Physical Meaning and Experimental Check of a Variational Principle for Macro-to-Micro Transition

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1. Boundary conditions in micro-macro problems

Basic requirement for the applicability of a micro-macro model:

Hill's macro-homogeneity condition: the micro-fields $\boldsymbol{\sigma}(\mathbf{x})$, $\mathbf{d}(\mathbf{x})$ fluctuate around well-defined macro-averages $\boldsymbol{\Sigma}$ and $\mathbf{D}$.

(Actually $\boldsymbol{\Sigma}$ and $\mathbf{D}$ usually not uniform, but vary slowly.)

Domain to be considered: any Representative Volume Element (RVE) . But even in a macro-homogeneous part, this means: *Boundary value unknown*, even *undetermined*

(varies from an RVE to another one)

Usual implicit postulate: the *exact* boundary data do not matter

→ assume data corresponding to a uniform field,

e.g. velocity $\mathbf{v}(\mathbf{x}) = \mathbf{D.x}$ for $\mathbf{x}$ at the boundary of the RVE

2. "Stochastic" features of the microscopic fields

A deformation process with non-linear constitutive equation =

An initial value Pb.

for a *non-linear* "dynamical" (= differential) system:

$$\frac{dY}{dt} = f(Y(t), t).$$

$Y(t) \equiv$ [displacement field $\mathbf{u}(\mathbf{x}^0, t)$, internal variables field $\mathbf{X}(\mathbf{x}^0, t)$]

$\Rightarrow \dfrac{dY}{dt}$ = [velocity field $\mathbf{v}(\mathbf{x}^0, t)$, evolution rate $\dot{\mathbf{X}}(\mathbf{x}^0, t)$]

= function of current $Y = (\mathbf{u}, \mathbf{X})$ *and* <u>current boundary data for $\mathbf{v}$</u>

↓

an "external forcing"

Non-linear constitutive equations ⇒ non-linear system,

$f(Y, t) \neq A(t).\ Y + B(t)$

⇒ Possible sensitivity to initial/boundary data (loss of stability?)

Recall: loss of stability in mechanics of materials appears as *strain localization*. (Cf. Considère's diffuse necking criterion.)

Microscopic strain localization is indeed the *rule* in plasticity (also in macro-homogeneous situations) :

- dislocation cells, | organized in
- slip lines, microscopic shear bands. | characteristic patterns

Consequences

1) The *microscopic strain field* (hence also the stress) has some *non-deterministic* features characteristic of non-linear dynamical systems, with *"self-organized" structures* emerging.

2) One should not simply *assume* some particular boundary data (e.g. $\mathbf{v}(\mathbf{x}) = \mathbf{D}.\mathbf{x}$, $\mathbf{x} \in \partial\Omega$) without checking the effect of other data

3) The *strain-rate heterogeneity*, $h \equiv \langle \, \| \, \mathbf{d} - \langle \mathbf{d} \rangle \, \| \, \rangle$, *depends* on the amount of microscopic localization.

Hence h is hardly predictable $\Rightarrow$ should be added to the microscopic information to make the data.

3. The principle of minimum heterogeneity

in the proposed micro-macro model

Microscopic constitutive eqns. assumed to derive from a *potential*:

e.g. for plasticity or viscoplasticity, $\boldsymbol{\sigma} = \frac{\partial u}{\partial \mathbf{d}}(\mathbf{d}, \mathbf{X})$.

X: variables that make u inhomogeneous ($\mathbf{X}=\mathbf{X}(\mathbf{x})$). E.g. crystal orientation, dislocation density, ...

Constituents: zones with constant **X**, say $\Omega_1, ..., \Omega_n$ (for $\mathbf{X}_1, ..., \mathbf{X}_n$)

$f_k \equiv \mathrm{Vol}(\Omega_k)/\mathrm{Vol}(\mathrm{RVE})$: volume fraction of constituent (k)

$\mathbf{D}_k$: volume average of the strain-rate **d** in constituent (k)

Unknown of the macro-to-micro transition: the distribution $(\mathbf{D}_k)$.

Let $(\mathbf{D}^*_k)$ be a candidate for this distribution.

$\Rightarrow$ average $\mathbf{D}^* \equiv f_1\, \mathbf{D}^*_1 + ... + f_n\, \mathbf{D}^*_n$ must be the macro-tensor **D**.

Heterogeneity of the distribution:

$$h = h((\mathbf{D}^*_k)) \equiv f_1 \|\mathbf{D}^*_1 - \mathbf{D}^*\| + ... + f_n \|\mathbf{D}^*_n - \mathbf{D}^*\|.$$

Model: Search $U_r\,(\mathbf{D}) \equiv \mathrm{Min}\,[f_1\, u_1(\mathbf{D}^*_1) + ... + f_n\, u_n(\mathbf{D}^*_n)]$

under constraints $\mathbf{D}^* = \mathbf{D}$ and $h = r$. (r assumed given).

Theorem: For any **D**, there exists a generically unique value $r_0\,(\mathbf{D})$ such that $U_{r_0}(\mathbf{D}) = U(\mathbf{D})$, the exact value of the macro-potential.

Micro-to-macro transition: the mere problem is to find r_0. One postulates a simple dependence $r_0 = r_0\,(\mathbf{D})$, e.g. $r_0 = a\,\|\mathbf{D}\|$, and one "adjusts" a from *one* mechanical test. (In easy cases, a is guessed.)

Macro-to-micro transition: one has to assume that the distribution solution $(\mathbf{D}^{sol}{}_k)$ is "the actual" distribution $(\mathbf{D}_k)$.

Theorem: the assumption $(\mathbf{D}^{sol}{}_k) = (\mathbf{D}_k)$ amounts to assuming a

Principle of minimum inhomogeneity:

Among distributions $(\mathbf{D}^*_k)$ that have the relevant macro-average **D** and that lead to the correct value of the macro-potential

[i.e. $U(\mathbf{D}) = f_1\, u_1(\mathbf{D}_1) +...+ f_n\, u_n\,(\mathbf{D}_n) = f_1\, u_1(\mathbf{D}^*_1) +...+ f_n\, u_n\,(\mathbf{D}^*_n)$],

the actual distribution $(\mathbf{D}_k)$ has the least heterogeneity h.

4. The maximum entropy principle

Consider a system of N "elementary constituents" (molecules in the kinetic theory of gases/ *Here:* small crystals with same volume) The state of each element^{y} const^{t} (velocity, position / *orientation, strain-rate*) is in one among M possible boxes, with $1 << M << N$.
Let l_i (i = 1, ..., M) be the number of elem^{y} const^{ts} in box (i).
The corresponding fraction is $p_i = l_i /N$ $(p_1 + ... + p_M = 1)$.

Macro-state: (pressure, density) / *here:* [volume fractions of the orientations f_k (k = 1, ..., n), macro strain-rate **D**, macro-power $\dot{W}$].
Must be computable from the probability distribution (p_i).

A given probability distrib^{n} (p_i) [or a given distrib^{n} (l_i), $l_i = Np_i$]
may be obtained by a large number Z of distinct *configurations:*
e.g. with N=12 elem^{y} const^{ts} and M=5 boxes, (l_i)=(2,1,3,1,5), as

Statistical Mechanics: the "real" distribution = the one that may be obtained by the *largest* number Z of distinct configurations compatible with the given macro-state.

Number of configur^{ns} (*ignoring the constraint* of the macro-state):

$$Z = \frac{N!}{l_1! \ldots l_M!} \quad \Rightarrow \quad \frac{1}{N}\,\mathrm{Log}Z \approx -\sum_{i=1}^{M} p_i \mathrm{Log} p_i \equiv S$$

S : *statistical entropy.*

⇒ In the "no constraint" case, Z = max ⇔ S = max.
Resulting distribution: *uniform*, $p_i = 1/M$ for $i = 1, \ldots, M$.

But the "S = max" principle is more general (now central in statistical physics). With constraints (= with *additional information*, e.g. macroscopic information): amounts to
selecting the ***broadest*** *probability distribution compatible with the available information* (Jaynes 1957). I.e., the "unbiased choice".

5. Minimum heterogeneity vs. maximum entropy (polycrystal)

Micro-state: (orientation **R**, strain-rate **d**)

$\mathbf{R} \in \{\mathbf{R}_1, \ldots, \mathbf{R}_n\}$, $\mathbf{d} \in \{\mathbf{D}^1, \ldots, \mathbf{D}^m\}$, $(\mathbf{D}^1 + \ldots + \mathbf{D}^m)/m = \mathbf{D}$.

Let $l_i = l^j{}_k$ = number of elementary crystals with µ-state $(\mathbf{R}_k, \mathbf{D}^j)$:

$$\Sigma_{j,k}\ l^j{}_k = N. \qquad i \Leftrightarrow (j, k), \qquad p^j{}_k = l^j{}_k / N.$$

The volume fractions of the orientations are given (= the texture):

$N_k \equiv l^1{}_k + \ldots + l^m{}_k$, or equivalently $f_k \equiv N_k / N$, are known.

Average strain-rate in orientation $\mathbf{R}_k$:

$$\mathbf{D}_k \equiv (l^1{}_k\, \mathbf{D}^1 + \ldots + l^m{}_k\, \mathbf{D}^m)/ N_k.$$

Heterogeneity: $h \equiv \sum_k f_k \left\| \mathbf{D}_k - \mathbf{D} \right\| = \sum_k \left\| \sum_j p^j{}_k\, \mathbf{D}^j - f_k \mathbf{D} \right\|.$

Since $p^1{}_k + \ldots + p^m{}_k = f_k$, the "$S$ = max" principle selects, in average over k and accounting for the constraints, the $(p^j{}_k)$ distribution closest possible to the uniform distribution $p^j{}_k = f_k/m$. But since $(\mathbf{D}^1 + \ldots + \mathbf{D}^m)/m = \mathbf{D}$, this means simply h minimum !!

Conclusions

1) In an inelastically deformed heterogeneous material, the microscopic fields have some *non-deterministic* features. These make difficult to envisage a micro-macro problem merely as a boundary value problem for a differential equation.

2) The proposed variational model is consistent with this remark: it considers the *strain heterogeneity* as a necessary *input* of the micro-macro model, in addition to the microscopic information.

3) The *principle of minimum inhomogeneity*, that justifies the macro-to-micro transition in the model, may be seen as a consequence of the *maximum entropy principle*.

4) The proposed model compares favourably with other models as to the *experimental agreement* - for the deformation textures of steels (other metals currently investigated).