))$ and $\mathrm{Diss}_{\mathcal{D}_\varepsilon}(q_\varepsilon, [0,t]) \to \mathrm{Diss}_{\mathcal{D}_0}(q_0, [0,t])$.

# 6. Rate-independent systems and a dislocation model

**Theorem.** Under the above and additional technical conditions we have:

**If** $q_\varepsilon : [0,T] \to \mathcal{Q}$ are energetic solutions for $(\mathcal{Q}, \mathcal{E}_\varepsilon, \mathcal{D}_\varepsilon)$ for $\varepsilon > 0$ and
$q_\varepsilon(0) \rightharpoonup q_0^0$ and $\mathcal{E}_\varepsilon(0, q_\varepsilon(0)) \to \mathcal{E}_0(0, q_0^0)$,

**then**, $q_\varepsilon(t) \rightharpoonup q_0(t)$ (for a subsequence),
$q_0 : [0,T] \to \mathcal{Q}$ is energetic solution of $(\mathcal{Q}, \mathcal{E}_0, \mathcal{D}_0)$, and
$\mathcal{E}_\varepsilon(t, q_\varepsilon(t)) \to \mathcal{E}_0(t, q_0(t))$ and $\mathrm{Diss}_{\mathcal{D}_\varepsilon}(q_\varepsilon, [0,t]) \to \mathrm{Diss}_{\mathcal{D}_0}(q_0, [0,t])$.

**$\Gamma$-convergence in the class of RIS only!**

# 6. Rate-independent systems and a dislocation model

**Theorem.** Under the above and additional technical conditions we have:

**If** $q_\varepsilon : [0,T] \to \mathcal{Q}$ are energetic solutions for $(\mathcal{Q}, \mathcal{E}_\varepsilon, \mathcal{D}_\varepsilon)$ for $\varepsilon > 0$ and
$q_\varepsilon(0) \rightharpoonup q_0^0$ and $\mathcal{E}_\varepsilon(0, q_\varepsilon(0)) \to \mathcal{E}_0(0, q_0^0)$,

**then**, $q_\varepsilon(t) \rightharpoonup q_0(t)$ (for a subsequence),
$q_0 : [0,T] \to \mathcal{Q}$ is energetic solution of $(\mathcal{Q}, \mathcal{E}_0, \mathcal{D}_0)$, and
$\mathcal{E}_\varepsilon(t, q_\varepsilon(t)) \to \mathcal{E}_0(t, q_0(t))$ and $\mathrm{Diss}_{\mathcal{D}_\varepsilon}(q_\varepsilon, [0,t]) \to \mathrm{Diss}_{\mathcal{D}_0}(q_0, [0,t])$.

**$\Gamma$-convergence in the class of RIS only!**

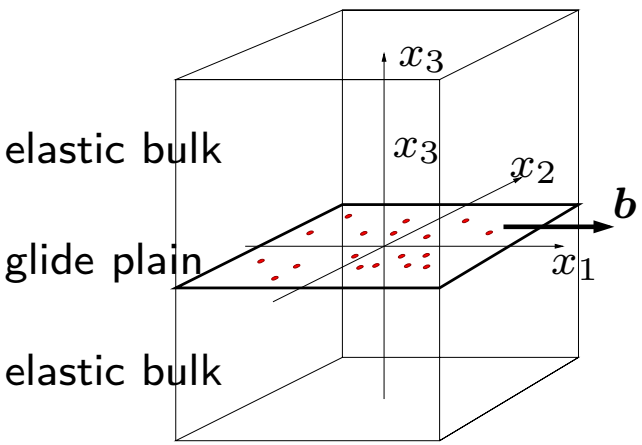
**Already many applications:**

- convergence to Younhg measures in models for shape-memory alloys
- damage-models converge to crack models
- homogenization of elastoplasticity or ferroelectricity
- derivation of a new elastoplastic plate model
- convergence of numerical approximation schemes

## Time-dependent dislocation model in the line-tension limit

modeling: Koslowski-Cuitino-Ortiz 2002

analysis: Garroni-Müller 2005–




$\Omega = \mathbb{T}^2 \times \mathbb{R} \subset \mathbb{R}^3$ unit cylinder in a crystal

$\mathbb{T}^2 = \mathbb{R}^2/\mathbb{Z}^2$ unit cell of slip plane

$\boldsymbol{b} = (1,0,0)^\top$ slip direction

$N_\varepsilon$ pinning sites of radius $\rho\varepsilon > 0$ in $\mathbb{T}^2$.

$u : \mathbb{T}^2 \to \mathbb{R}$ slip between the upper and lower part

$$U^{\mathsf{3D}}(x_1, x_2, 0^+) - U^{\mathsf{3D}}(x_1, x_2, 0^-) = \begin{pmatrix} \boldsymbol{b}u(x_1, x_2) \\ 0 \\ 0 \end{pmatrix}$$

## Energy storage

$$\mathcal{E}_\varepsilon(t,u) = \frac{1}{\varepsilon N_\varepsilon} \iint_{\mathbb{T}^2\times\mathbb{T}^2} K(x-y)(u(x)-u(y))^2 \,\mathrm{d}xy \qquad \text{elastic bulk energy}$$

$$+ \frac{1}{\varepsilon^2 N_\varepsilon} \int_{\mathbb{T}^2} \mathrm{dist}(u(x),\mathbb{Z})^2 \,\mathrm{d}x \qquad \text{Peierls energy}$$

$$- \int_{\mathbb{T}^2} f^\varepsilon_{\mathsf{ext}}(t,x)u(x)\,\mathrm{d}x \qquad \text{ext. shear loading}$$

## Energy storage

$$\mathcal{E}_\varepsilon(t,u) = \frac{1}{\varepsilon N_\varepsilon}\iint_{\mathbb{T}^2\times\mathbb{T}^2} K(x-y)(u(x)-u(y))^2\,\mathrm{d}xy \qquad \text{elastic bulk energy}$$

$$+\frac{1}{\varepsilon^2 N_\varepsilon}\int_{\mathbb{T}^2} \mathrm{dist}(u(x),\mathbb{Z})^2\,\mathrm{d}x \qquad \text{Peierls energy}$$

$$-\int_{\mathbb{T}^2} f^\varepsilon_{\mathsf{ext}}(t,x)u(x)\,\mathrm{d}x \qquad \text{ext. shear loading}$$

**Dissipation** via work against pinning sites

$$\mathcal{D}_\varepsilon(u_{\mathsf{old}},u_{\mathsf{new}}) = \frac{1}{\varepsilon^2 N_\varepsilon}\int_{\mathbb{T}^2}\sum_{i=1}^{N_\varepsilon} \underbrace{\psi\big(\tfrac{1}{\varepsilon}(x-x^i_\varepsilon)\big)}_{\text{pinning strength}} \big|u_{\mathsf{new}}(x)-u_{\mathsf{old}}(x)\big|\,\mathrm{d}x$$

# 6. Rate-independent systems and a dislocation model

We have a rate-independent systems $(\mathcal{Q}, \mathcal{E}_\varepsilon, \mathcal{D}_\varepsilon)$ where $\mathcal{Q} = \mathsf{L}^2(\mathbb{T}^2)$

**Challenge:** Find $\Gamma$-limit for critical scaling $N_\varepsilon = \Lambda \left|\log \varepsilon\right| / \varepsilon$

# 6. Rate-independent systems and a dislocation model

We have a rate-independent systems $(\mathcal{Q}, \mathcal{E}_\varepsilon, \mathcal{D}_\varepsilon)$ where $\mathcal{Q} = \mathsf{L}^2(\mathbb{T}^2)$

**Challenge:** Find $\Gamma$-limit for critical scaling $N_\varepsilon = \Lambda \, |\log \varepsilon| \, / \varepsilon$

Joint work with St. Müller in DFG-Research Unit 797 MICROPLAST

Preliminary result for simplified dissipation distance (homogenized pinning) $\overline{\mathcal{D}}_\varepsilon = \overline{\mathcal{D}}$ with $\overline{\mathcal{D}}(u_{\mathsf{old}}, u_{\mathsf{new}}) = \psi_0 \|u_{\mathsf{new}} - u_{\mathsf{old}}\|_{\mathsf{L}^1}$

# 6. Rate-independent systems and a dislocation model

We have a rate-independent systems $(\mathcal{Q}, \mathcal{E}_\varepsilon, \mathcal{D}_\varepsilon)$ where $\mathcal{Q} = \mathsf{L}^2(\mathbb{T}^2)$

**Challenge:** Find $\Gamma$-limit for critical scaling $N_\varepsilon = \Lambda \, |\log \varepsilon| \, / \varepsilon$

Joint work with St. Müller in DFG-Research Unit 797 MICROPLAST

Preliminary result for simplified dissipation distance (homogenized pinning) $\overline{\mathcal{D}}_\varepsilon = \overline{\mathcal{D}}$ with $\overline{\mathcal{D}}(u_{\mathsf{old}}, u_{\mathsf{new}}) = \psi_0 \|u_{\mathsf{new}} - u_{\mathsf{old}}\|_{\mathsf{L}^1}$

**Theorem.** For $N_\varepsilon = \Lambda \, |\log \varepsilon| \, / \varepsilon$ and $\overline{\mathcal{D}}_\varepsilon = \overline{\mathcal{D}}$ we have

$$(\mathcal{Q}, \mathcal{E}_\varepsilon, \overline{\mathcal{D}}) \quad \overset{\Gamma}{\to} \quad (\mathcal{Q}, \mathbb{E}, \overline{\mathcal{D}})$$

where $\mathbb{E}$ is the line-tension energy

$$\mathbb{E}(t,u) = \begin{cases} \int_{S(u)} \gamma(\nu) |[\![u]\!]| \mathrm{d}\mathcal{H}^1 & \text{for } u \in \mathsf{BV}(\Omega;\mathbb{Z}), \\ \infty & \text{otherwise.} \end{cases}$$

Proof of above theorem is a slight generalization of Garroni-Müller'06 ARMA
Challenge means to construct **mutual recovery sequences** for $(\mathcal{Q}, \mathcal{E}_\varepsilon, \mathcal{D}_\varepsilon)$.

# Overview

1. Introduction
2. Convergence of functionals and forces
3. GENERIC and coarse graining
4. Nonlinear Schrödinger equation
5. From viscous to dry friction
6. Rate-independent systems and a dislocation model
7. **Conclusion**

# 7. Conclusion

- Evolutionary multiscale systems are mathematically quite challenging
- Systems driven by functionals enjoy special benefits
  - conservation of energy, growth of entropy
  - geometric structures are helpful and organize the mathematics
  - driving forces may converge automatically

$$\Big(u_\varepsilon \rightharpoonup y \text{ and } \mathcal{F}_\varepsilon(u_\varepsilon) \to \mathcal{F}_0(y)\Big) \implies \mathsf{D}\mathcal{F}_\varepsilon(u_\varepsilon) \rightharpoonup \mathsf{D}\mathcal{F}_0(y)$$

# 7. Conclusion

- Evolutionary multiscale systems are mathematically quite challenging
- Systems driven by functionals enjoy special benefits
  - conservation of energy, growth of entropy
  - geometric structures are helpful and organize the mathematics
  - driving forces may converge automatically

$$\Big(u_\varepsilon \rightharpoonup y \text{ and } \mathcal{F}_\varepsilon(u_\varepsilon) \to \mathcal{F}_0(y)\Big) \implies \mathrm{D}\mathcal{F}_\varepsilon(u_\varepsilon) \rightharpoonup \mathrm{D}\mathcal{F}_0(y)$$

- Multiscale passage within one class relatively easy
- Passages between different dissipation classes remain a major challenge

# 7. Conclusion

- Evolutionary multiscale systems are mathematically quite challenging
- Systems driven by functionals enjoy special benefits
  - conservation of energy, growth of entropy
  - geometric structures are helpful and organize the mathematics
  - driving forces may converge automatically

$$\Big(u_\varepsilon \rightharpoonup y \text{ and } \mathcal{F}_\varepsilon(u_\varepsilon) \to \mathcal{F}_0(y)\Big) \implies \mathrm{D}\mathcal{F}_\varepsilon(u_\varepsilon) \rightharpoonup \mathrm{D}\mathcal{F}_0(y)$$

- Multiscale passage within one class relatively easy
- Passages between different dissipation classes remain a major challenge

**Thank You for Your Attention**