

# Física y Aplicaciones de la Materia Granular

Discrete element modeling of strongly deformed particles in dense shear flows

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- Grandes deformaciones de partículas blandas
- Método de los elementos discretos
- Empaquetamientos altamente densos
- Fuerzas de contacto: MC-DEM

## Discrete element modeling of strongly deformed particles in dense shear flows

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### ABSTRACT

The discrete element method (DEM) proposed by Cundall and Strack [1] is a widely used numerical approach to study the fundamentals of particulate matter at the particle scale. In our present study, the flow behavior of dense configurations of soft particles was studied by means of a new formulation of the multi-contact force closure for the DEM. The first step was to verify the response of the new force closure, and calibrate its parameters based on a comparison of the results for simple uniaxial compression with results from a reference simulation. This reference simulation used a highly accurate nonlocal formulation of contact mechanics in the quasi-static limit [2], which accounts for the interplay of deformations due to multiple contact forces acting on a single particle. The newly developed and calibrated model results show significant improvement over those derived via the existing multi-contact model. Also, the dependence of the stress in the sheared granular matter on the Poisson's ratio was unveiled when using the newly derived advanced multi-contact force closure. Therefore, an extensive campaign of simple shear flow simulations was performed (at a fixed volume of the simulation box) to probe the effect of particle volume fraction and the speed of shearing. These simulations show that the stress at particle volume fractions larger than a critical value depends not only on the friction coefficient and particle stiffness, but also on the Poisson's ratio of the material. Finally, we report a response surface for the pressure in a sheared particle bed as a function of all key influence parameters. This response surface is beneficial for calibrating DEM model parameters in extremely dense flow configurations.

- Integración de las ecuaciones de movimiento
- Fuerzas de contacto de a pares
- DEM:

$$\delta_c = (r_i + r_j) - (\mathbf{x}_i - \mathbf{x}_j \cdot \mathbf{n})$$

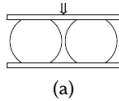
- MC-DEM:

$$\delta_{k \rightarrow c} = -\gamma \frac{(1 + \nu)F_k}{2\pi E d_k} \left\{ (\mathbf{n}_k \cdot \mathbf{u}_{kc})(\mathbf{n}_c \cdot \mathbf{u}_{kc}) + (3 - 4\nu)\mathbf{n}_k \cdot \mathbf{n}_c - (1 - 2\nu) \frac{(\mathbf{n}_k + \mathbf{u}_{kc}) \cdot \mathbf{n}_c}{1 + \mathbf{n}_k \cdot \mathbf{u}_{kc}} \right\}$$

- Aplicable a varias leyes de contacto. Hertz:  $F \propto (\delta_c + \sum_k \delta_{k \rightarrow c})^{3/2}$

## Usual DEM model

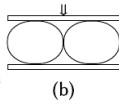
- Independent contacts  $F_c = f(\delta_c)$
- Nondeformable spheres



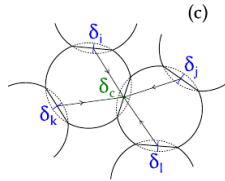
(a)

## Proposed model

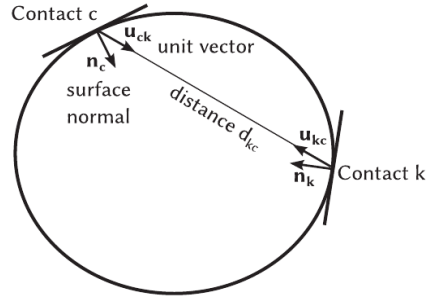
- Multiple contacts
- $F_c = f(\delta_c, \delta_i, \delta_j, \delta_k, \delta_l)$
- Surface deformations create new contacts



(b)



(c)

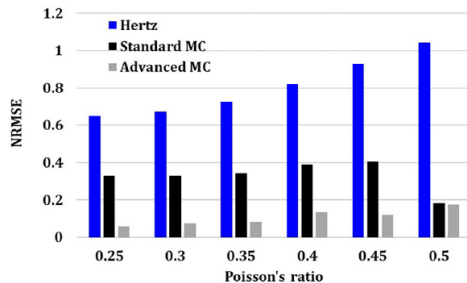


Modelo multicontacto.

- $MPR = \delta_{max}/r_i$
- $F_k = \begin{cases} f(\delta_c) & \text{si } \delta_{k \rightarrow c} > \delta_{max} \\ f(\delta_c + \sum_k \delta_{k \rightarrow c}) & \text{si } \delta_{k \rightarrow c} \leq \delta_{max} \end{cases}$
- Los parámetros MPR y  $\gamma$  deben calibrarse para cada configuración

Caso testigo: compresión uniaxial de partículas de hidrogel.

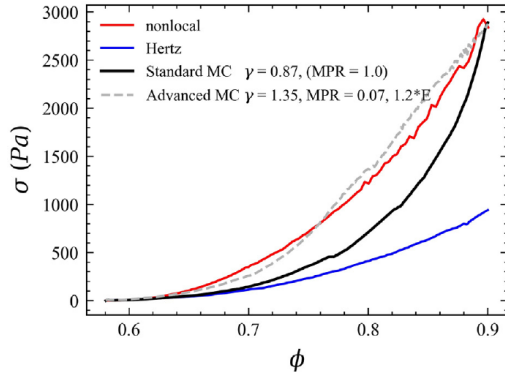
- 514 partículas,  $\phi$  inicial = 0,58
- Comparación con modelos *nonlocal*, Hertz y MC estándar
- Ajuste de los parámetros  $\gamma$  y  $E$ : dependencia lineal con  $\nu$



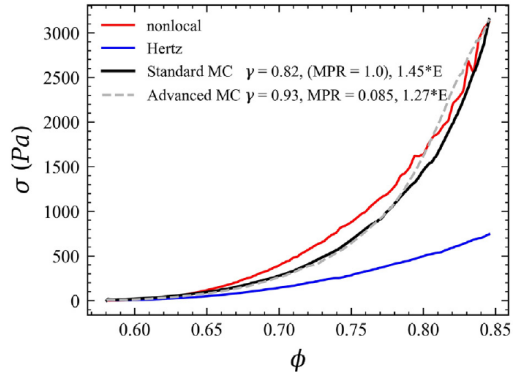
Error cuadrático medio normalizado.

# Verificación y calibración

e)  $\nu = 0.45$

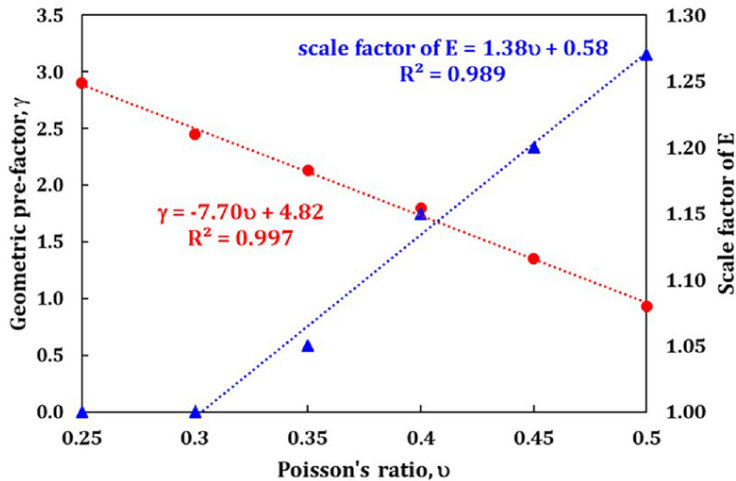


f)  $\nu = 0.50$



Tensión vs fracción de volumen sólido.

# Verificación y calibración

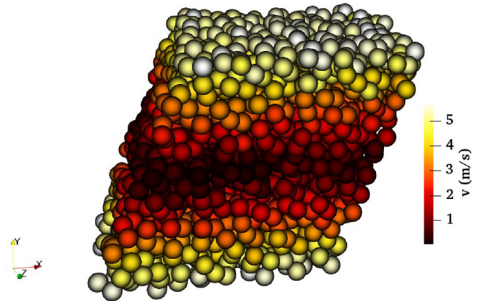


Prefactor  $\gamma$  y  $E$  calibrados como función de  $\nu$ .



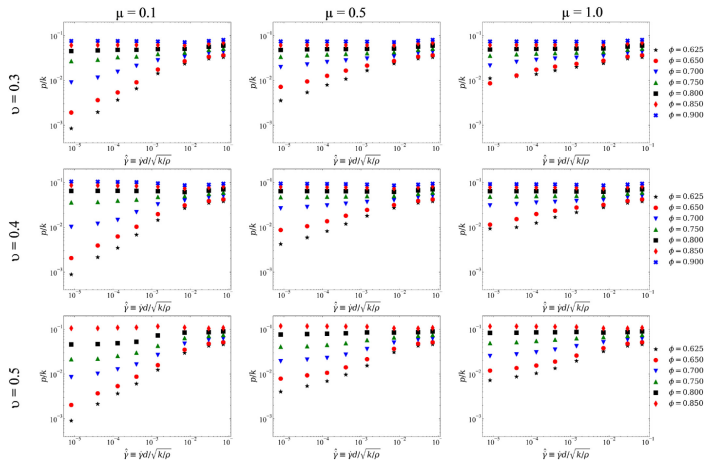
# Flujo de corte simple

- Simulación de cubo en caja de simulación periódica con condiciones de borde Lees-Edward
- 20 000 partículas monodispersas
- $\phi = 0,625; 0,65; 0,7; 0,75; 0,8; 0,85$  y  $0,9$



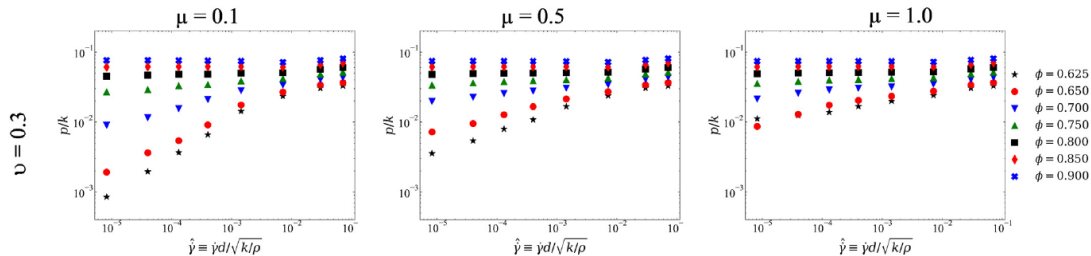
Materia granular en flujo de corte simple,  $\phi = 0,9$ .

# Resultados



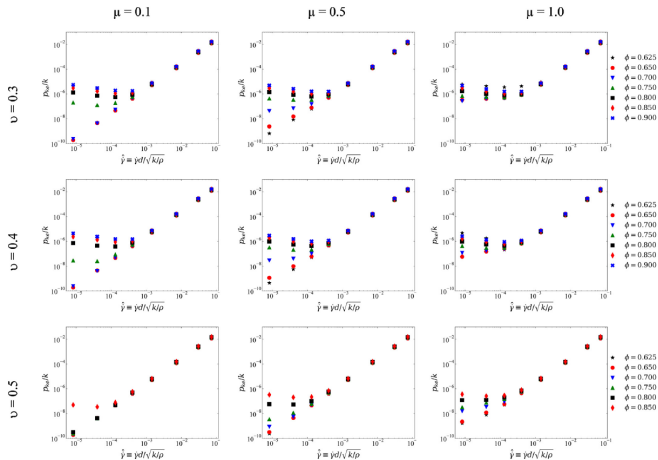
Presión adimensional vs. tasa de corte adimensional.

# Resultados



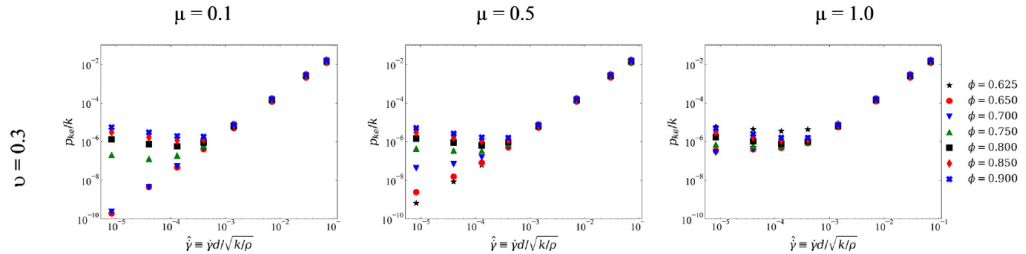
Detalle de la presión adimensional vs. tasa de corte adimensional.

# Resultados



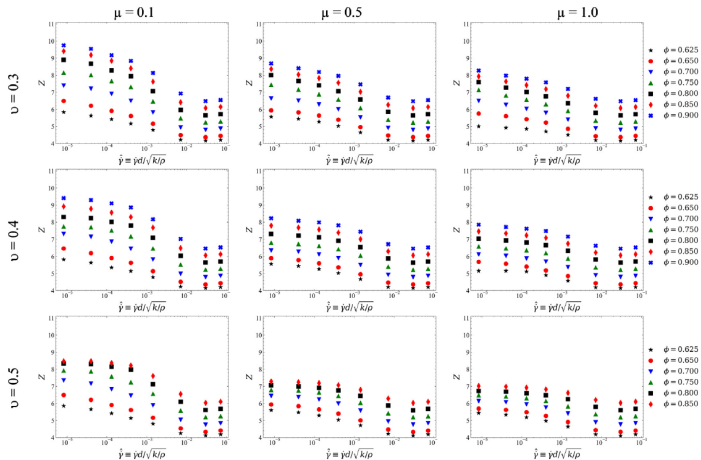
Presión cinemática adimensional vs. tasa de corte adimensional.

# Resultados



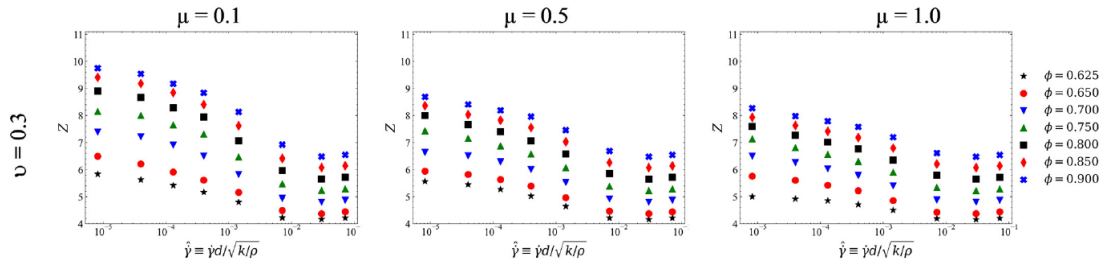
Detalle de la presión cinemática adimensional vs. tasa de corte adimensional.

# Resultados



Número de coordinación promedio vs. tasa de corte adimensional.

# Resultados



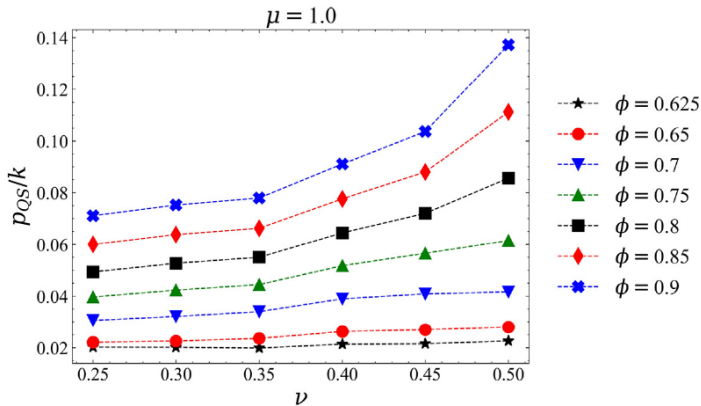
Detalle del número de coordinación promedio vs. tasa de corte adimensional.

# Resultados

La presión en el régimen cuasi estático puede modelarse como:

$$p_{QS}/k = \alpha_{QS} |\phi - \phi_C|^\beta$$

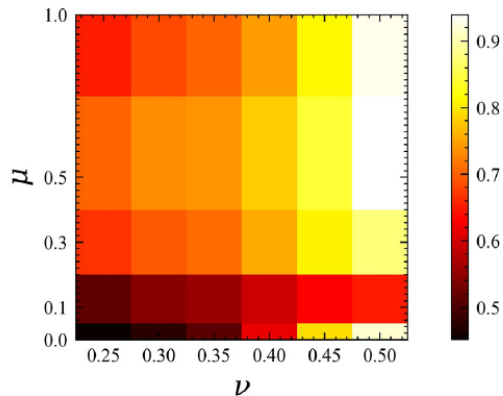
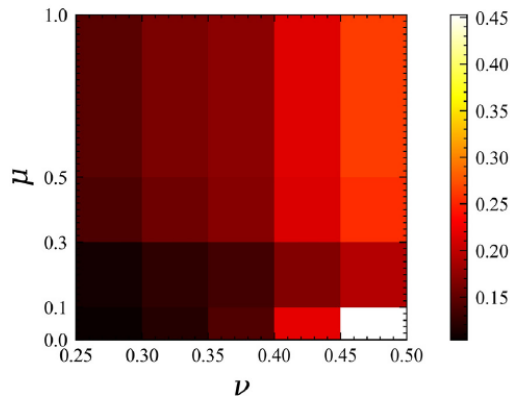
- $\alpha_{QS}$  depende del coeficiente de fricción
- $\beta$  depende del modelo de contacto



Presión cuasi estática promedio vs.  $\nu$ .



# Resultados



$\alpha_{QS}$  y  $\beta$  para varios coeficientes de fricción y coeficiente de Poisson.

# Conclusiones

- Se mejoró el modelo multicontacto estándar y se calibraron sus parámetros
- MPR cambia entre DEM y MC-DEM, y permite simulación de configuraciones con  $\phi > 0,7$
- Cuando las partículas se vuelven incompresibles ( $\nu$  se aproxima a 0,5) debe ajustarse el módulo de Young.
- Para flujos de corte simples por encima del punto de atascamiento la presión cuasiestática depende tanto del coeficiente de fricción como del coeficiente de Poisson

# Muchas Gracias