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Stochastic Homogenization of a two Dimensional Granular Medium

M. Najib(*), M. Arminjon(**) and H. Smaoui(*)¹

Abstract

In order to describe the macroscopic behavior of granular media, a statistical micro to macro level transition model is first developed, based on Jaynes' principle of maximum entropy. The model formulation translates into a strictly convex, nonlinear optimization problem. It is tested by solving model examples of two dimensional granular structures. Next, a Lagrangian dual formulation of the maximum entropy problem is derived and analyzed. The dual formulation, which is confirmed to be computationally more efficient than the primal one, is applied in solving an evolution problem for a regular granular structure subjected to a biaxial compression loading with a prescribed lateral stress. Results show that the model is capable of predicting the response, in terms of stress and strain, throughout the evolution of the structure, and a satisfactory agreement is observed with the physical solution that is known a priori. **Keywords:** granular media, statistical mechanics, statistical entropy, micro-macro transition, Lagrangian duality.

1 Introduction

Despite all the progress made in the analysis and modelling of the behaviour of granular media [3, 6, 7, 8, 10, 13], the development of relationships between the macroscopic and microscopic properties for these media is continues to be a challenging research objective. The present paper is an attempt to contribute to the current trend aiming at the development of behavior models for granular materials based on micro-macro transition. The discrete nature of granular materials at the particle scale and the large number of geometric and mechanical characteristics that govern the behaviour at the local scale [12], motivated the use of a statistical mechanics approach [4, 8]. The proposed approach is precisely a statistical one, based on Jaynes' principle of

maximum entropy ("MAXENT") [9]. This principle actually holds a fundamental status since it underlies the entire range (scope) of modern statistical physics [5]. The maximum entropy principle is applied in search for a discrete probability distribution (p_i), over a finite set of M elements, when only the averages of some quantities in the sense of this distribution law are known. It consists in selecting the distribution that minimizes the statistical entropy statistique

$$S = \sum_i p_i \log p_i, \quad (1)$$

subject to the condition that the known averages Q (with $Q \ll M$) are specified quantities. In a previous work [2], a formulation of the principle of maximum entropy was established and successfully applied to the probleme of macro-micro transition for a heterogeneous continuum. The objective here is to adapt this formulation to the case of a discrete medium which presumably constitutes an interesting test for this new approach. Such an adaptation is far from being obvious, as the previous work [2] was concerned with a heterogeneous but microscopically continuous medium. In particular, for a heterogeneous continuum, both at the micro and macro scales there exists a behaviour law that relates the "solicitation" tensors to the "response" (e.g. strain rate and Cauchy stress), and the aim is simply to establish the scale transition in this behaviour law. A direct application of the existing approach [2] would lead to a granular medium model consisting of an assembly of deformable grains and a second phase (air or water, or both). Such a "porous medium" approach would be extremely difficult to manage in a practical problem where the issue of unilateral contact is of primary importance. For a granular aggregate governed by dry friction type contacts, one is confronted with the task of modelling the strain of an assembly of rigid grains undergoing a quasi-static evolution while interacting according to a Coulomb contact law.

Although some of the physics of the problem is lost due to the assumption of quasi-static evolution as pointed out in [6], it is adopted here in a simple framework as a first approximation for the study of granular materials. The proposed approach is an adaptation of the work in [2] to granular materials which consists essentially in: **i**) partitioning the aggregate into Voronoi cells, each of them containing a unique intergranular contact point, and **ii**) replacing the "solicitations" and "responses" considered in [2] by the "dynamic microscopic variables" representing the dynamic state of the

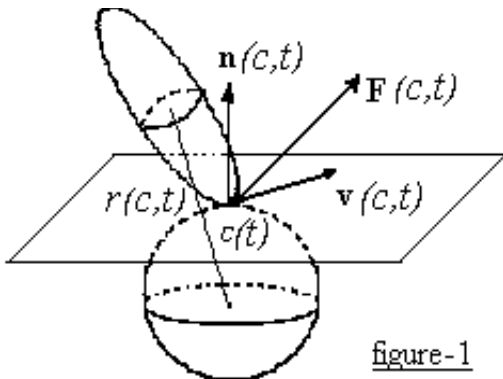
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contact at hand. It is then possible to model the strain of the aggregate using MAXENT. This leads to a convex optimization problem, and it is, subsequently, found that the dual form the problem is more convenient for numerical solution.

2 Statistical Model and Primal Problem

A representative elementary volume V [1] of a granular material is considered. The particles are assumed to be rigid and interaction among them to obey Coulomb's dry friction law with unilateral contact. The fundamental microscopic variables chosen for describing the structure and the local behavior of the granular material are: the list $C(t)$ of contact points at a given instant ² of time t ; the contact forces $\mathbf{F}(c, t)$, $c \in C(t)$, mutually applied between particles, the directions $\mathbf{n}(c, t)$ that are normal to the contact tangent plane ³, the norms $r(c, t)$ of the "branch" vectors which connect the centroids of the particles in contact, and their relative velocities at the contact points ⁴



The intergranular void has been integrated in the model by considering a partition of the granular domain into Voronoi cells, associated to the set of contact points $C(t)$ at time t . This is achieved by attributing at

² The same index c is maintained at all times t for a given contact which naturally involves two interacting particle, each contact being continuously followed through time when applicable.

³ By convention, the chosen outward normal is that of the particle which exerts the force $\mathbf{F}(c, t)$ onto the other particle sharing the contact $c \in C(t)$.

⁴ The relative velocity is defined as the velocity of the particle for which the normal $\mathbf{n}(c, t)$ is directed inwards, with respect to that of the particle with an outward normal (figure-1).

each instant t and almost every point x of the granular domain V , the contact point $c(x, t)$ that is the closest to x , in the sense Euclidian norm, defined by:

$$\|x - c(x, t)\| = \min_{c \in C(t)} \|x - c\| \quad (2)$$

As a result, each Voronoi cell is a convex polyhedron which contains a unique contact and has as boundaries the mediator planes of the segments joining the only contact point of the cell to the "neighboring" contact points. With this partition of the volume V into material cells, each containing a unique contact point, the discrete granular material can be described as a continuum. Then the variables $\mathbf{F}(x, t)$, $\mathbf{n}(x, t)$, $r(x, t)$ and $\mathbf{v}(x, t)$ are defined, at each instant t and at almost every point x in V , by their values at the closest contact point $c(x, t)$ given by (2).

The individual behaviour of each particle is not of interest here. What matters however, is the overall behaviour of the medium as a whole which is described in terms of the local states which are the parameters selected for the representation of the structure of the medium without having the interpretation of thermodynamic states. For each instant t and almost every point x in V , the local state of the granular medium is defined by the list of pairs

$$X(x, t) = (\mathbf{n}(x, t), r(x, t)) \quad (3)$$

Moreover, for each instant t and almost every point x in V , the pair

$$\xi(x, t) = (\mathbf{v}(x, t), \mathbf{F}(x, t)). \quad (4)$$

is considered to represent what will be called the "microscopic dynamic variables" (MDV). These variables play the role of the solicitation and response tensors in the model developed in [2]. As in most statistical mechanics models, the key variables of the problem, namely the states and the VDM for the present model, are restricted to a set of discrete values. Although some states in the granular medium are discrete in nature

$$\mathbf{n} \in \{\mathbf{n}_c \in [0, 2\pi] \times [0, \pi] / c \in C_1 \text{ and } C_1 \subset C\},$$

$$r \in \{r_c \in \mathbb{R}^+ / c \in C_2 \text{ and } C_2 \subset C\}.$$

different discretizations are considered for modeling purpose. For instance, regularly spaced angular orientation values may be chosen for the discrete values)

$$\begin{cases} \mathbf{n} \in \{\mathbf{n}_k \in [0, 2\pi] \times [0, \pi] / 1 \leq k \leq K\} \\ r \in \{r_l \in \mathbb{R}^+ / 1 \leq l \leq L\} \end{cases} \quad (5)$$

so that

$$X_{kl}(t) = \{(\mathbf{n}_k(t), r_l(t)) / 1 \leq k \leq K \text{ and } 1 \leq l \leq L\}. \quad (6)$$

Similarly, discretization of the MDV's can be expressed by

$$\begin{cases} \mathbf{v} \in \{\mathbf{v}^m \in \mathbb{R}^2 / 1 \leq m \leq M\} \\ \mathbf{F} \in \{\mathbf{F}^q \in \mathbb{R}^2 / 1 \leq q \leq Q\} \end{cases} \quad (7)$$

so that

$$\xi^{mq}(t) = \{(\mathbf{v}_k^m(t), \mathbf{F}^q(t)) / 1 \leq m \leq M \text{ and } 1 \leq q \leq Q\}. \quad (8)$$

Thus, for each time t one can establish a partition of volume V into sub-domains $V_{kl}^{mq}(t)$, defined for $1 \leq k \leq K$, $1 \leq l \leq L$, $1 \leq m \leq M$ and $1 \leq q \leq Q$ by

$$\begin{cases} V_{kl}^{mq}(t) = \{x \in V / X(x, t) = (\mathbf{n}_k(t), r_l(t))\} \\ \xi(x, t) = (\mathbf{v}^m, \mathbf{F}^q) \end{cases} \quad (9)$$

which conveys an aggregate structure to the medium [1].

A basic assumption is the a priori knowledge of the volume fractions ρ_{kl} of the states X_{kl} that are present in the model.

For each time instant t , the discrete distribution of volume fractions $V_{kl}^{mq}(t)$ is considered. It is alternatively denoted

$$p_{kl}^{mq}(t) \quad (10)$$

$1 \leq k \leq K$, $1 \leq l \leq L$, $1 \leq m \leq M$ and $1 \leq q \leq Q$ as it represents the probability of joint occurrence of the state kl and MVD mq . In a granular medium, the average stress is given by [11, 14]

$$\sigma = \frac{1}{V} \sum_{c \in C} \mathbf{F}^c \otimes \mathbf{l}^c \quad (11)$$

where \mathbf{F}^c represents the contact force at contact c between a pair of particles, and \mathbf{l}^c is the vector connecting their centroids. In terms of the states chosen here, this average stress is expressed by

$$\sigma(t) = \frac{1}{V} \left[\sum_{0 \leq q \leq Q} \sum_{\substack{0 \leq k \leq K \\ 0 \leq l \leq L}} N_{kl}^q(t) \mathbf{F}^q \otimes r_l(t) \mathbf{n}_k(t) \right] \quad (12)$$

where $N_{kl}^q(t)$ is the number of contacts where the contact force and the state take on the discrete values \mathbf{F}^q and $X_{kl}(t) = (\mathbf{n}_k(t), r_l(t))$ respectively.

The maximum entropy (MAXENT) model consists in solving the following variational problem (\mathbf{P}), in which

one seeks to determine, at every time t , the discrete distribution $p_{kl}^{mq}(t)$ of probabilities of occurrence of state which maximizes the statistical entropy S [9] defined by:

$$S(p_{kl}^{mq}(t)) = - \sum_{\substack{0 \leq m \leq M \\ 0 \leq q \leq Q}} \sum_{\substack{0 \leq k \leq K \\ 0 \leq l \leq L}} p_{kl}^{mq}(t) \text{Log}[p_{kl}^{mq}(t)]$$

subject to the constraints 1-6 defined next.

Thus, the formulation of MAXENT for each time t consists in the constrained optimization problem (\mathbf{P}):

$$\max \left[- \sum_{\substack{0 \leq m \leq M \\ 0 \leq q \leq Q}} \sum_{\substack{0 \leq k \leq K \\ 0 \leq l \leq L}} p_{kl}^{mq}(t) \text{Log}[p_{kl}^{mq}(t)] \right] \quad (13)$$

subject to

1) Nonnegativity of probabilities

$$0 \leq p_{kl}^{mq}(t) \leq 1 \quad (14)$$

$1 \leq k \leq K$, $1 \leq l \leq L$, $1 \leq m \leq M$ et $1 \leq q \leq Q$

2) Expressions of known volume fractions of states

$$\sum_{m,q} p_{kl}^{mq}(t) = \rho_{kl} \quad (1 \leq k \leq K \text{ et } 1 \leq l \leq L). \quad (15)$$

3) Kinematic boundary conditions: prescribed components D_{ij} of the macroscopic strain rates $\mathbf{D}(t)$ at t ,

$$\sum_{\substack{0 \leq m \leq M \\ 0 \leq q \leq Q}} \sum_{\substack{0 \leq k \leq K \\ 0 \leq l \leq L}} p_{kl}^{mq}(t) L_{ij}(\mathbf{n}_k(t), r_l(t), \mathbf{v}^m) = D_{ij}(t), \quad (16)$$

where $\mathbf{L}(\mathbf{n}_k(t), r_l(t), \mathbf{v}^m)$ is the local strain rate gradient (tensor) defined at the state level and expressed in terms of the local variables.

4) Stress boundary conditions : components σ_{ij} of applied macroscopic stress tensor $\sigma(t)$ which are complementary to the prescribed components of \mathbf{D} ,

$$\sum_{\substack{0 \leq m \leq M \\ 0 \leq q \leq Q}} \sum_{\substack{0 \leq k \leq K \\ 0 \leq l \leq L}} p_{kl}^{mq}(t) \Phi_{ij}(\mathbf{n}_k(t), r_l(t), \mathbf{F}^q) = \sigma_{ij}(t), \quad (17)$$

where $\Phi(\mathbf{n}_k(t), r_l(t), \mathbf{F}^q)$ is the local stress tensor defined at the state level and given, for spherical particles, by the expression

$$\Phi(\mathbf{n}_k(t), r_l(t), \mathbf{F}^q) = \frac{N_c \mathbf{F}^q \otimes r_l(t) \mathbf{n}_k(t)}{V} \quad (18)$$

where N_c is the total number of contacts in the representative volume V [1].

5) Energy balance condition

$$\sum_{\substack{0 \leq m \leq M \\ 0 \leq q \leq Q}} \sum_{\substack{0 \leq k \leq K \\ 0 \leq l \leq L}} p_{kl}^{mq}(t) [V \cdot [\sigma(t) \otimes \mathbf{L}(\mathbf{n}_k(t), r_l(t), \mathbf{v}^m) + \Phi(\mathbf{n}_k(t), r_l(t), \mathbf{F}^q) \otimes \mathbf{D}(t)] + W_i(\mathbf{F}^q, \mathbf{v}^m)] = 0 \quad (19)$$

where $W_i(\mathbf{F}^q, \mathbf{v}^m)$ is the work of internal forces defined for the state level description expressed by $W_i(\mathbf{F}^q, \mathbf{v}^m) = \mathbf{F}_T^q \cdot \mathbf{v}_T^m$, \mathbf{F}_T^q and \mathbf{v}_T^m denoting respectively the tangential components of \mathbf{F}^q and \mathbf{v}^m

6) Unilateral contact and Coulomb dry friction conditions

$$p_{kl}^{mq}(t) = 0 \quad (20)$$

When the variables \mathbf{v}^m ou \mathbf{F}^q fail to satisfy the unilateral contact or the Coulomb dry friction conditions if

$$\mathbf{F}_N^q < 0 \quad \text{for } 1 \leq q \leq Q \quad (21)$$

where \mathbf{F}_N^q denotes the normal component of \mathbf{F}^q or

$$\mathbf{v}_N^m < 0 \quad \text{for } 1 \leq m \leq M \quad (22)$$

where \mathbf{v}_N^m designates the normal component of \mathbf{v}^m or

$$\mathbf{F}_N^q \mathbf{v}_N^m \neq 0 \quad (23)$$

or

$$\|\mathbf{F}_T^q\| > \mu \mathbf{F}_N^q \quad (24)$$

where μ denotes Coulomb's dry friction coefficient. which is assumed to be uniform for all contacts.

3 Biaxial compression test problem

As a test example the problem of biaxial compression of a 2D sample of regular granular material is considered. The solicitation is defined by specified velocity gradient D_{yy} and an imposed lateral confining stress σ_{xx} . The regular arrangement of the particles, depicted in Figure-2, makes it easy to analytically determine the response at the microscopic and macroscopic scales, providing a reference solution for comparison with the results of the MAXENT model.

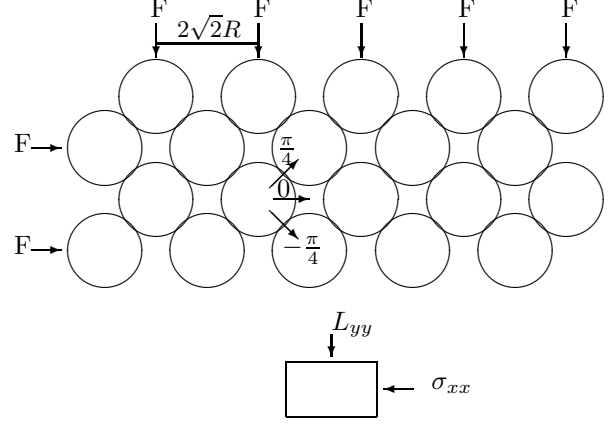


Figure-2-

The model formulation leads to a convex nonlinear programming problem. It can be noted that, with the exception of the constraint in Equation(16), which expresses the average strain rate, all the problem constraints are linear. There exist a number of formulae in the literature [3, 7, 10] that relate the average strain rate tensor to the interparticle relative c. The expression adopted in the present model

$$\mathbf{L}(\mathbf{n}_k(t), r_l(t), \mathbf{v}^m) = \frac{\mathbf{n}_k(t) \otimes \mathbf{v}^m}{r_l(t)}. \quad (25)$$

is one that is presented in [10] and subjected to a correction factor raised by the author [10] and confirmed by analytical calculation for the regular arrangement of the present example. The main advantage of this averaging formula is that it involves precisely the local variables $X(x, t) = (\mathbf{n}(x, t), r(x, t))$ and $v(x, t)$ adopted in the present model. Furthermore, a convenient feature is its linear form which makes the MAXENT problem a linearly constrained, convex one.

3.1 Formulation of the MAXENT problem

Using the expression of equation (16) for the average strain rate, the MAXENT problem can be written, in its primal form (\mathbf{P}), as

$$\min \sum_{i=1}^{KLMQ} X_i \text{Log} X_i \quad (26)$$

$$AX = b \quad 0 \leq X_i \leq 1$$

where $X(t)$ denotes the vector formed by the probabilities $p_{kl}^{mq}(t)$, A is the $(KLMQ + 3) \times (KLMQ)$ defined by

$$A = \begin{pmatrix} e_1 & e_1 & e_1 & \dots & e_1 \\ e_2 & e_2 & e_2 & \dots & e_2 \\ e_3 & e_3 & e_3 & \dots & e_3 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ e_{KL} & e_{KL} & e_{KL} & \dots & e_{KL} \\ \mathbb{L}_1 & \mathbb{L}_2 & \mathbb{L}_3 & \dots & \mathbb{L}_{KL} \\ \Phi_1 & \Phi_2 & \Phi_3 & \dots & \Phi_{KL} \\ \Pi_1 & \Pi_2 & \Pi_3 & \dots & \Pi_{KL} \end{pmatrix} \quad (27)$$

where $e_i = e_{(k,l)}$ is the i^{th} canonical row vector of dimension MQ for $1 \leq i \leq KL$, $\mathbb{L}_i = \mathbb{L}_{(k,l)}$, $1 \leq i \leq KL$, are the row vectors in \mathbb{R}^{MQ} defined by

$$\mathbb{L}_{(k,l)} = \mathbf{L}(\mathbf{n}_k(t), r_l(t), \mathbf{v}^{(m,q)})_{\substack{0 \leq m \leq M \\ 0 \leq q \leq Q}} \quad (28)$$

with $\mathbf{v}^{(m,q)} = \mathbf{v}^m$ for all $1 \leq q \leq Q$, $\Phi_i = \Phi_{(k,l)}$, $1 \leq i \leq KL$, are the row vectors in \mathbb{R}^{MQ} given by

$$\Phi_{(k,l)} = \Phi(\mathbf{n}_k(t), r_l(t), \mathbf{F}^{(m,q)})_{\substack{0 \leq m \leq M \\ 0 \leq q \leq Q}} \quad (29)$$

with $\mathbf{F}^{(m,q)} = \mathbf{F}^q$ for all $1 \leq q \leq Q$, $\Pi_i = \Pi_{(k,l)}$, $1 \leq i \leq KL$, are the row vectors in \mathbb{R}^{MQ} defined by

$$\Pi_{(k,l)} = (V \cdot [\sigma(t) \otimes \mathbf{L}(\mathbf{n}_k(t), r_l(t), \mathbf{v}^m) + \quad (30)$$

$$\Phi(\mathbf{n}_k(t), r_l(t), \mathbf{F}^q) \otimes \mathbf{D}(t)] + \Pi(\mathbf{F}^q, \mathbf{v}^m))_{\substack{0 \leq m \leq M \\ 0 \leq q \leq Q}}$$

and b is the vector in \mathbb{R}^{KLMQ+3} defined by

$$b = (\rho_1, \rho_2, \rho_3, \dots, \rho_{kl}, D, \sigma, 0)^t \quad (31)$$

where $\rho_i = \rho_{KL}$, $1 \leq i \leq KL$, denotes the volume fraction of the state $(\mathbf{n}_k(t), r_l(t))$. The problem (\mathbf{P}) is solved using the MATLAB procedure *fmincon* after a regularization of the entropy function over the hyperplanes $X_i = 0$ where it is not defined.

3.2 Regularization of the entropy function

The statistical entropy function S expressed in (11) is actually not defined for $p_{kl}^{mq}(t) = 0$

Therefore, in order to make it suitable for numerical solution it is subjected to regularization via prolongation. This is achieved by approximating the entropy function S in the neighborhood of the hyperplanes $X_i(t) = 0$, $i = 1, KLMQ$ as follows. Using the notation

$$S(X) = \sum_{i=1}^{KLMQ} S_i(X_i), S_i(X_i) = X_i \text{Log}(X_i) \quad (32)$$

the regularized entropy is obtained as the separable sum of regularized scalar functions \overline{S}_i , where \overline{S}_i denotes the regularization of S_i near the origin. The function \overline{S}_i is constructed so that it meets the following requirements:

- 1) being defined for all $X_i \geq 0$,
- 2) coinciding with S over the interval $[\varepsilon, +\infty[$,
- 3) satisfying C^0 continuity at the origin and C^1 continuity at ε ,
- 4) closely approximating S in the interval $]0, \varepsilon[$, ε being a small positive scalar.

A suitable candidate for such a prolongation is the function

$$\overline{S}(X_i) = \alpha x_i^\beta \quad X_i \in [0, \varepsilon]$$

where $\alpha = \text{Log}(\varepsilon)/e$ and $\beta = (1 + \text{Log}(\varepsilon))/\text{Log}(\varepsilon)$. A further advantage of the chosen regularization is that, similarly to the function S_i the slope at the origin is infinite.

3.3 Implementation and numerical results

In a first series of runs, a gross discretization of the local variables has been considered in order to keep the problem size minimal. By carefully eliminating, by construction, the physically impossible MDVs, the number of variables amounted to 56. The problem was solved with and without friction and the results in terms of macroscopic response were in total agreement with the predicted solutions. However, the distribution of MDVs is fundamentally different. Indeed, in the reference solution the applied forces are assumed to be uniformly distributed among all the surface particles, and the load transfer among the internal grains follows a single pattern as shown in Figure-2, whereas in the solution by MAXENT a large number of patterns are present according to some probability distribution. In particular,

a combination of scenarios of distributions of applied force at the surface particles is observed. In attempting to run examples with finer discretizations, difficulties arised with the procedure *fmincon* as the number of variables exceeded the 100 barrier. This handicap was overcome by adopting the dual formulation of the problem which appears to be spectacularly more efficient to solve than the primal.

4 Dual formulation

Due to the separable structure of problem (D) and to the very limited number of constraints compared to the number of variables the dual form of th MAXENT problem is definitely more attractive for numerical solution. Indeed, the dual problem (D) is unconstrained and the number of dual variables is very small and is independent of the degree of discretization of the MDVs.

4.1 Formulation of the dual problem

The primal problem (P) is a strictly convex problem, therefore it exhibits no duality gap. Moreover, it is separable and linearly constrained, which makes the dual formulation easy. The Lagrangian function is written as

$$L(X, \lambda) = \sum_{i=1}^{KLMQ} [X_i \text{Log } X_i + \sum_{q=1}^{KL+3} \lambda_q (A_{qi} X_i - b_q)] \quad (33)$$

and the dual function is defined by

$$\begin{aligned} \omega(\lambda) &= \min_{X \in [0,1]^{KLMQ}} L(X, \lambda) \quad (34) \\ &= \min_{X \in [0,1]^{KLMQ}} \left\{ \sum_{i=1}^{KLMQ} X_i [\text{Log } X_i + \sum_{q=1}^{KL+3} \lambda_q A_{qi}] - \sum_{q=1}^{KL+3} \lambda_q b_q \right\} \end{aligned}$$

Denoting

$$L_i(X_i, \lambda) = X_i [\text{Log } X_i + \sum_{q=1}^{KL+3} \lambda_q A_{qi}] \quad (35)$$

for $1 \leq i \leq KLMQ$ and using separability, the dual function takes on the form

$$\omega(\lambda) = \sum_{i=1}^{KLMQ} \left\{ \min_{X_i \in [0,1]} L_i(X_i, \lambda) - \sum_{q=1}^{KL+3} \lambda_q b_q \right\} \quad (36)$$

Moreover, the minima in (36) are given by

$$\begin{cases} \bar{X}_i = \exp[-(1 + \sum_{q=1}^{KL+3} \lambda_q A_{qi})], & \text{if } 1 + \sum_{q=1}^{KL+3} \lambda_q A_{qi} \geq 0 \\ \bar{X}_i = 1 & \text{otherwise} \end{cases} \quad (37)$$

and the dual problem (D) is then written as

$$\max_{\lambda \in \mathbb{R}^{KL+3}} \omega(\lambda)$$

where ω is the dual function defined using (33,34 and 37) by

$$\omega(\lambda) = \sum_{i=1}^{KLMQ} [\text{Log } \bar{X}_i + \sum_{q=1}^{KL+3} \lambda_q A_{qi}] \bar{X}_i - \sum_{q=1}^{KL+3} \lambda_q b_q \quad (38)$$

4.2 Results of the dual formulation

As expected, the dual implementation is found to be far more efficient than the primal and makes possible the solution of problems with very fine discretizations that may reach tens of thousands of MDVs while maintaining robustness. In order to simulate an evolution problem the MAXENT model has been coupled with an incremental macroscopic law. Given a macroscopic strain increment $\delta\varepsilon$ between instants t and $t + \delta t$, and assuming the macroscopic stress tensor $\sigma(t)$ to be known, the MAXENT solution at time t leads to the stress $\sigma(t + \delta t)$. Results of the evolution problem, expressed in terms of the responses $\sigma_{yy}(t)$ and $D_{xx}(t)$ in time, are in good agreement with the analytical solutions as shown in figures 3 and 4

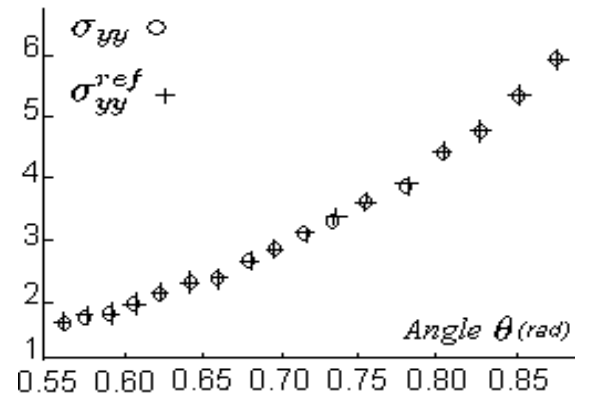


figure-3

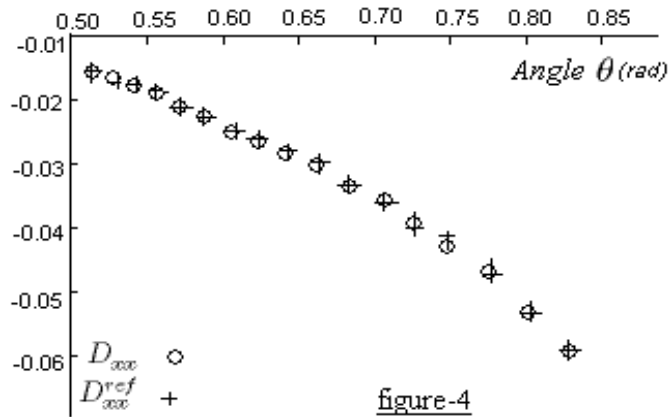


figure-4

5 Discussion and perspectives

The proposed model is a genuine maximal entropy model, defined by the equation (12) and the constraints 1-6. It was implemented numerically for a regular arrangement of circular particles, for which an explicit solution, considered as a reference solution, is known. This problem is characterized by local force boundary conditions which are consistent with the specified values for D_{yy} and σ_{xx} . However, other microscopic boundary conditions may alternatively lead to the same specified boundary values which are macroscopic quantities and are the only ones that intervene in MAXENT. Thus, the explicit solution only serves as a reference for comparison and should not be taken as the exact or the only solution to the problem of micro-macro transition at hand. The solution provided by MAXENT is, indeed, different from this reference solution. For instance, interparticle sliding and nonzero normal forces are distributed in a more balanced way among the possible combinations. This is reasonable since the reference problem and the MAXENT problem are, in essence, different : MAXENT does not actually recognize the real boundary conditions; instead, it adopts a statistical definition of the constraints and the aim is not to satisfy equilibrium in the mechanics sense, but to achieve the least biased repartition of volume fractions $p_{kl}^{mq}(t)$ of the states.

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