Anisotropic contiguity calculations of many-grain aggregates using the Fast Multipole Boundary Element Method

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1. Overview

The microstructure of partially molten rock strongly influences the macroscopic properties of the grain-melt aggregate. Partially molten rock under elevated pressure and temperature deforms in a time-dependent, viscous manner. The evolution of the aggregate under these conditions is controlled by the physical properties of the grains and melt. Viscosity differences between the grains and melt produce stress along the grain-melt interface that affects the grains' ability to deform [1, 2, 3, 4, 5]. Surface tension forces along the grain-melt interface drive viscous deformation within a grain, which can affect nearby grains [5]. Previous work has shown that the viscosity ratio between the grains and the melt, along with the grains' surface tension, can impact the contiguity of an aggregate [6, 7].

Our work uses a numerical acceleration technique that allows us to simulate the evolution of a mesoscale grain-melt aggregate subjected to an imposed velocity for a range of physical parameters. We use the results of the simulations to derive emperical relationships between the properties of the microstructure. Specifically, we use secondary testing to obtain relationships between the deformation and anisotropy of the contiguity tensor for an evolving grain-melt aggregate.

2. Governing equations and boundary integrals

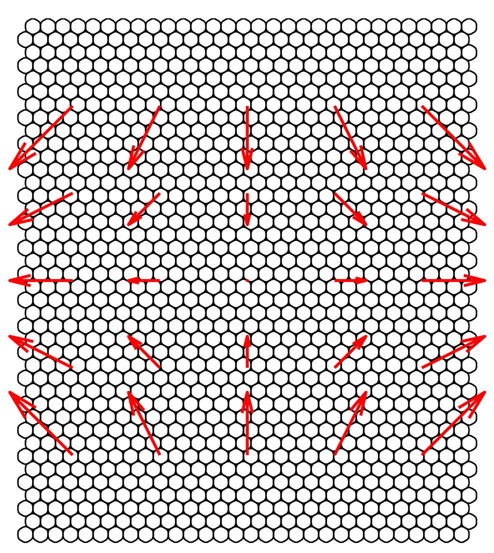


Figure 1: The initial grain aggregate and the imposed pure shear velocity. The Fast Multipole Boundary Element Method is used to solve the Stokes velocity. The geometry evolves through creeping flow governed by the kinematic condition.

The evolution of a grain-melt aggregate is governed by a coupled viscous flow within the grains and melt. The P grains and melt are treated as incompressible fluids, and as such the velocity of the flow, u_i, throughout the aggregate, is divergence free,

$$u_{i,i} = 0. \qquad (1)$$

Conservation of momentum within each grain and the melt requires, in the absence of a body force,

$$T_{ij,i} = 0, \qquad (2)$$

where the stress tensor T_{ij} for a fluid with viscosity μ and pressure field P is given by

$$T_{ij} = -P + \mu\left(u_{i,j} + u_{j,i}\right). \qquad (3)$$

Following [8] and [9], we derive the boundary integral equation (BIE) for (1-3):

$$u_j(\boldsymbol{x}_0) = \frac{2}{1+\lambda^{(q)}}\left[u_j^{\infty}(\boldsymbol{x}_0) - \frac{1}{4\pi\mathcal{C}a}\sum_{p=1}^{P}\int_{\Gamma_p}\Delta f_i(\boldsymbol{x})\mathcal{U}_{ij}(\boldsymbol{x},\boldsymbol{x}_0)\,d\Gamma_p + \sum_{p=1}^{P}\frac{1-\lambda^{(p)}}{4\pi}\int_{\Gamma_p}^{\mathcal{PV}} u_i(\boldsymbol{x})\mathcal{T}_{ijk}(\boldsymbol{x},\boldsymbol{x}_0)\hat{n}_k(\boldsymbol{x})\,d\Gamma_p\right], \qquad (4)$$

where $\mathcal{U}_{ij}(\boldsymbol{x},\boldsymbol{x}_0)$ and $\mathcal{T}_{ijk}(\boldsymbol{x},\boldsymbol{x}_0)$ are the Stokeslet and Stresslet, $\Delta f_i(\boldsymbol{x})$ is the jump in surface traction across the grain-melt interface Γ_p, $\lambda^{(p)} = \mu_p/\mu_m$ is the viscosity ratio between the p^{th} grain and melt, and $\mathcal{C}a = \frac{\mu_m u_c}{\gamma_c}$ is the capillary number. Velocity $u_j^{\infty}(\boldsymbol{x}_0)$ represents the velocity of the melt absent the grains.

Each integral is broken into N_p boundary element integrals by dividing a boundary into boundary elements such that

$$\int_{\Gamma_p} \cdot\, d\Gamma_p = \sum_{e=1}^{N_p}\int_{\Gamma_{p,e}} \cdot\, d\Gamma_{p,e}. \qquad (5)$$

The resulting linear system is rewritten in matrix notation as

$$\left(\frac{1+\lambda}{2}\boldsymbol{I} - \frac{1-\lambda}{4\pi}\boldsymbol{T}\right)\boldsymbol{u} = \boldsymbol{u}^{\infty} - \frac{1}{4\pi\mathcal{C}a}\boldsymbol{U}\Delta\boldsymbol{f}. \qquad (6)$$

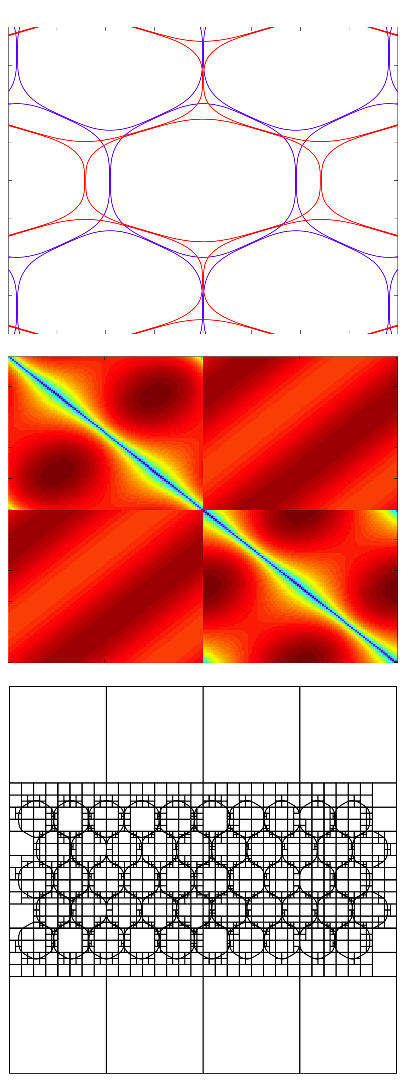
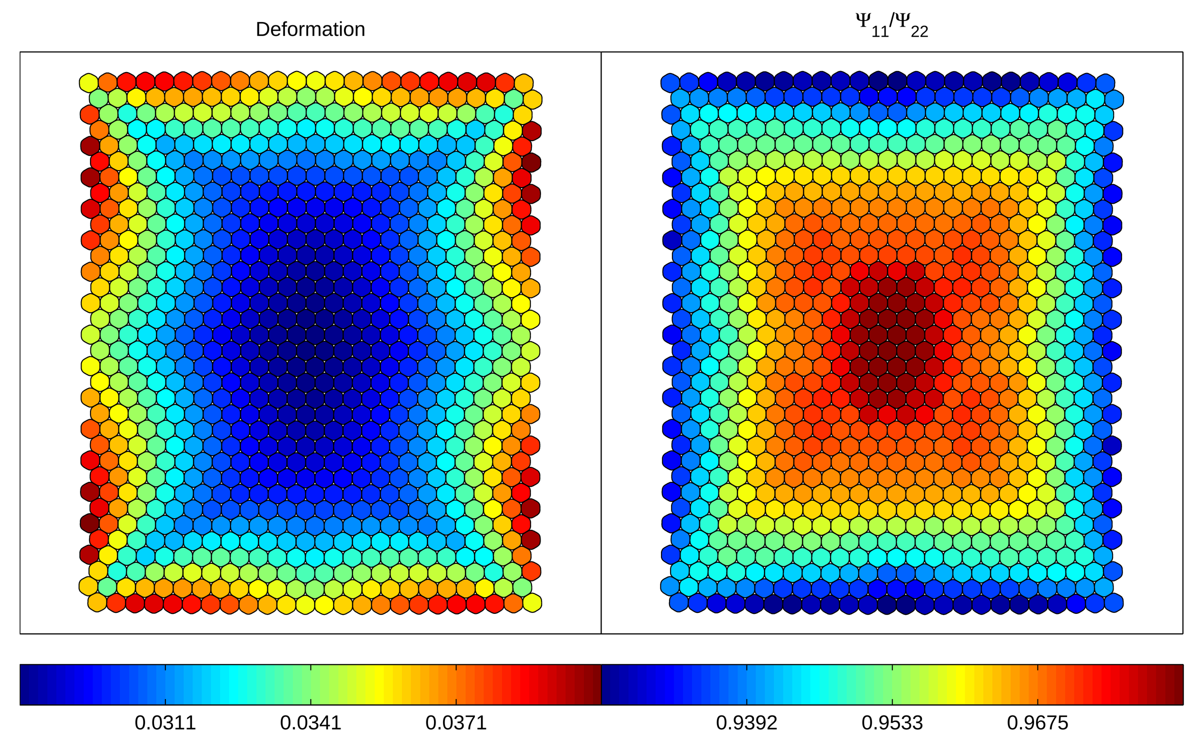


Figure 2: (Top) Deformation of a patch of grains in a pure shear flow. (Middle) Dense Stokeslet matrix generated by the BIE. (Bottom) Adaptive domain partitioning of smaller grain-melt aggregate for FMM expansions.

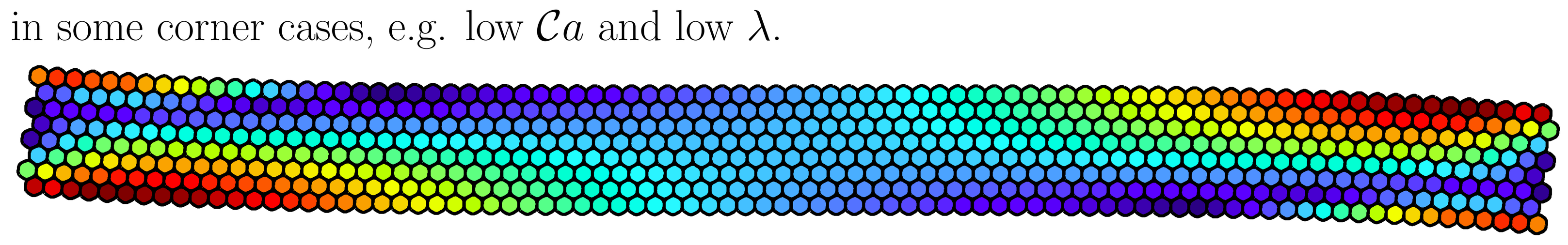
The system of linear algebraic equations arising from discretization of (4) is generally dense and asymmetric. The lack of matrix structure requires using direct solvers for which computing the solution is $\mathcal{O}(N^3)$ in time, where N is the number of pole points used in the discretization. The Fast Multipole Method (FMM) accelerates the convergence to a numerical solution by approximating matrix-vector multiplication in $\mathcal{O}(N\log(N))$ time and storage compared to the standard $\mathcal{O}(N^2)$ for dense matrices [10][11].

3. Numerical Results



The results of the simulations are used to compute the deformation, D, and anisotropy of the contiguity tensor, Ψ_{11}/Ψ_{22}, over the aggregate. The contiguity tensor measures the amount of normal inter-grain contact for each grain. Parameter λ is varied over $[1.0, 2.0, 5.0, 50.0]$, and parameter $\mathcal{C}a$ is varied over $[1, 0.7, 0.5, 0.3, 0.1, 0.05]$.

We then test for relationships between the deformation of a grain, D, and the anisotropy of the contiguity tensor, Ψ_{11}/Ψ_{22}, for grains in the prescribed flow. Across all simulations, the outer grains buffered the inner grains from immediate deformation and anisotropy. Overall behavior is strongly dependent on λ with $\mathcal{C}a$ only having an impact on the evolution in some corner cases, e.g. low $\mathcal{C}a$ and low λ.



4. Discussion

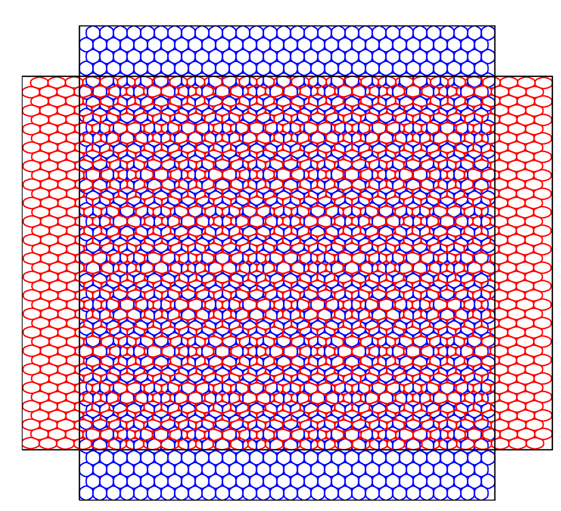


Figure 5: Our method can be used in conjunction with continuous macroscopic models that take into account the microscopic behaviors and relationships between anisotropy of the contiguity tensor and deformation in grains.

For a parcel of grain-melt matrix in the continuous aggregate, a mesoscale simulation can find relationships between microscopic dependent properties.

Using the Fast Multipole Boundary Element Method, we can feasibly simulate the evolution of a large grain-melt matrix.

The microscopic properties computed from the numerical simulations are analyzed and used to derive emperical relationships between them. For the pure shear test case, we found an emperical relationship between anisotropy of the contiguity and deformation given by:

$$\Psi_{11}/\Psi_{22} \sim e^{-4D} \qquad (7)$$

with $R^2 = 0.997789$. The relationship holds for all tested values of $\mathcal{C}a$ and λ.

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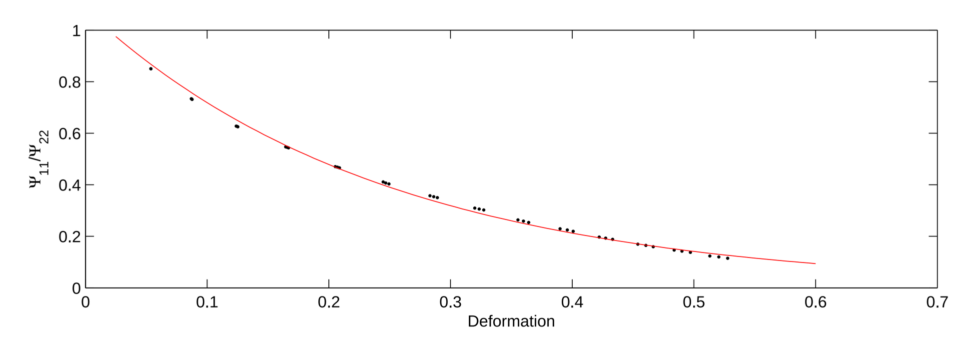

Figure 6: Using the numerical simulations, we derive an empirical relationship between the deformation and anisotropy in the contiguity tensor.

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