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Upscaling of Dislocation Dynamics

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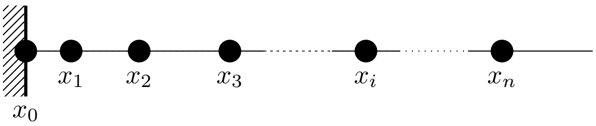
1. Application: plasticity of metals

Plastic behaviour of metals on the macro scale results from many dislocations interacting on the micro scale. The main question is:

> How to obtain the macroscopic evolution equation from the dynamics at the micro scale?

2. Microscopic model: particle system



Unknowns: $0 < x_1 < \ldots < x_n$

Parameter: $1 \lesssim \beta_n \lesssim n$, $\beta_n \approx \frac{\text{interaction energy}}{\text{external load}}$

Energy:

$$E_n(x) := \underbrace{\frac{1}{n^2}\sum_{j<i}\sum V_n(x_i - x_j)}_{\text{interaction}} + \underbrace{\frac{1}{n}\sum_{i=1}^{n} x_i}_{\text{external load}}$$

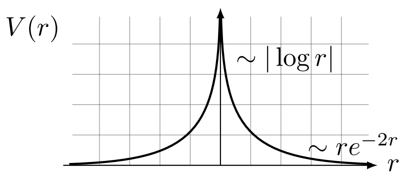


Figure 1. Singular and non-local interaction potential $V_n(r) := \beta_n V(\beta_n r)$.

Gradient flow: $\begin{cases} \dot{x}(t) = -n\nabla E_n(x(t)), & t > 0 \\ x(0) = x^0 \end{cases}$

3. Re-interpretation: empirical measure

Let $\pi_n : \mathbb{R}^n \to \mathcal{P}([0,\infty))$, $\qquad \pi_n(x) = \frac{1}{n}\sum_{i=1}^{n}\delta_{x_i}$

$$E_n(\mu_n) = \begin{cases} E_n(x) & \text{if } \mu_n := \pi_n(x) \\ \infty & \text{otherwise.} \end{cases}$$

4. Main Theorem: macroscopic evolution equation

Assume $\pi_n(x^0) \to \mu^0$ in the Wasserstein metric. Then $\pi_n(x(t))$ converges to $\mu(t)$ in the Wasserstein metric, pointwise in time a.e., in which $x(t)$ is the solution to the microscopic dynamics, and $\mu(t)$ solves the Wasserstein gradient flow

$$\frac{\partial}{\partial t}\mu = \operatorname{div}\left(\mu\nabla E(\mu)\right).$$

5. The macroscopic energy E

regime	macroscopic energy $E(\rho)$
$\beta_n \to c$	$\int_0^\infty x\rho + \frac{c}{2}\int_0^\infty\int_0^\infty V(c(x-y))\rho(x)\rho(y)\,dydx$
$1 \ll \beta_n \ll n$	$\int_0^\infty x\rho + \left(\int_0^\infty V(r)\,dr\right)\int_0^\infty \rho^2(x)\,dx$
$\frac{\beta_n}{n} \to c$	$\int_0^\infty x\rho + c\int_0^\infty \Psi\left(\frac{c}{\rho(x)}\right)\rho(x)\,dx$

Table 1. The expressions are infinite if $\rho := \frac{d\mu}{d\mathcal{L}} \notin L^1$. In the third expression, we use $\Psi(r) := \sum_{k=1}^\infty V(kr)$.

6. Proof

To conclude that the gradient flows converge, it is enough [1] to show that:

- E_n Γ-converges to E both in the narrow topology [2] and in the Wasserstein topology [3],
- E_n and E are convex, and
- (E_n) is equi-coercive in the narrow topology.

7. Extensions

The same upscaling result holds for:

- $\beta_n \ll 1$ and $\beta_n \gg n$ [2], and
- the case in which there is a second hard wall at the right end [4].

8. Current research

- Characterizing the boundary layer at $x = 0$.
- Upscaling the related 2-dimensional particle system.
- Adding temperature, and using techniques from statistical mechanics.

References

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[2] M. G. D. Geers, R. H. J. Peerlings, M. A. Peletier, and L. Scardia. Asymptotic behaviour of a pile-up of infinite walls of edge dislocations. *Archive for Rational Mechanics and Analysis*, 209:495–539, 2013.

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