

# Analysis of the Effect of a Heat Bath on a Rate-Independent System

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# Introduction

- Many deterministic physical processes are modeled by evolution laws that incorporate not just energetics but also dissipation, *i.e.* loss of energy due to frictional effects. Mathematically, these processes can be modelled as **gradient descents** — in the case of 1-homogenous dissipation, they are **rate-independent processes**.
- Also, many physical processes are subject to some randomness, perhaps due to the presence of a heat bath, which supplies additional (uncorrelated) energy to the process.

## Question

How does a gradient descent (in particular, a rate-independent system) behave when placed in contact with a heat bath?

To investigate this, we introduce a notion of **thermalized gradient descent**.

# Introduction

- The thermalization procedure is quite general, and in the case of 2-homogenous dissipation it corresponds to additive  $\text{It}\bar{o}$  noise.
- In the case of 1-homogeneous dissipation (a rate-independent system), something unexpected happens: the heat bath destroys the rate-independence in a controlled way and yields a **deterministic nonlinear gradient descent**; the thermalized dissipation potential is a “smoothing out” of the original one.
- As a toy model, consider a rough block sitting on a sandpaper table and subject to forces (springs, external loads, & c.) weaker than the frictional resistance of the sandpaper/block interface. Intuition suggests that
  - at “**zero temperature**”, the block shouldn’t move at all;
  - at “**positive temperature**” (shaking the table), the block might move — will it move deterministically? randomly?

## Some Notation

- $P$  will denote a **finite partition** of an interval of time  $[0, T]$ :

$$P = \{0 = t_0 < t_1 < t_2 < \cdots < t_N = T\}.$$

- $\Delta$  will denote the **backward difference operator** acting on sequences, finite or infinite, taking values in  $\mathbb{R}$ ,  $\mathbb{R}^n$ , or any vector space  $\mathcal{Z}$ :

$$\Delta z_i := z_i - z_{i-1}.$$

- $\bar{z}^{(P)}: [0, T] \rightarrow \mathcal{Z}$  will denote the **piecewise-constant càdlàg interpolation** of  $z_0, z_1, \dots, z_N \in \mathcal{Z}$  on the partition  $P$ :

$$\bar{z}^{(P)}(t) := z_i \text{ for all } t \in [t_i, t_{i+1}).$$

- $\llbracket P \rrbracket$  will denote the **mesh size** of  $P$ :

$$\llbracket P \rrbracket := \max_{i=1, \dots, N} |\Delta t_i|.$$

## Gradient Descents — The Basics

- Many evolutionary models for physical processes are posed in terms of a quantity/field of interest,  $z: [0, T] \rightarrow \mathcal{Z}$ ,  $\mathcal{Z}$  being some (suitably nice) linear space (e.g. Hilbert, Banach,  $BV(\Omega; \mathbb{R}^3)$ , ...).
- The evolution of  $z$  is determined by an initial condition, an **energetic potential**  $E: [0, T] \times \mathcal{Z} \rightarrow \mathbb{R} \cup \{+\infty\}$  and a **dissipation potential**  $\Psi: \mathcal{Z} \rightarrow [0, +\infty]$ .

### Example

In  $\mathcal{Z} = \mathbb{R}^n$  with dissipation  $\Psi = \frac{1}{2} \|\cdot\|_2^2$ , we have the **classical gradient descent**

$$\dot{z}(t) = -\nabla E(t, z(t)).$$

Along a trajectory, the energy satisfies the **energy balance**

$$\frac{d}{dt} E(t, z(t)) = -\|\dot{z}(t)\|_2^2 + (\partial_t E)(t, z(t)).$$

# Gradient Descents — Energetic Solutions

## Definition

$z: [0, T] \rightarrow \mathcal{Z}$  is said to be an **energetic solution** of the gradient descent problem in  $E$  and  $\Psi$  if  $z$  is absolutely continuous, satisfies the prescribed initial condition, and, Lebesgue-a.e. in  $[0, T]$ , the **energy balance**

$$\frac{d}{dt}E(t, z(t)) = -(\Psi(\dot{z}(t)) + \Psi^*(DE(t, z(t)))) + (\partial_t E)(t, z(t)),$$

where  $\Psi^*: \mathcal{Z}^* \rightarrow \mathbb{R} \cup \{+\infty\}$  is the **convex conjugate** of  $\Psi$ :

$$\Psi^*(\ell) := \sup\{\langle \ell, x \rangle - \Psi(x) \mid x \in \mathcal{Z}\}.$$

Much of this carries over to state spaces with no linear structure: see Ambrosio, Gigli & Savaré (2008), *Gradient Flows in Metric Spaces and in the Space of Probability Measures*.

## Gradient Descents — Incremental Formulation

- Typically, existence and uniqueness questions for gradient descents, as well as computation, are addressed using the Moreau–Yosida (implicit Euler) incremental formulation: given  $z_i \approx z(t_i)$ , find  $z_{i+1} \approx z(t_{i+1})$  to minimize

$$\mathcal{W}_{i+1}: \tilde{z} \mapsto \underbrace{E(t_{i+1}, \tilde{z}) - E(t_i, z_i)}_{\text{energy difference}} + \underbrace{\Delta t_{i+1} \Psi \left( \frac{\tilde{z} - z_i}{\Delta t_{i+1}} \right)}_{\text{dissipation}}. \quad (\text{MY})$$

- The idea now is to generate a **thermalized gradient descent**  $\mathcal{Z}$  by seeking densities  $\rho(t, z)$  that minimize a functional in which (MY) competes with an entropy term.
- For simplicity, we now restrict our attention to  $\mathcal{Z} = \mathbb{R}^n$ , and “entropy” will mean **relative entropy with respect to  $n$ -dimensional Lebesgue measure**.



## Thermalized Gradient Descent

Consider the following incremental problem for the PDF  $\rho(t, \cdot)$  of  $Z_t$  with respect to Lebesgue measure on  $\mathbb{R}^n$  at times  $0 = t_0 < t_1 < \dots < t_N = T$ :

- Consider the “prior” density  $\rho_i \approx \rho(t_i, \cdot)$  on  $\mathbb{R}^n$ .
- Find a new joint density  $\rho_{i,i+1}(\cdot, \cdot)$  on  $(\mathbb{R}^n)^2$ , with first marginal  $\rho_i$ , that minimizes

$$\tilde{\rho} \mapsto \iint [\mathcal{W}_{i+1}\tilde{\rho} + \varepsilon\tilde{\rho} \log \tilde{\rho}],$$

where

$$\mathcal{W}_{i+1}(z_i, z_{i+1}) = E(t_{i+1}, z_{i+1}) - E(t_i, z_{i+1}) + \Delta t_{i+1} \Psi \left( \frac{\Delta z_{i+1}}{\Delta t_{i+1}} \right)$$

is the Moreau–Yosida “cost” of changing from state  $z_i$  to state  $z_{i+1}$  in the absence of the heat bath.

- Integrate/marginalize over the first slot of  $\rho_{i,i+1}(\cdot, \cdot)$  to get a “posterior” density  $\rho_{i+1}$  on  $\mathbb{R}^n$  for time  $t_{i+1}$ .

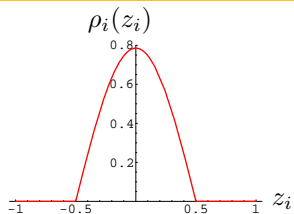


Figure: One step of the incremental thermalized gradient descent problem.

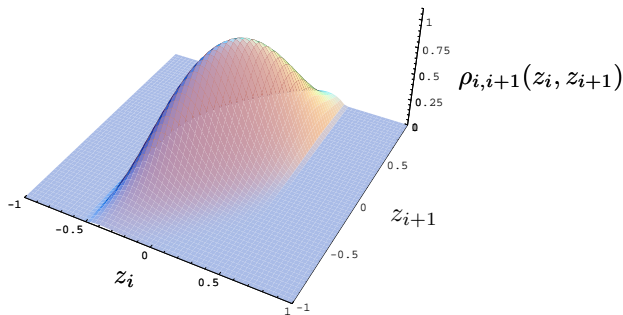
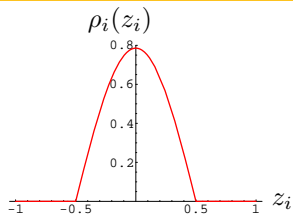


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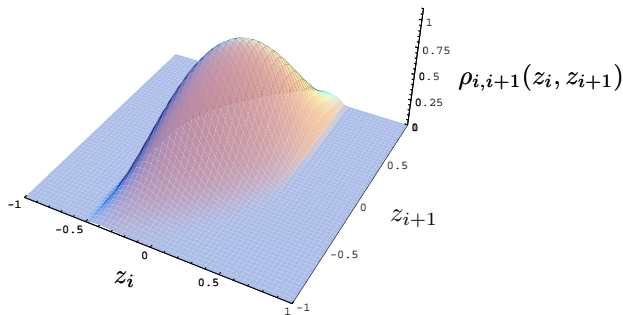
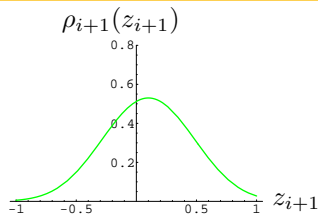
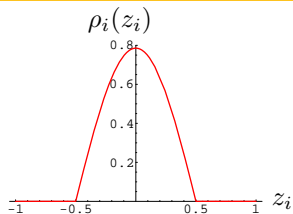


Figure: One step of the incremental thermalized gradient descent problem.

# Thermalized Gradient Descent

## Lemma

*Subject to mild regularity and growth conditions, the single-step increments follow a Gibbs–Boltzmann-type distribution with respect to the Moreau–Yosida incremental cost function:*

$$\rho_{i+1}(z_{i+1}|z_i) = \frac{1}{C(z_i)} \exp\left(-\mathcal{W}_{i+1}(z_i, z_{i+1})/\varepsilon\right).$$

## Definition

On a partition  $P$  of  $[0, T]$ , we will call the Markov chain  $Z^{(P)}$  so generated the (discrete-time) **thermalized gradient descent** in  $E$  and  $\Psi$ .

**Question.** What limit, if any, does the càdlàg process  $\bar{Z}^{(P)}$  have as  $\|P\| \rightarrow 0$ ?

# Thermalized Gradient Descent

## Example

For “nice” potentials  $E$  and the 2-homogeneous dissipation potential

$$\Psi := \frac{1}{2} \|\cdot\|_2^2,$$

the incremental scheme makes sense. As  $\llbracket P \rrbracket \rightarrow 0$ , the piecewise constant càdlàg interpolation  $\bar{Z}^{(P)} : \Omega \times [0, T] \rightarrow \mathbb{R}^n$  of  $Z^{(P)}$  converges in law on  $\mathcal{C}^0([0, T]; \mathbb{R}^n)$  to the solution  $Y$  of the Itô stochastic gradient descent

$$\dot{Y}(t) = -\nabla E(t, Y(t)) + \sqrt{\varepsilon} \dot{W}(t);$$

*i.e.*, the thermalized gradient descent scheme is a plausible model for “linear kinetics + noise”.

# Thermalizing a Rate-Independent Process

Consider a “nice” rate-independent system in  $\mathbb{R}^n$ :

- an energetic potential  $E: [0, T] \times \mathbb{R}^n \rightarrow \mathbb{R}$  — convex, time derivative in  $W^{1,\infty}$ , space derivative in  $C^1$ ;
- a dissipation potential  $\Psi: \mathbb{R}^n \rightarrow [0, +\infty)$  — homogeneous of degree one and strictly convex (*i.e.* non-degenerate).  $\Psi$  is the convex conjugate of the characteristic function of a convex compact set  $\mathcal{E} \subsetneq (\mathbb{R}^n)^*$  that has  $0 \in \overset{\circ}{\mathcal{E}}$ , the *elastic region*:

$$\Psi(v) = \sup\{\langle \ell, v \rangle \mid \ell \in \mathcal{E}\}.$$

Study the process  $Z^{(P)}$  by studying its increments:

$$\Delta Z_i^{(P)} := Z_i^{(P)} - Z_{i-1}^{(P)}.$$

What are the moments of the increments,  $\mathbb{E}[\Delta Z_i^{(P)}]$ ,  $\text{Var}[\Delta Z_i^{(P)}]$  & *c.*?

# Effective (Dual) Dissipation Potential

## Definition

Define an **effective dual dissipation potential**

$$\tilde{\Psi}^* : (\mathbb{R}^n)^* \rightarrow \mathbb{R} \cup \{+\infty\}$$

by

$$\tilde{\Psi}^*(\ell) := \log \int_{\mathbb{R}^n} \exp(-(\langle \ell, x \rangle + \Psi(x))) \, dx.$$

(Cf. the cumulant-generating function of the measure  $d\psi = e^{-\Psi(x)} \, dx$ )

Define the **effective dissipation potential** by convex conjugation:

$$\tilde{\Psi}(x) = \tilde{\Psi}^{**}(x) := \sup \{ \langle \ell, x \rangle - \tilde{\Psi}^*(\ell) \mid \ell \in (\mathbb{R}^n)^* \}.$$

Note that  $\tilde{\Psi}$  is determined purely by the dissipation functional  $\Psi$  (or, equivalently, the elastic region  $\mathcal{E} \subsetneq (\mathbb{R}^n)^*$  associated to  $\Psi$ ).



$$\tilde{\Psi}^*(\ell) := \log \int_{\mathbb{R}^n} \exp(-(\langle \ell, x \rangle + \Psi(x))) \, dx.$$

$$\tilde{\Psi}(x) := \sup_{\ell} [\langle \ell, x \rangle - \tilde{\Psi}^*(\ell)].$$

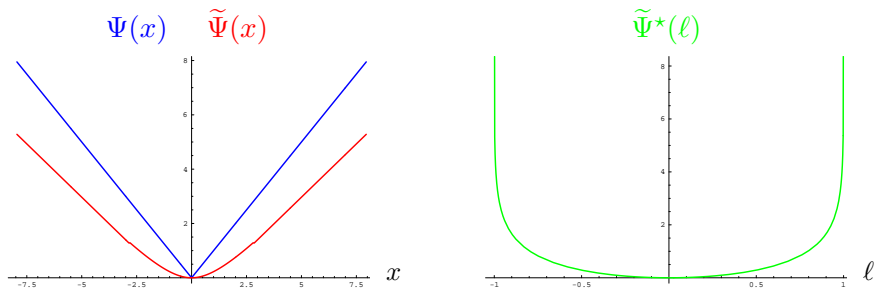


Figure: The effective (dual) dissipation potential in dimension one for  $\Psi(x) = |x|$ .  $\tilde{\Psi}^*$  blows up like the logarithm of the distance to the yield surface  $\partial\mathcal{E}$ .  $\tilde{\Psi}$  is smooth and is asymptotic to  $\Psi$  at infinity.

## Explicit Examples

### Example

If  $\Psi$  is the weighted  $\ell^1$  norm  $\Psi(x) := \sigma_1|x^1| + \dots + \sigma_n|x^n|$ , with weights  $\sigma_i > 0$ , then (up to an additive constant)

$$\tilde{\Psi}^*(\ell) = - \sum_{i=1}^n \log(\sigma_i^2 - |\ell_i|^2).$$

### Example

If  $\Psi$  is a multiple of the Euclidean norm,  $\Psi(x) := \sigma\|x\|_2$ ,  $\sigma > 0$ , then

$$\begin{aligned} \tilde{\Psi}^*(\ell) &= \log \int_{\mathbb{S}^{n-1}} \frac{(n-1)!}{(\langle \ell, \omega \rangle + \sigma)^{-n}} d\mathcal{H}^{n-1}(\omega) \\ &= -\frac{n+1}{2} \log(\sigma^2 - \|\ell\|_2^2). \end{aligned}$$

## Why $\tilde{\Psi}$ ?

- The reason that  $\tilde{\Psi}$  is so important is that the change of variables  $Z_{i+1} \rightsquigarrow \Delta Z_{i+1}/\varepsilon_{i+1}$  yields (modulo higher-order error terms):

$$\mathbb{E}[\Delta Z_{i+1} | Z_i = z_i] \approx -\varepsilon_{i+1} D\tilde{\Psi}^*(DE(t_{i+i}, z_i));$$

$$\text{Var}[\Delta Z_{i+1} | Z_i = z_i] \approx -\varepsilon_{i+1}^2 \left\| D^2\tilde{\Psi}^*(DE(t_{i+i}, z_i)) \right\|_2 \ll \varepsilon_{i+1}.$$

- Hence, it looks like the continuous-time limit with  $\varepsilon_{i+1} = \theta \Delta t_{i+1}$  should satisfy the deterministic ordinary differential equation

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# Convergence Result

## Theorem (Convergence to Nonlinear Gradient Descent)

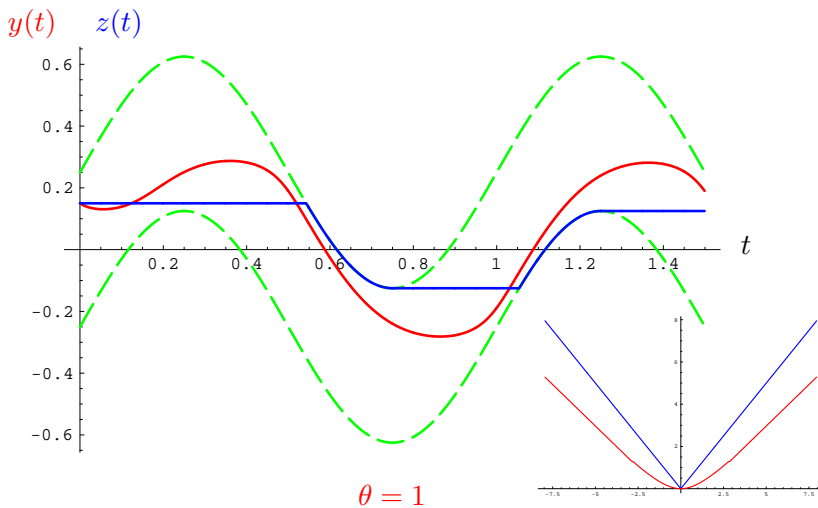
If  $(t, x) \mapsto \tilde{\Psi}^*(DE(t, x))$  is convex in  $x$  for each  $t \in [0, T]$ , then the piecewise constant càdlàg interpolation  $\bar{Z}^{(P)} : \Omega \times [0, T] \rightarrow \mathbb{R}^n$  converges in probability as  $\llbracket P \rrbracket \rightarrow 0$  to the solution of

$$D\tilde{\Psi} \left( -\frac{\dot{y}(t)}{\theta} \right) = DE(t, y(t)).$$

More precisely, for any  $\lambda > 0$ , as  $\llbracket P \rrbracket \rightarrow 0$ ,

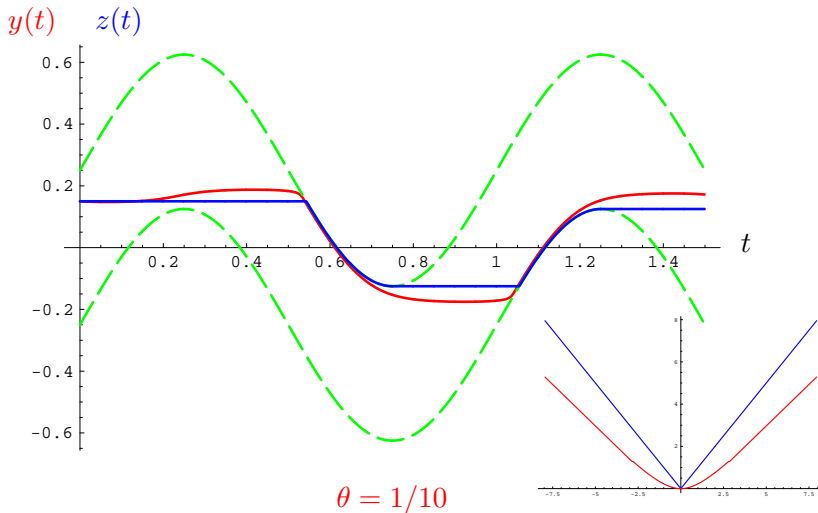
$$\mathbb{P} \left[ \sup_{t \in [0, T]} \left\| \bar{Z}^{(P)}(t) - y(t) \right\|_2 \geq \lambda \right] \in O(\llbracket P \rrbracket^{1/2}).$$

(If  $D^2E \equiv 0$ , then the order of convergence is  $O(\llbracket P \rrbracket)$ .)



Indicated in green is the frontier of the stable region,

$$\mathcal{S}(t) := \{x \in \mathbb{R}^n \mid -DE(t, x) \in \mathcal{E}^{\circ}\}.$$



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## Andrade's Creep Law

- In 1910, Andrade reported that as a function of time,  $t$ , the creep deformation,  $\xi$ , of soft metals at constant temperature and applied stress can be described by a power law  $\xi(t) \sim t^{1/3}$ . Similar behavior has been observed in many classes of materials, including non-crystalline materials.
- Morally, macroscopic creep should be observed as a change in the mean of the microscopic slip field.
- We will study this using the Koslowski–Cuitiño–Ortiz phase field model for a material sample along a single slip plane, thought of as the unit torus,  $\mathbb{T}^2$ .
- The **phase field**  $u \in H^{1/2}(\mathbb{T}^2; \mathbb{R})$  measures the total amount of slip at each point:  $u(x) \in \mathbb{R}$  is the slip (in multiples of the Burgers vector  $b$ ) at  $x \in \mathbb{T}^2$ .

## KCO Phase Field Model — Details

In the KCO model the **energetic potential** is

$$E(s, u) := \sum_{k \in \mathbb{Z}^2 \setminus \{0\}} \frac{\mu b^2}{4} \frac{1}{1/K + d/2} |\hat{u}(k)|^2 - (s \cdot b) \int_{\mathbb{T}^2} u(x) \, dx,$$

where  $\hat{u}$  is the Fourier transform of  $u$ ,  $k \in \mathbb{Z}^2$  is the wavenumber,

$$K := \frac{1}{1 - \nu} \sqrt{k_1^2 + k_2^2} - \frac{\nu}{1 - \nu} \frac{k_2^2}{\sqrt{k_1^2 + k_2^2}},$$

$b$  is the Burgers vector,  $s$  is the applied shear stress,  $\nu$  is Poisson's ratio and  $d$  is the interplanar distance. For  $\mu > 0$  (the shear modulus), the **dissipation potential** is

$$\Psi(u) = \mu \sum_{p \in \mathcal{O}} \int_{\mathbb{B}_r(p)} |u(x)| \, dx.$$

## Reduction of the KCO Model

- In KCO, the dissipation  $\Psi$  is not positive-definite on  $H^{1/2}(\mathbb{T}^2; \mathbb{R})$ : it is concentrated over discs of radius  $0 < r \ll 1$  centred on a (random) point set of obstacles,  $\mathcal{O}$ . Hence, only the values of the phase field over  $\mathcal{O}$  experience dissipation.
- Schur complementation (minimizing out those degrees of freedom that do not experience dissipation) yields a reduced finite-dimensional model posed in  $\mathbb{R}^{\mathcal{O}}$ . The reduced energetic potential is a quadratic form in  $\xi := u|_{\mathcal{O}}$ :

$$E_{\text{red}}(s, \xi) = \frac{1}{2} \xi \cdot G \xi - (s \cdot b) \tau \cdot \xi + \frac{h}{2} (s \cdot b)^2$$

and the reduced dissipation  $\Psi_{\text{red}}$  is a non-degenerate weighted  $\ell^1$  norm.

## Mean Field Model

- Write  $\xi$  as the sum of its mean and the fluctuation about the mean:

$$\bar{\xi} := \frac{1}{\#\mathcal{O}} \sum_{p \in \mathcal{O}} \xi_p \in \mathbb{R}, \quad \hat{\xi} := \xi - \bar{\xi} \mathbf{1}.$$

- Creep is a “bulk phenomenon” in the sense that it is a change of the **mean field**  $\bar{\xi}$  of the overall phase field. Numerical experiments bear out the hypothesis that the fluctuations  $\hat{\xi}$  of the phase field about its mean are small (in the sense that they dissipate very little energy).
- Therefore, we narrow the focus of our study to the one-dimensional mean field  $\bar{\xi}$ . The resulting model is of the form

$$E_{\text{MF}}(s, \bar{\xi}) = -(s \cdot b) \bar{\tau} \bar{\xi}; \quad \Psi_{\text{MF}}(\bar{\xi}) = \sigma |\bar{\xi}|,$$

where  $\sigma = \mu \cdot \pi r^2 \cdot \#\mathcal{O}$ .

# Convergence Result

- In this case, the effective dual dissipation potential for the mean field is

$$\tilde{\Psi}_{\text{MF}}^*(\bar{\ell}) = -\log(\sigma^2 - (s \cdot b)^2 \bar{\tau}^2).$$

- Under the assumption of linear strain hardening (*i.e.*  $\sigma = \sigma_0 \bar{\xi}$ ) the resulting effective ordinary differential equation is

$$\frac{d\bar{\xi}(t)}{dt} = \frac{2\theta(s \cdot b)\bar{\tau}}{(\sigma_0 \bar{\xi}(t))^2 - (s \cdot b)^2 \bar{\tau}^2}.$$

- For fixed  $\theta$  and  $0 < (s \cdot b)\bar{\tau} \ll \sigma$  (*i.e.* constant temperature and constant small applied stress), solutions grow in accord with Andrade's creep law:

$$\bar{\xi}(t) \sim t^{1/3}.$$

# Conclusions

Given a reference measure and hence a notion of entropy, gradient descents can be thermalized and the resulting Markov chain models analyzed.

- In the case of 2-homogeneous dissipation, the TGD scheme describes the effect of adding  $\text{It}\bar{o}$  noise.
- In the case of 1-homogeneous dissipation, the TGD scheme yields a deterministic gradient flow in an effective dissipation potential  $\tilde{\Psi}$  that is a nonlinear transformation (“smoothing-out”) of the original dissipation potential  $\Psi$ .
- As an application, this analysis can be used to derive Andrade’s creep law for soft metals under the assumption of linear strain hardening.

# Outlook

Can this analysis be extended to

- second-order equations of motion (inertial effects, non-Markovian processes)? Difficulty: increments are very badly behaved, variances can blow up in short time.
- infinite-dimensional and/or non-linear state spaces? Difficulty: with respect to what reference measure will entropy be calculated?

**“Commutativity Question”**. The Andrade creep law should follow directly from applying the TGD method to the Koslowski–Cuitiño–Ortiz model in  $H^{1/2}(\mathbb{T}^2)$  and *then* examining the mean field, not passing to a mean field model first and then applying TGD.

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