

# The unusual problem of upscaling isostaticity theory for granular matter

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Isostaticity theory (IT) provides stress field equations for marginally rigid packs of non-cohesive particles, interacting through hard-core forces. Its main advantage over strain-based theories is by closing the stress equations with stress-structure, rather than stress-strain, relations, which enables modelling the stress chains, often observed in experiments and simulations. The usefulness of IT has been argued to extend beyond its applicability at the jamming point. IT has been shown to be derivable from first principles in two-dimensions, with the structure quantified by a fabric tensor that couples to the stress field. However, upscaling IT to the continuum is done currently empirically by postulating convenient closure equations. The problem is that a volume average of the fabric tensor vanishes in the continuum limit, trivialising the closure equation. This poses an unusual upscaling problem, necessitating a new approach. Such an approach is developed here, resolving the problem for planar granular assemblies. The new method is developed firstly for idealised 'unfrustrated' packs and it is then extended to general realistic systems. The applicability of the method is illustrated with a tractable example.

## About Bob:

Bob Behringer was one of the main players in the field of granular matter and contributed more than many to better understanding of these systems. When I first saw the beautiful images of force chains, produced by his experiments on photo-elastic particles [1], I remember thinking that this person had just tore a window in the wall of mystery surrounding the poorly understood granular systems. By devising a way to visualise force propagation paths in such media he made it possible to peer inside them and start to sort out the confusion surrounding them at the time. Indeed, his experiments gave rise to a new generation of predictive modelling.

And then I met the man and realised that there was much more to Bob than his experiments. Bob impressed me immensely well beyond his science. The combination of his levelheadedness and his love of life was inspiring. Very notable was his default 'cool, calm and collected' mode, with a pen between his teeth and a glint of humour in his eye. But that mode would last only until I described to him a potential new idea. The cool mode would disappear and he would react with the enthusiasm of a child. Indeed, his boundless curiosity made it easy to get him excited with good science. Beyond the science there were his a lot of generosity and kindness. It was a pleasure to discuss with him anything, from fundamental science, through music and swimming to the meaning of life in general. Each such discussion felt like embarking on a voyage of discovery and almost always resulted in some more dots being connected and a better understanding emerging. Often, our discussions would meander into bantering, at which he was very good. It was very easy to forget how important his contribution had been to the development of the field and simply love him as a human being. Bob's death left a large gap in the field, as well as a hole in the hearts of many. The field is not the same without him.

## Introduction:

Granular materials (GMs) form an important and ubiquitous state of matter, playing a major role in our everyday life. They support and transmit stress significantly differently than conventional solids, often in the form of non-uniform stress chains [6]-[14]. Having a fundamental theory to predict the stress that develops in such media under given boundary loads is extremely significant for a wide range of applications in fields beyond science and engineering. All continuum static stress theories are based on balance conditions of force and torque:

$$\begin{aligned}\nabla \cdot \boldsymbol{\sigma} + \mathbf{F}_{\text{ext}} &= \mathbf{0} \\ \boldsymbol{\sigma} &= \boldsymbol{\sigma}^T,\end{aligned}\tag{1}$$

where  $\boldsymbol{\sigma}$  is the stress tensor,  $\boldsymbol{\sigma}^T$  its transpose, and  $\mathbf{F}$  includes all external and body forces on the medium. These equations must be supplemented by one constitutive relation in two dimensions (three in three dimensions). In elasticity theory, this is achieved by imposing compatibility conditions on the strain and relating the strain to the stress. This procedure results in elliptic equations whose solutions cannot be the observed stress chains. Alternative approaches, such as Critical State theory, popular in the engineering literature, rely on closures that relate the stress components when the medium is on the 'yield surface', which is a surface in the space spanned by the stress components. This approach gives a hyperbolic set of equations, yielding stress chains, or slip lines, but it is phenomenological in nature and lacks predictive power [15].

At the jamming point, GMs are minimally connected, possessing the lowest possible mean number of force-carrying contacts per particle, at which the structure is at mechanical equilibrium. In this marginally rigid, or isostatic, state, the intergranular forces in the assembly can be determined from balance conditions alone. This makes the strain, and hence stress-strain relations, redundant as input at the grain level. Since the continuum stress field is a coarse-grained representation of

the spatial distribution of those forces then continuum strain-based constitutive properties are also redundant. For this reason, such theories, which includes elasticity, are inadequate for GMs.

Isostaticity stress theory resolves the problem [16]-[25]. Most GMs in nature are not precisely isostatic, but sufficiently close to this state, they contain isostatic regions whose sizes depend on the proximity to it [22], making this theory relevant also in its vicinity. Moreover, there exist realistic systems that are close to marginal rigidity, e.g. within shear bands or by careful preparation [23, 24].

The irrelevance of strain for marginally rigid systems leaves structure as the only usable constitutive property for closing the stress equations. The most general form of such a relation in 2D is [16]-[19]

$$\sum_{ij} q_{ij} \sigma_{ij} \equiv \mathbf{Q} : \boldsymbol{\sigma} = \mathbf{0} , \quad (2)$$

where  $\mathbf{Q}$  is a symmetric fabric tensor, quantifying the local structure in a specific way. Following empirical [16, 17] and mean-field [19] proposals for the form of  $\mathbf{Q}$ , a first-principle theory derived it directly from the local grain-scale microstructure [20]. Specifically, around a grain  $g$

$$\mathbf{Q}_g = \frac{1}{2} \boldsymbol{\epsilon}^{-1} \cdot [\mathbf{C}_g + (\mathbf{C}_g)^T] \cdot \boldsymbol{\epsilon} , \quad (3)$$

where  $\boldsymbol{\epsilon} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$  is a  $\pi/2$ -rotation matrix and

$$\mathbf{C}_g = \sum_c \mathbf{C}_{cg} = \sum_c \mathbf{r}_{cg} \otimes \mathbf{R}_{cg} , \quad (4)$$

with the sum running over the loops  $c$  that surround grain  $g$ . The quadrilateral, whose diagonals are the vectors  $\mathbf{r}_{cg}$  and  $\mathbf{R}_{cg}$  (see Fig. 1), is called 'quadron', and it is the structure's most basic volume element [27]. For brevity, I index the quadrons in the following  $cg$  by  $q$  rather than  $cg$ . This structural tensor, which has a 3D equivalent [28], is useful for most GMs except when the grains are extremely non-convex [29]. The quadrons surrounding grain  $g$  are said to belong to it and their number equals its number of contacts with neighbouring grains. This description allows us both to quantify the disordered local structure unambiguously and close the stress equations with a stress-structure coupling tensor  $\mathbf{Q}$ .

It can be readily verified that  $\text{Tr}\{\mathbf{Q}_g\} = \sum_{q \in g} \text{Tr}\{\mathbf{Q}_q\} = \sum_{q \in g} \mathbf{r}_q \cdot \mathbf{R}_q$ , where  $q$  are the sum is over the quadrons belonging to grain  $g$ . Therefore,  $\text{Tr}\{\mathbf{Q}_g\}$  quantifies the deviation of the quadrons around grain  $g$  from a kite form and, consequently, this is a measure of the net rotation of grain  $g$  relative to a global mean, which must be zero [20]. In other words, this quantity describes a local rotational fluctuation. It is constructive to consider

$$\mathbf{P}_g = \boldsymbol{\epsilon} \mathbf{Q}_g \boldsymbol{\epsilon}^{-1} = \sum_q (\mathbf{s}_q \mathbf{s}_q - \mathbf{t}_q \mathbf{t}_q) / 2 , \quad (5)$$

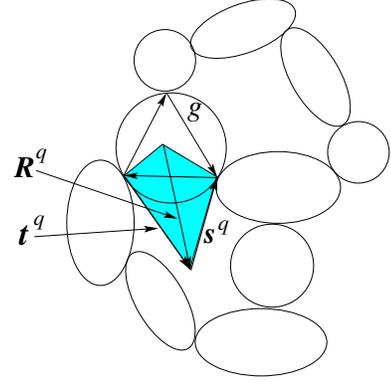


FIG. 1. The loop sides of the quadron  $q$ , whose diagonals are  $\mathbf{r}_q$  and  $\mathbf{R}_q$  and whose area is  $A_q$ , are the vectors  $\mathbf{s}_q$  and  $\mathbf{t}_q$ . The symmetric tensor  $\mathbf{P}_g$  can be written in terms of these vectors,  $\mathbf{P}_g = \frac{1}{2} \sum_q (\mathbf{s}_q \otimes \mathbf{s}_q - \mathbf{t}_q \otimes \mathbf{t}_q)$ , with  $q$  being all the quadrons belonging to grain  $g$ . Note that  $\mathbf{t}_q = -\mathbf{s}_{q'}$  if  $q'$  is adjacent to  $q$ . Therefore, the sum over  $\mathbf{P}_q$  inside a loop  $c$  vanishes identically irrespective of the loop shape.

where  $\mathbf{s}_q$  and  $\mathbf{t}_q$  are shown in Fig. 1. The antisymmetric part of  $\mathbf{C}_q$  can be written as  $\mathcal{A}\{\mathbf{C}_q\} = A_q \boldsymbol{\epsilon}$ , with  $A_q = \frac{1}{2} |\mathbf{r}_q \times \mathbf{R}_q|$  being the area of the quadron  $q$ . The area associated with grain  $g$  is  $A_g = \sum_q A_q = \mathcal{A}\{\mathbf{C}_g\}$  and the total area of the system is  $A_{sys} = \sum_g A_g$ .

#### The problem:

The first-principles derivation and, in particular, the ability to derive  $\mathbf{Q}_g$  from local structural characteristics [20] were an important development, but a new problem emerged. The equations of a complete stress theory should have the same form when upscaled, which requires that  $\mathbf{Q}_g$  can be coarse-grained systematically to arbitrarily large length-scales. This is problematic because the volume-average of  $\mathbf{Q}_g$  over any region of space vanishes except for contributions from the region's boundary. This renders the closure relation (2) a useless trivial identity in the continuum limit. To see this, consider a region  $\Gamma$ , of boundary  $\partial\Gamma$ , area  $A_\Gamma$ , and  $N_\Gamma \sim L^2$  grains. We have  $\mathbf{Q}_\Gamma = \langle \mathbf{Q}_g \rangle_\Gamma = \boldsymbol{\epsilon} \langle \mathbf{P}_g \rangle_\Gamma \boldsymbol{\epsilon}^{-1} = \mathbf{P}_\Gamma$  and the volume-average of  $\mathbf{P}$  is

$$\mathbf{P}_\Gamma = \frac{1}{2A_\Gamma} \sum_q (\mathbf{s}_q \otimes \mathbf{s}_q - \mathbf{t}_q \otimes \mathbf{t}_q) . \quad (6)$$

Let us partition the sum over neighbouring pairs in contact,  $g$  and  $g'$ , surrounding loop  $c$ . These terms cancel in pairs inside the loop because  $\mathbf{t}_{q \in c} = -\mathbf{s}_{q' \in c}$ . It follows that the contribution of loops, fully enclosed within  $\Gamma$ , to the sum (6) vanishes - only that of the quadrons along the boundary  $\partial\Gamma$  survives because those are not cancelled by neighbour quadrons. The vanishing of this sum is independent of the structural geometry, topology and grain shapes. It follows that  $\mathbf{P}_\Gamma \sim 1/L \rightarrow 0$  as  $L$  increases, rendering (3) a trivial identity.

The upscaling method:

#### I. Packs with staggered order

The resolution of this problem is based on the observation that eq. (3) can be rewritten in terms of only half the degrees of freedom in systems possessing a staggered order (SO) [20]. SO in granular packs means that grains can be labeled + and -, such that any + grain is in contact only with - grains and vice versa. This is tantamount to the condition that each loop is surrounded by an even number of grains. The upscaling procedure in such systems involves three steps: partitioning the assembly into pairs of + and - in contact; deriving the constitutive equation for unit pairs in terms of half the degrees of freedom; upscaling the constitutive equation.

The general force moment on grain  $g$  is  $\mathcal{F}_g = \sum_h \boldsymbol{\rho}_{gh} \times \mathbf{f}_{gh}$ , where  $h$  are the neighbours of  $g$ ,  $\mathbf{f}_{gh}$  the force that grain  $h$  exert on  $g$ , and  $\boldsymbol{\rho}_{gh}$  are the position vectors of the contacts between  $g$  and  $h$ . The local stress on grain  $g$  is then  $\boldsymbol{\sigma}_g = \mathbf{F}_g/A_g$ . The mean and differential stresses of a +/- pair are, respectively,  $\boldsymbol{\sigma}_m = (\mathcal{F}_+ + \mathcal{F}_-)/A_{pair}$  and  $\boldsymbol{\sigma}_d = (\mathcal{F}_+ - \mathcal{F}_-)/A_{\pm}$ , where  $A_{\pm} = A_+ + A_-$  is the area associated with the pair. Averaged over a large region,  $\Gamma$ ,  $\langle \boldsymbol{\sigma}_m \rangle_{\Gamma}$  converges to the traditional continuum stress field, with the local stress fluctuations  $\langle \boldsymbol{\sigma}_d \rangle_{\Gamma} \rightarrow 0$ . We combine the constitutive equations (3) for the pair, rearrange:

$$\begin{aligned} (\mathbf{Q}_+ + \mathbf{Q}_-) : \boldsymbol{\sigma}_m + (\mathbf{Q}_+ - \mathbf{Q}_-) : \boldsymbol{\sigma}_d &= 0 \\ (\mathbf{Q}_+ - \mathbf{Q}_-) : \boldsymbol{\sigma}_m + (\mathbf{Q}_+ + \mathbf{Q}_-) : \boldsymbol{\sigma}_d &= 0, \end{aligned} \quad (7)$$

and average over  $\Gamma$ . The first equation becomes a trivial identity. The correlation between the two small quantities,  $\langle \boldsymbol{\sigma}_d (\mathbf{Q}_+ + \mathbf{Q}_-) \rangle_{\Gamma}$  also decays with size, which leaves  $\langle (\mathbf{Q}_+ - \mathbf{Q}_-) : \boldsymbol{\sigma}_m \rangle = 0$ , in which the subscript  $\Gamma$  was dropped for brevity. The averages of  $\mathbf{Q}$  and  $\boldsymbol{\sigma}$  decouple as  $\Gamma$  increases:

$$\langle (\mathbf{Q}_+ - \mathbf{Q}_-) : \boldsymbol{\sigma}_m \rangle = \langle \mathbf{Q}_+ - \mathbf{Q}_- \rangle : \langle \boldsymbol{\sigma}_m \rangle. \quad (8)$$

Since  $\langle \mathbf{Q}_+ + \mathbf{Q}_- \rangle = 0$  then  $\langle \mathbf{Q}_+ \rangle = -\langle \mathbf{Q}_- \rangle$  and we can substitute this into (8) to obtain the upscaled relation

$$\langle \mathbf{Q}_+ \rangle : \langle \boldsymbol{\sigma}_m \rangle = 0. \quad (9)$$

This constitutive relation is a consistent coarse-grained version of the original one. Moreover, it has the significant advantage that the average of the constitutive quantity  $\mathbf{Q}_+$  does not vanish identically on coarse-graining like the original equation. Thus, this resolves the coarse-graining problem in SO systems.

## II. Extension to general GMs

In general GMs, there are almost always loops surrounded by odd numbers of grains (OL), which ‘frustrates’ the SO, as at least two same-sign grains must be in contact.

The extension of the above method to general systems is by renormalising the structure to lift the frustration. Consider a single OL, within a region of only even-edged loops, such as sketched in Fig. 2. Label the grains around it as + and - in the clockwise direction, alternately. The last grain,  $g_f$ , is in contact with the first one,  $g_0$ , and they are both +. Starting from a neighbour

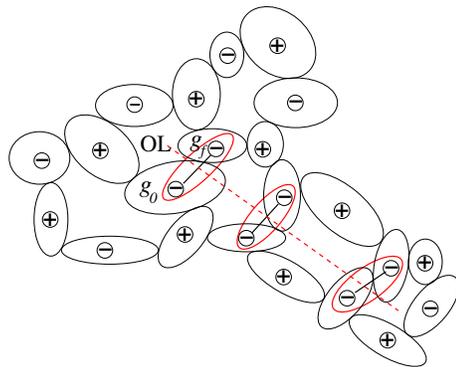


FIG. 2. The frustration around an OL surrounded by even-edged loops. Labelling the grains around it alternately by + and -, leaves two neighbouring ‘frustrated’ grains with the same sign ( $g_0$  and  $g_l$ ). Starting from a neighbour of  $g_0$  and labelling the next shell (thick lines), leaves another frustrated pair lying adjacent to the first one. Continuing this procedure shell by shell around the original OL, results in a line of such frustrated grain pairs emanating from it. This line is capped when it is incident on another OL.

of  $g_0$ , which does not belong to the OL, label similarly the first shell of loops surrounding the OL. With this shell’s loops being even-edged, it must contain exactly one frustrated pair of grains and these, which is adjacent to the pair  $g_0$ - $g_f$ . Repeating this process shell by shell outwards, a continuous line of same-sign pairs emanates from the single OL, as sketched in Fig. 2. This line extends to the system boundary. However, if the line is ‘incident’ on another OL, it ends, as sketched in Fig. 2.

This observation is the key to renormalising the structure for lifting the frustration. Isolating same-sign grain pairs into lines and regarding each such pair as a rigid super-grain, we recover a SO structure! The procedure is the following. Firstly, identify all the OLs in the network. Next, partition the OLs into nearest pairs, minimising the overall number of contacts between them. Thirdly, identify a ‘frustration’ line between each OL pair, using the above method and avoiding crossing of these lines. Finally, declare each frustrated pair of grains a super-grain and compute its fabric tensor,  $Q$  as the sum of the fabric tensors of its constituents. The result is a system of rigid objects, some the original grains and some the super-grains, possessing a SO. Finally, use the above coarse-graining procedure to upscale the constitutive relation to regions of required size, namely, containing sufficient numbers of loops each.

Although his renormalisation changes the local topology, it does not alter the forces on the original grains. Turning two grains into a super-grain eliminates the contact between them and consequently some quadrans, which are the descriptors and basic elements of the local structure. Since the structure tensor of the super-grain is the sum of those of its constituents,  $\mathbf{C}_{\pm} = \mathbf{C}_+ + \mathbf{C}_-$ , then the area associated with the super-grain is  $A_{\pm}\epsilon = \mathcal{A}\{\mathbf{C}_{\pm}\} = (\mathcal{A}\{\mathbf{C}_+\} + \mathcal{A}\{\mathbf{C}_-\}) = (A_+ + A_-)\epsilon$ , as ex-

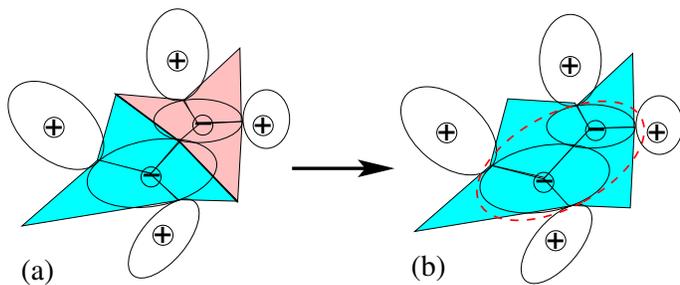


FIG. 3. The frustrated pair in (a) is joined into a super-grain, denoted by a dashed red line, in (b). The area of the super-grain is the sum of the areas of its constituents, which is also the coefficient of the antisymmetric part of the renormalised geometric tensor  $\mathbf{C}_{\text{pair}}$ . Since the renormalised fabric tensor  $\mathbf{P}$  is the sum over the tensors of the frustrated grains, their common vectors  $\mathbf{s}$  and  $\mathbf{t}$  between the joined pair (thick black lines in (a)) are also eliminated in (b), disposing of the effect of the contact point in the structural description. The stress field is unaffected by this because these vectors cancelled out anyway in the original structure. Therefore, the joining procedure is self-consistent.

pected. Another feature of the procedure concerns the physics of the stress field. Considering eq. (4), eq. (6) and Fig. 3, note that the vectors  $\mathbf{s}$  and  $\mathbf{t}$ , which originally extended between the eliminated contact point and the centres of the loops flanking it, cancel out and they do not play any role in the renormalised tensor  $\mathbf{Q}_{\pm}$  that results from the pair of the eliminated grains. Since the stress-structure coupling can be mediated only by grain contacts, the removal of the effect of the eliminated contact point by the local renormalisation is significant - it underpins the self-consistency of the procedure with its local structural and geometrical interpretation.

#### Example:

To illustrate the method, consider the granular pack shown in Fig. 4. The underlying structure is ordered on a honeycomb lattice, possessing SO. A defect has been introduced by expanding one hexagonal loop into an octagon, generating two pentagonal neighbours. The latter are OLs, introducing two sources of local frustration. The structure tensor  $\mathbf{C}$  is purely antisymmetric in the regular hexagonal regions and  $\mathbf{Q}_{\mathbf{g}}$  vanishes. The frustration defects, highlighted by ellipses in the figure, introduce a local finite fluctuation in the fabric tensor and we wish to calculate the renormalised effect on the constitutive relation after renormalising to SO. Carrying out the above joining procedure on the frustrated grains, and summing over the resulting  $\mathbf{Q}$  tensors of the positive grains, we obtain the renormalised contribution:

$$\mathbf{Q}_{\text{defect}} = \begin{pmatrix} -\frac{3}{10} & -\frac{4\sqrt{3}}{5} \\ -\frac{4\sqrt{3}}{5} & -\frac{3}{2} \end{pmatrix}. \quad (10)$$

Substituting into (9), the local constitutive around the defect is then

$$\sigma_{xx} + 5\sigma_{yy} + \frac{16}{\sqrt{3}}\sigma_{xy} = 0. \quad (11)$$

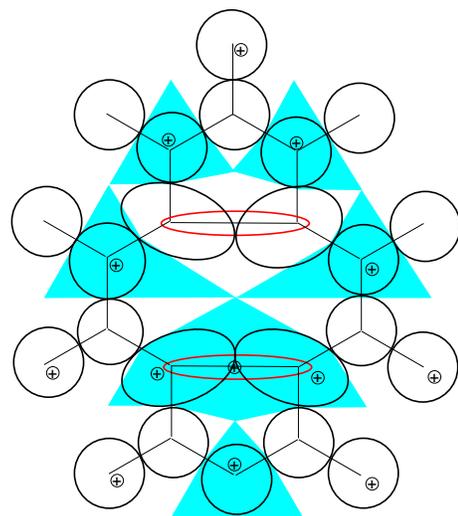


FIG. 4. A granular structure, based on a honeycomb lattice, is ordered except for a defect consisting of an octagonal loop flanked by two pentagonal loops, which introduce two frustrated grain pairs. The coarse-graining is over all the positive grains, but only those near the defect with irregular areas (shown shaded) have a finite fabric tensor.

This can now be used, together with eqs. (1), to calculate the local stress. However, if the system includes a random distribution of such defects, we may wish to coarse-grain over larger regions. This is done simply by calculating the local fabric tensors, as above, and averaging them over volumes of any desirable size to obtain an upscaled constitutive relation.

#### Conclusion:

In summary, the problem of upscaling the stress equations of isostatic GMs is unique in that the volume average of the constitutive fabric tensor, which couples to the stress to close the field equations, vanishes in the large-scale limit. This has led to imposing phenomenological or empirical fabric tensors. Particular examples of such closures are the yield conditions, such as Mohr-Coulomb, in Critical State Theory. This problem is resolved here from first-principles by developing a specialised upscaling method. The method is based on the observation that the constitutive relation can be written in terms of only half the degrees of freedom in ideally unfrustrated granular packs. Unlike for the full system, the volume average of the resulting constitutive relation for grain pairs need not vanish identically in the continuum limit. The method is extended to more realistic frustrated systems by developing a renormalisation scheme which joins frustrated grain pairs and restores the unfrustrated SO. The procedure leads to a renormalisation of the local fabric tensor and an example of such a calculation for a simple system including two defects in an otherwise honeycomb-like structure has been illustrated.

It would be interesting to test the method on systems in which both the structure and the forces can be visualised, such as the many examples produced in the lab

of Bob Behringer [1]. Moreover, the problem is still outstanding for three-dimensional systems, which have not

been discussed here. Work on extension of the method to such systems is ongoing.

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