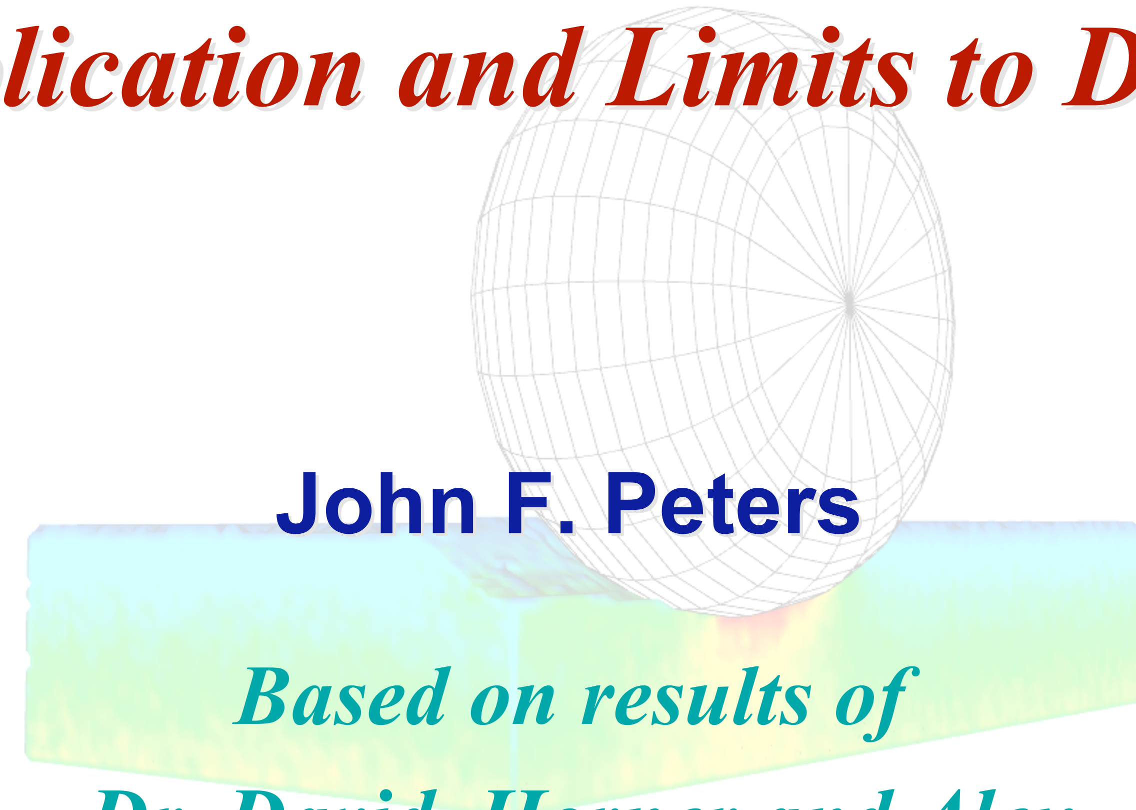
Application and Limits to DEM

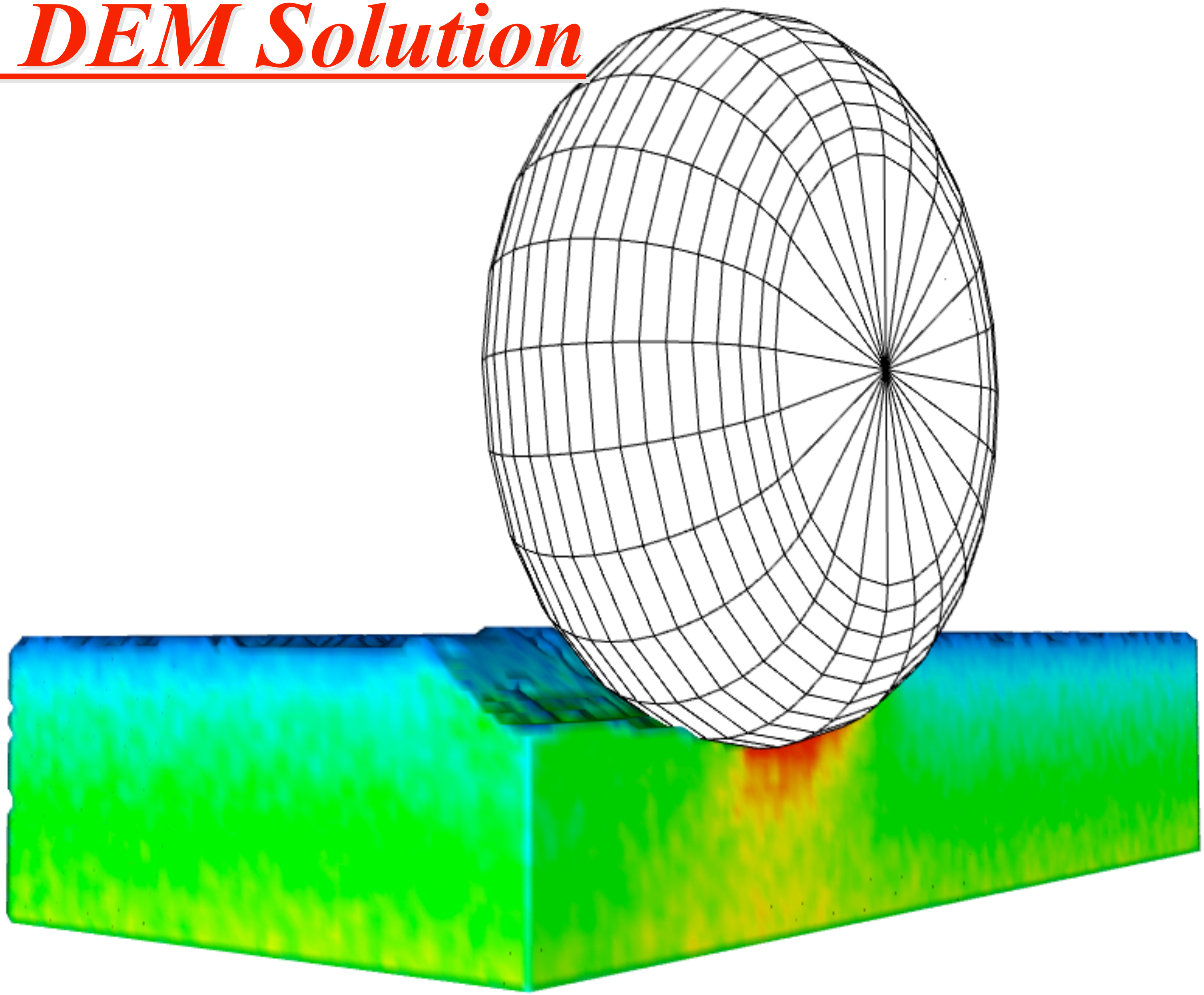


John F. Peters

Based on results of

Dr. David Horner and Alex Carrillo

The DEM Solution



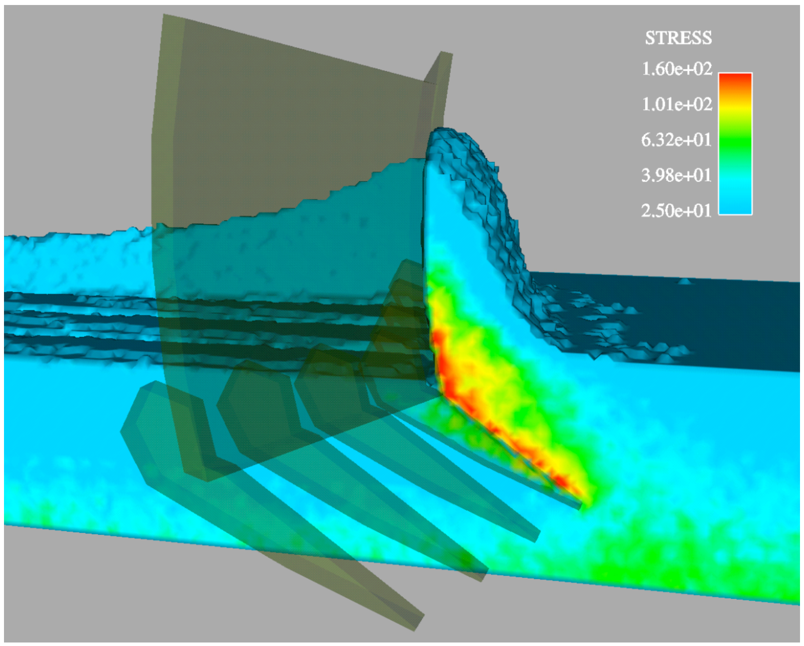
Soil Deformation: Technical Challenges

- Changing geometry (Difficult to describe from either material or spatial framework alone)

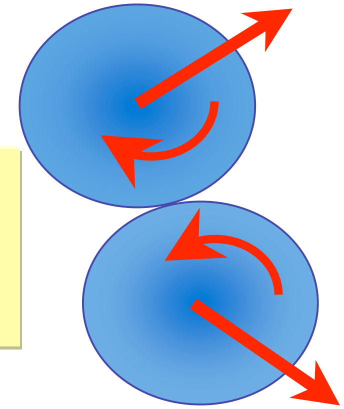
- Changing topology (Real motions are non-affine)

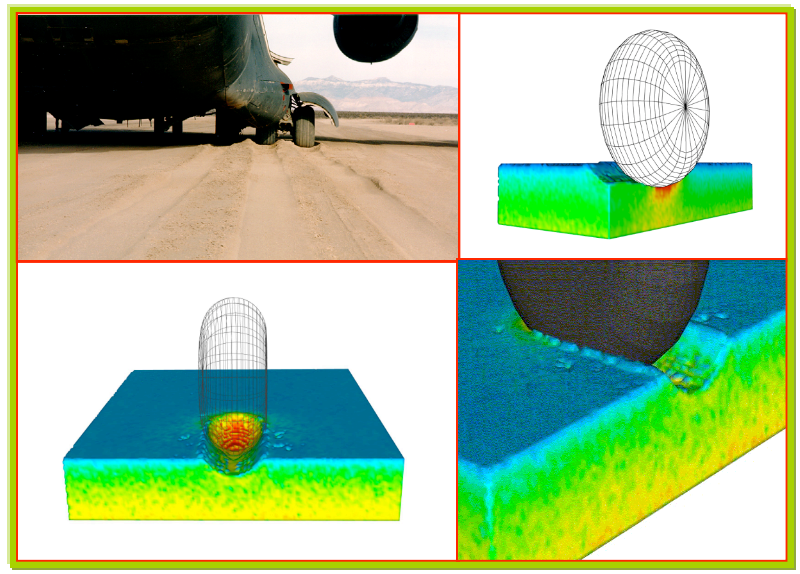
- No adequate phenomenological constitutive theory available. Key issues must be resolved at more fundamental level

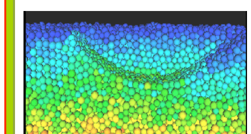
The computational solution



- Discrete element models are fundamentally simple and display realistic *emergent* behavior.



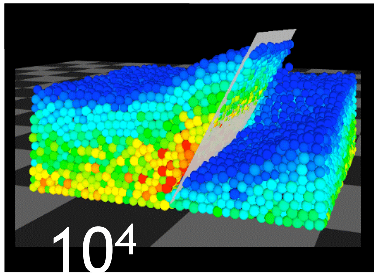


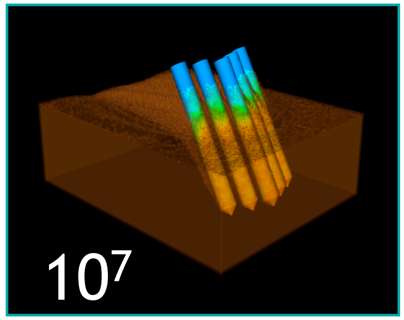


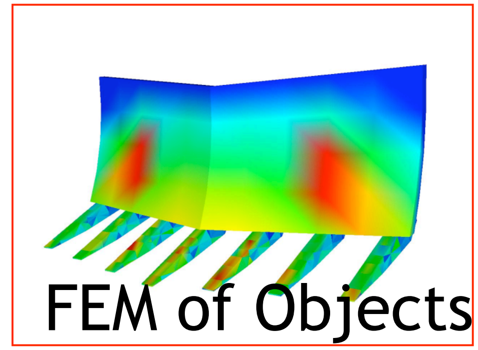
- The discrete element method depends on high performance computing resources.

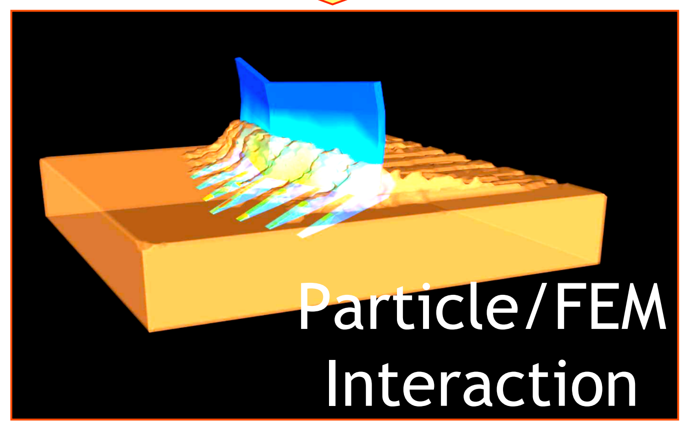
- DEM is in its formative stages but with HPC support will become a powerful analysis tool

The Development Trend

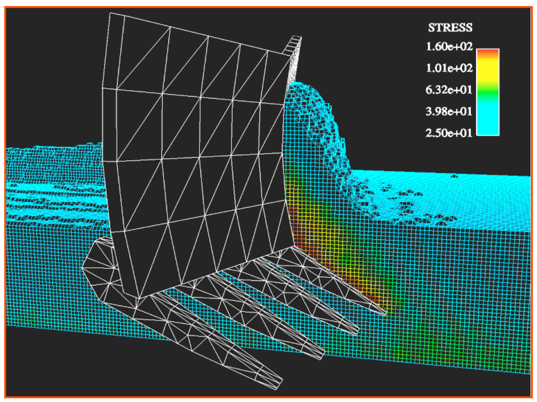








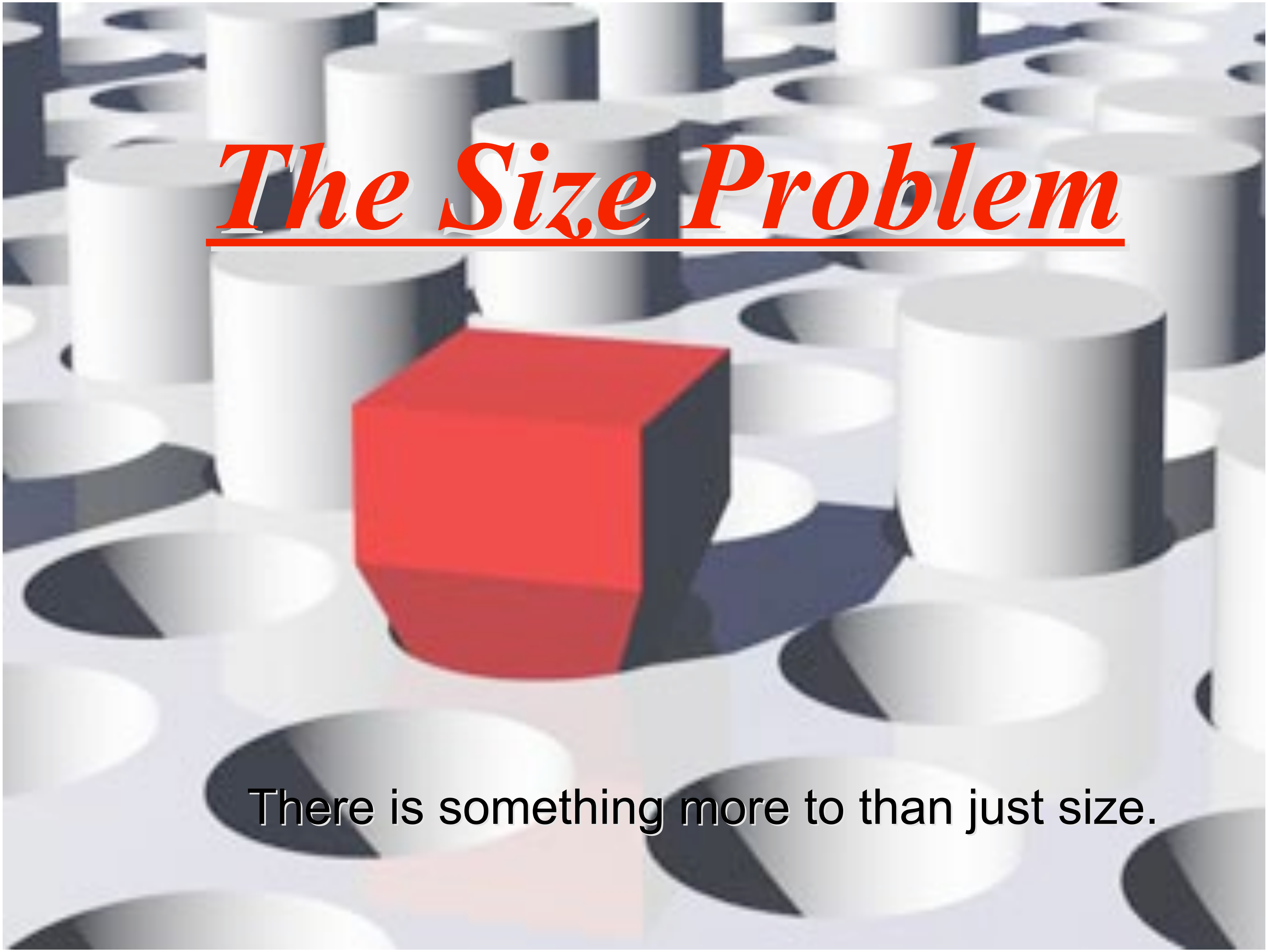
Current Capability



Virtual Laboratory

Current work will provide the resources to make this transition possible.

The Size Problem



There is something more to than just size.

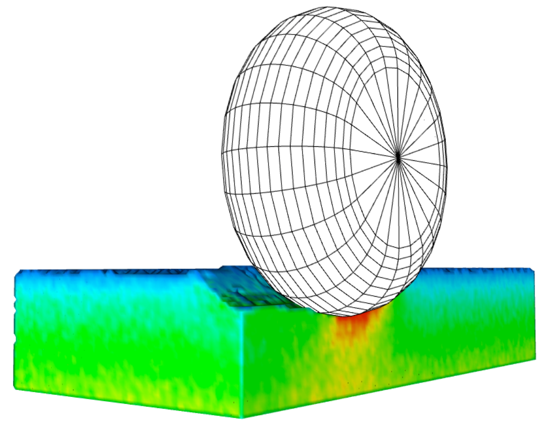
Discrete Element Modeling

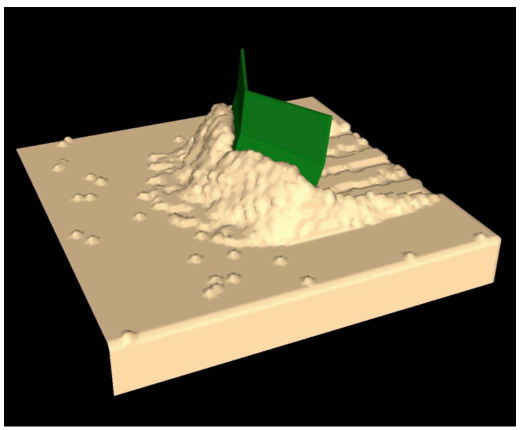
- Model particles in detail as a tool to understand micromechanics of granular media.

✓ Use discrete elements to capture prototype-scale behavior dominated by non-affine motion, shear bands and other non-continuum behavior.

Prototype Scale Analysis

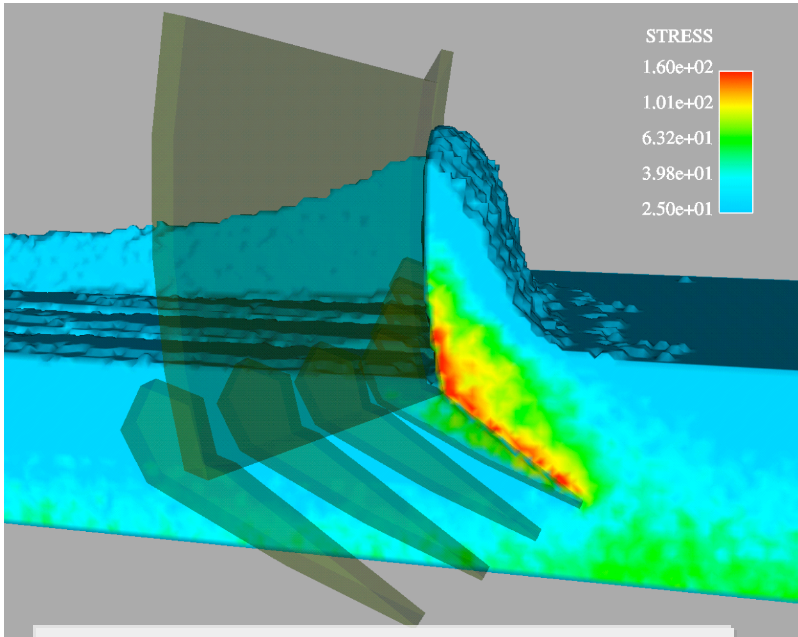
- Particles used in simulation are larger than in prototype.
- Satisfying micromechanics not required.
- Equivalence is based on bulk behavior of material.

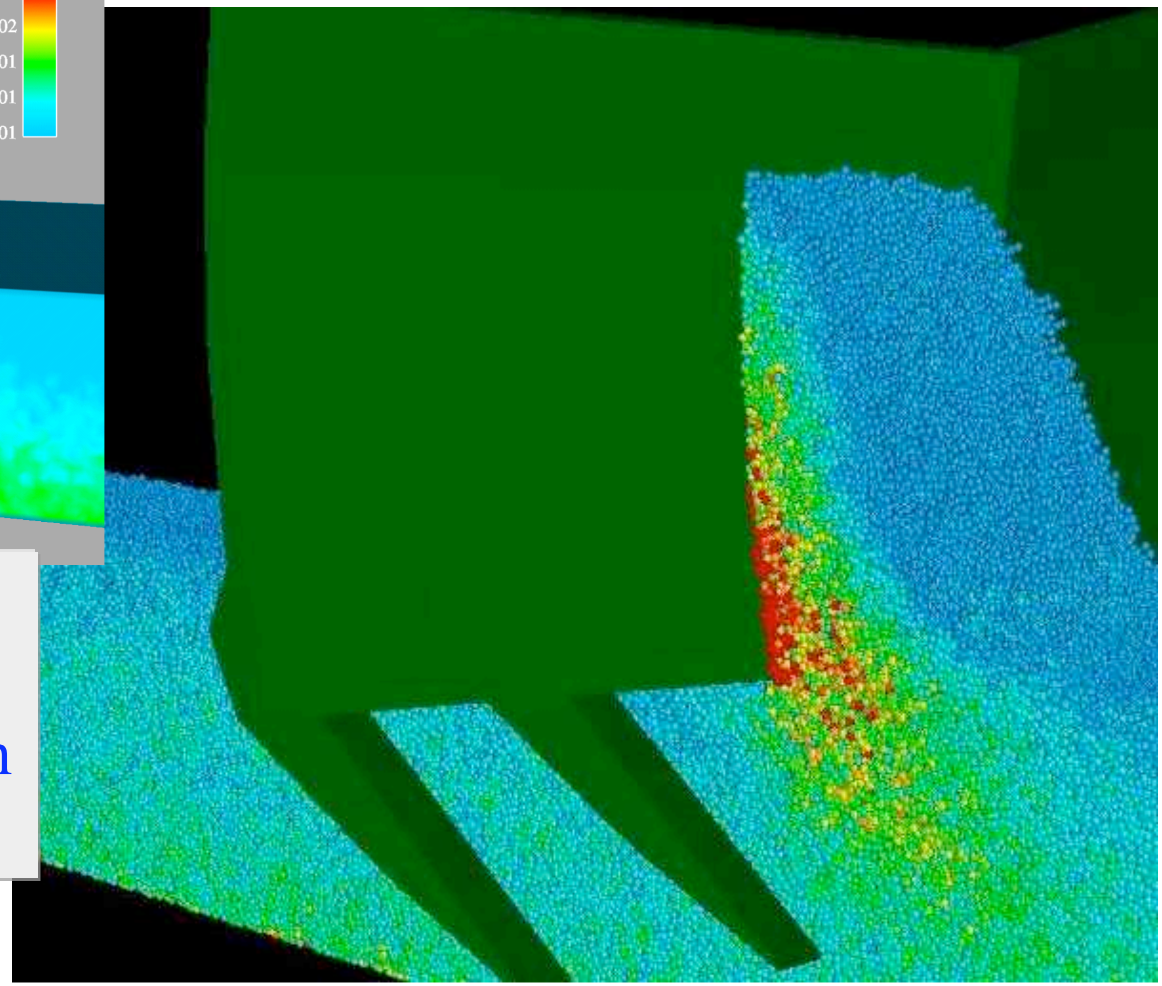




- Some have used arguments based on dimensional analysis similar to geotechnical centrifuge.
- Size effects result from two sources:
  - Cosserat rotations
  - Force chains
- Particle interaction laws an open issue

The Particle Scale



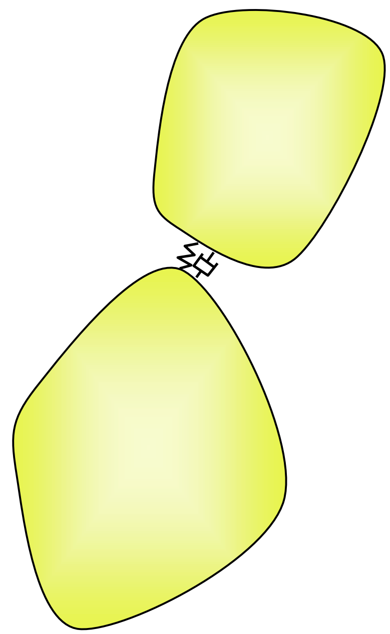


Cutaway View of Discrete Element Simulation of Plowing in Soil

Critical Question for Prototype Scale Simulation by DEM

Can properties be determined to capture bulk properties of material?

- Contact stiffness and damping
- Rotational inertia
- Particle distribution
- Particle shape



Principal Themes

1. You cannot compute what you do not resolve. *The Numerical Sage*

2. Numerical error appears as real physics but at the wrong scale.

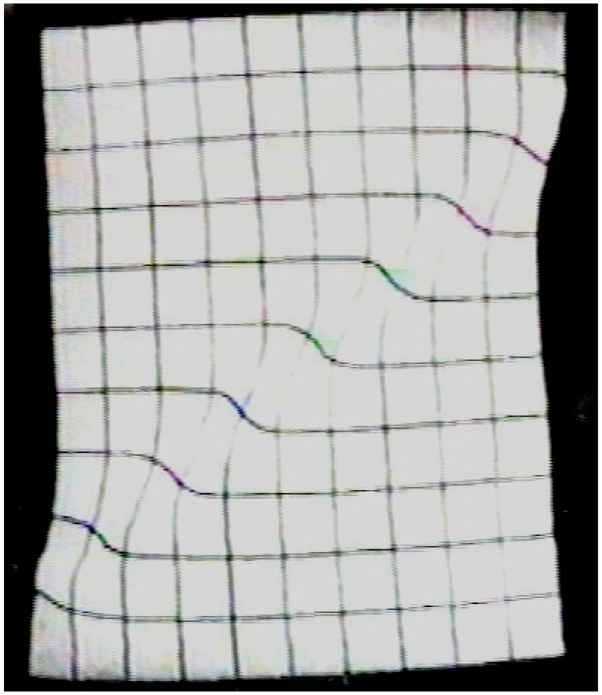
DEM versus Numerical Modeling

Numerical: Discrete system as approximation to partial differential equations with well established concepts of consistency, stability and convergence.

DEM: Discrete system as approximation to finer discrete system but without established theory on error created by scale.

The Shear-Band Problem

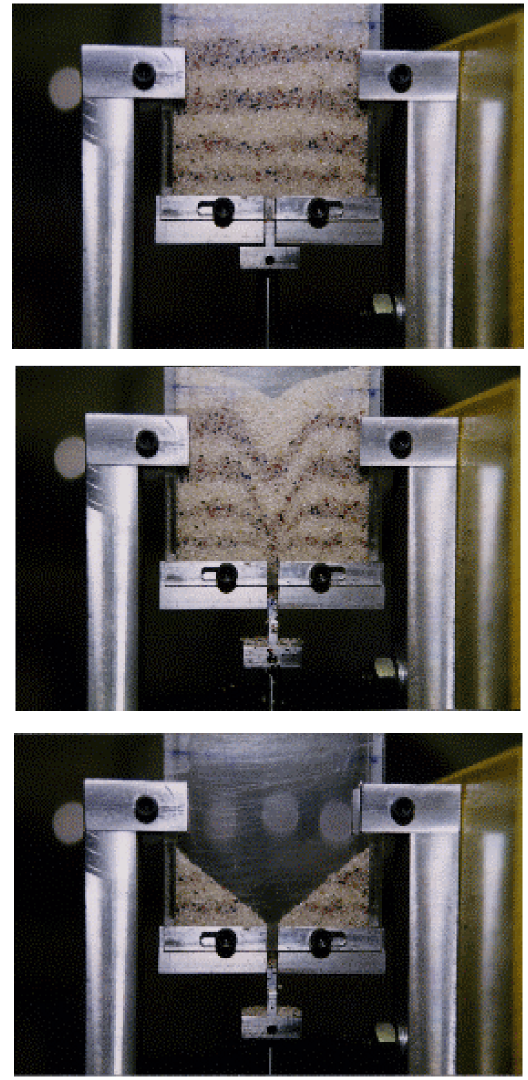
- Shear band thickness influenced by particle size
- Thickness could affect failure kinematics

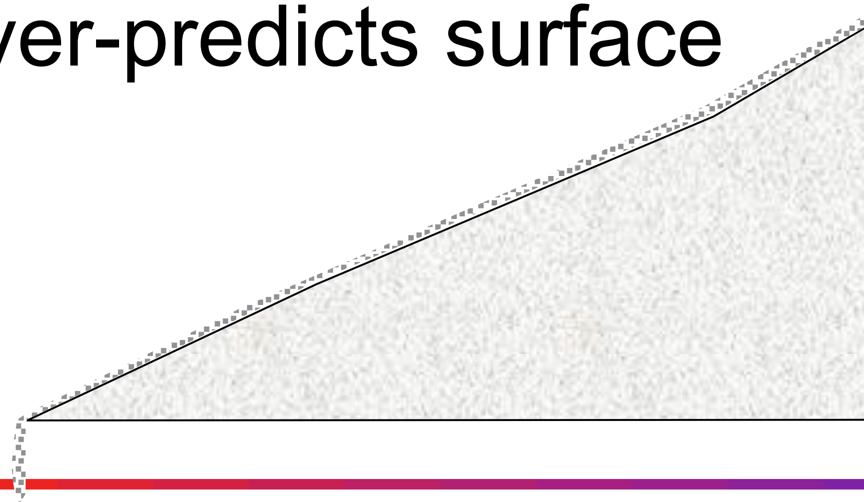


The Avalanche Problem

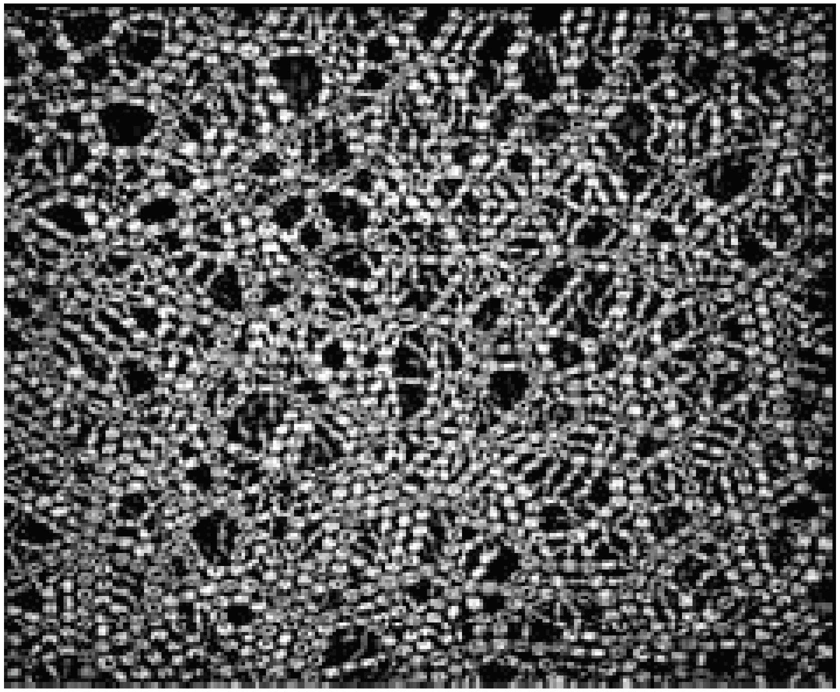
- Without rotations, near-surface behavior not captured properly

- Rotation effect in over-sized media over-predicts surface layer



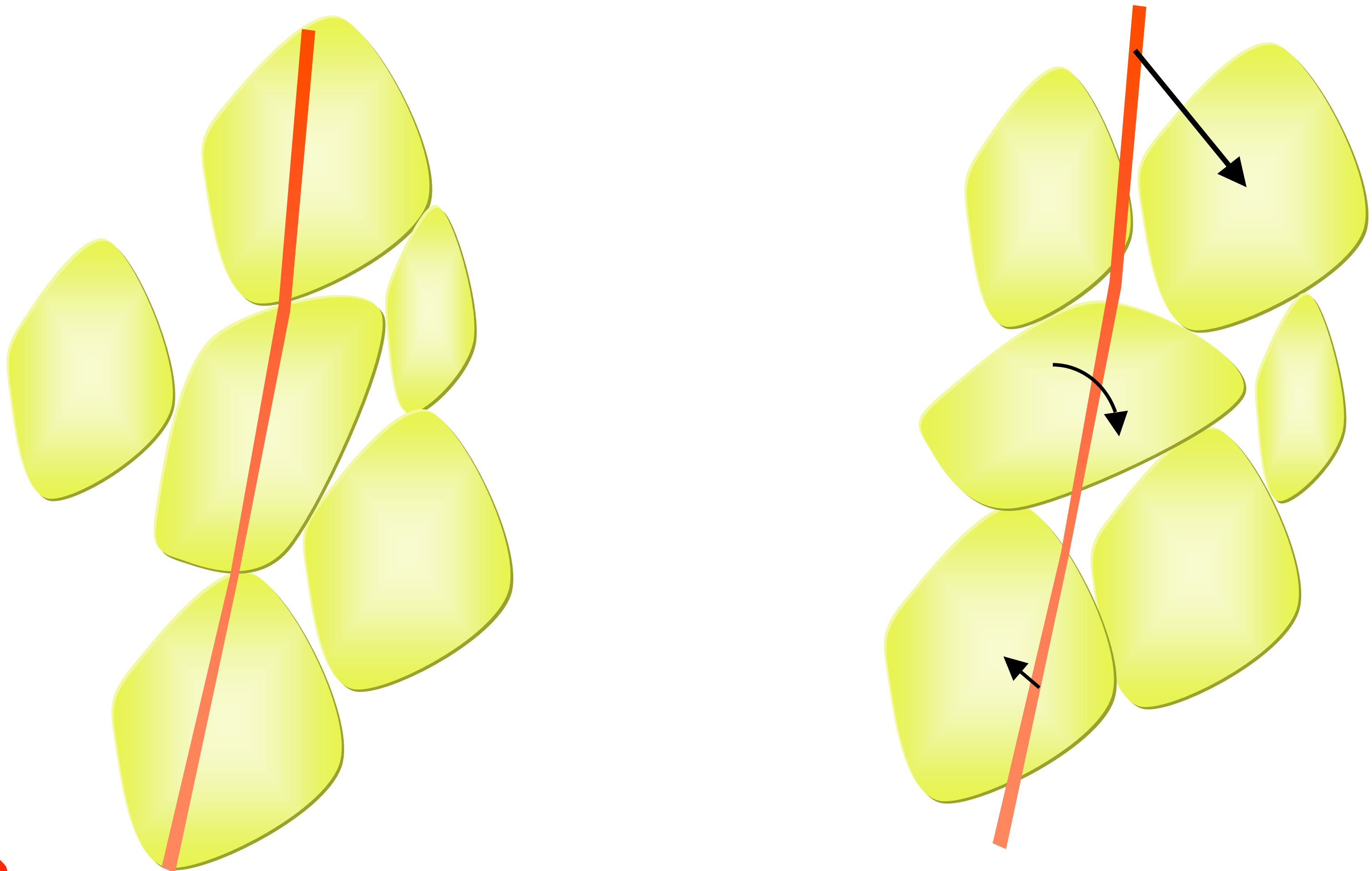


Force Chains

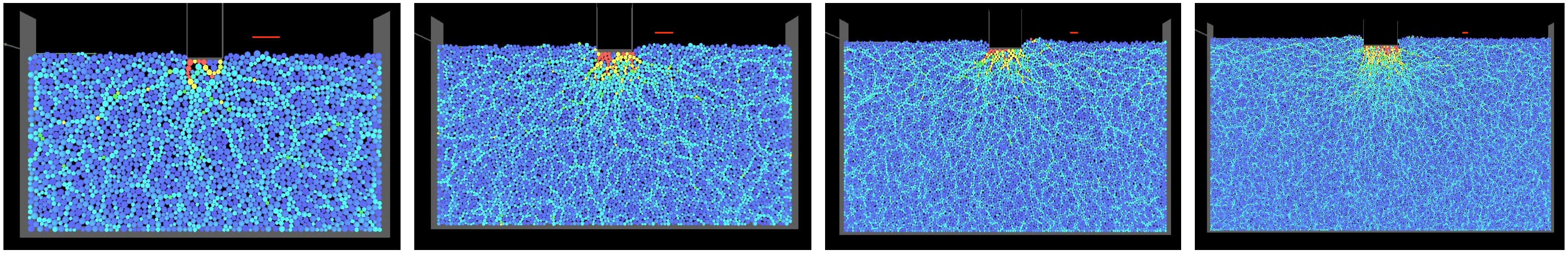


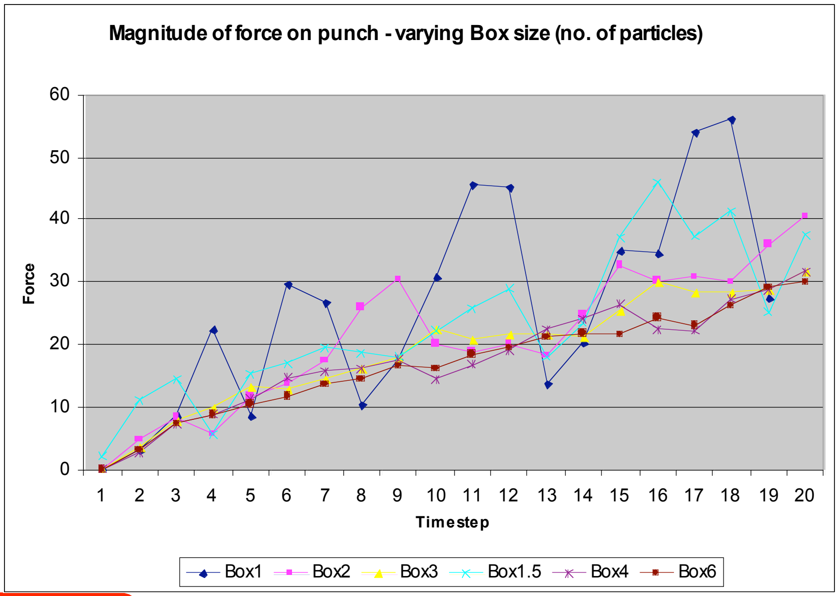
"Stress" chains in assembladge of photoelastic discs (Behringer)

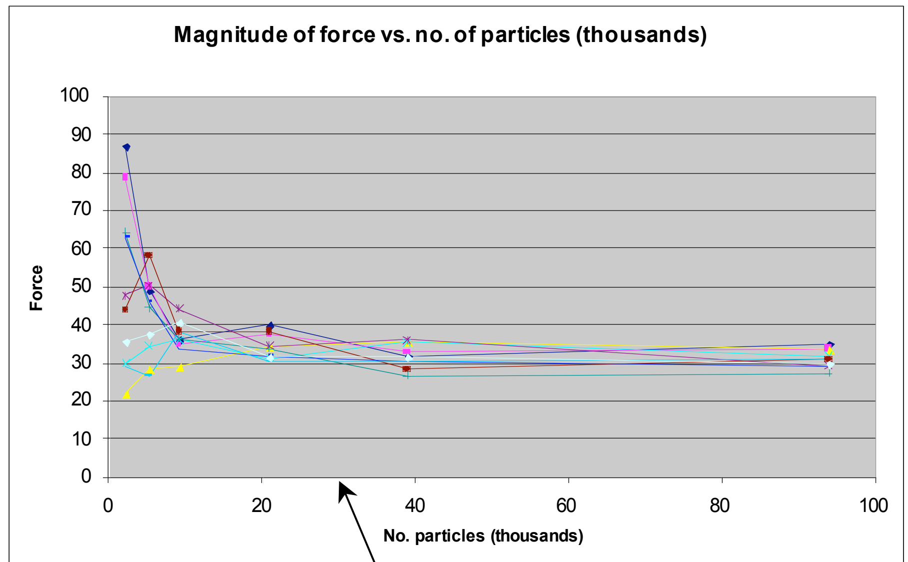
Particle Buckling



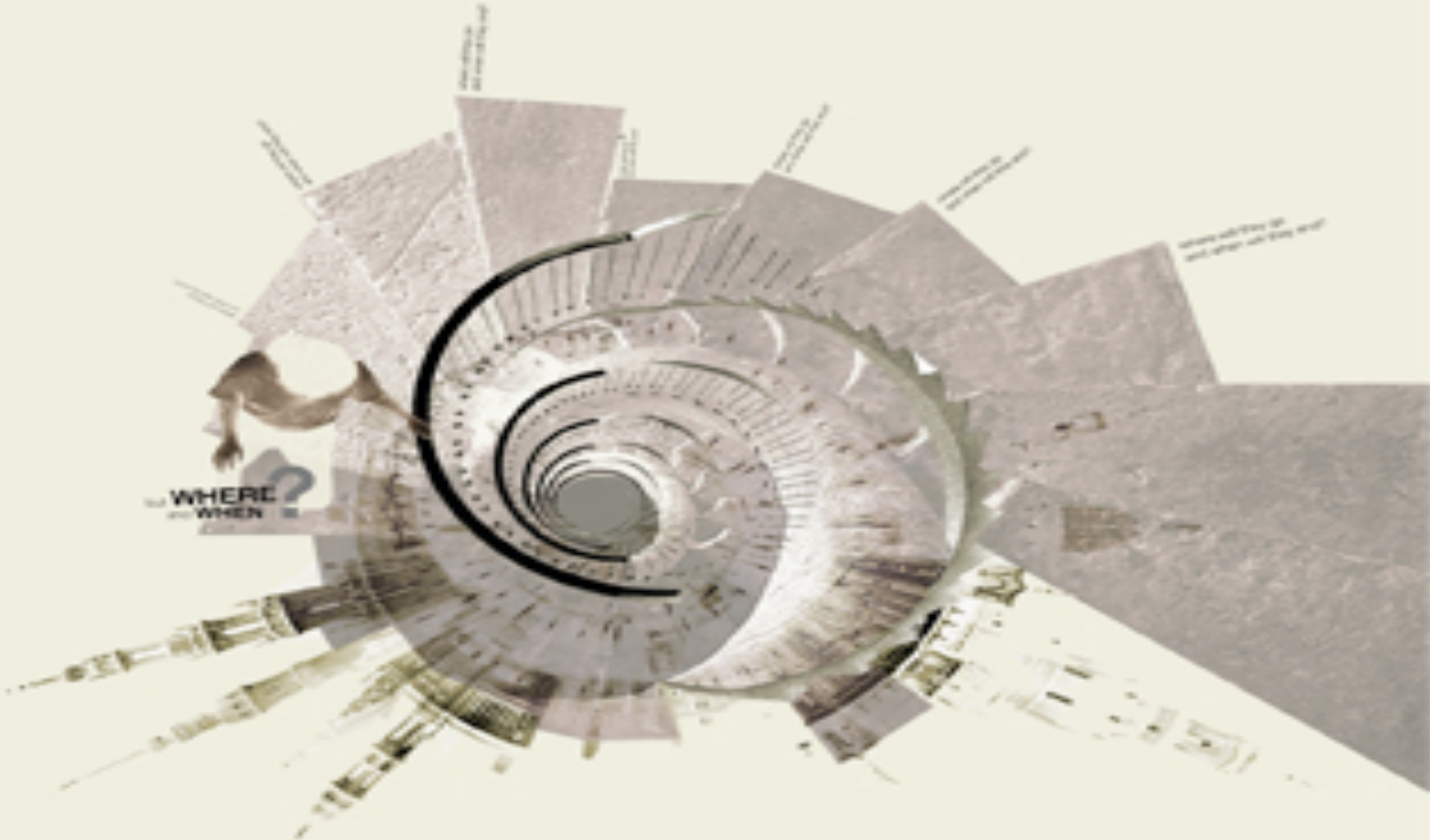
Calibration Issues and Convergence







6.4 million for 3D



The Granular Continuum

neuferth.files.wordpress.com

Continuum as Reference

- Very large scale separation between simulation and actual soil
- Granular behavior falls within scope of continuum mechanics (although much more progress needed!).
- A continuum description is an avenue to analysis.

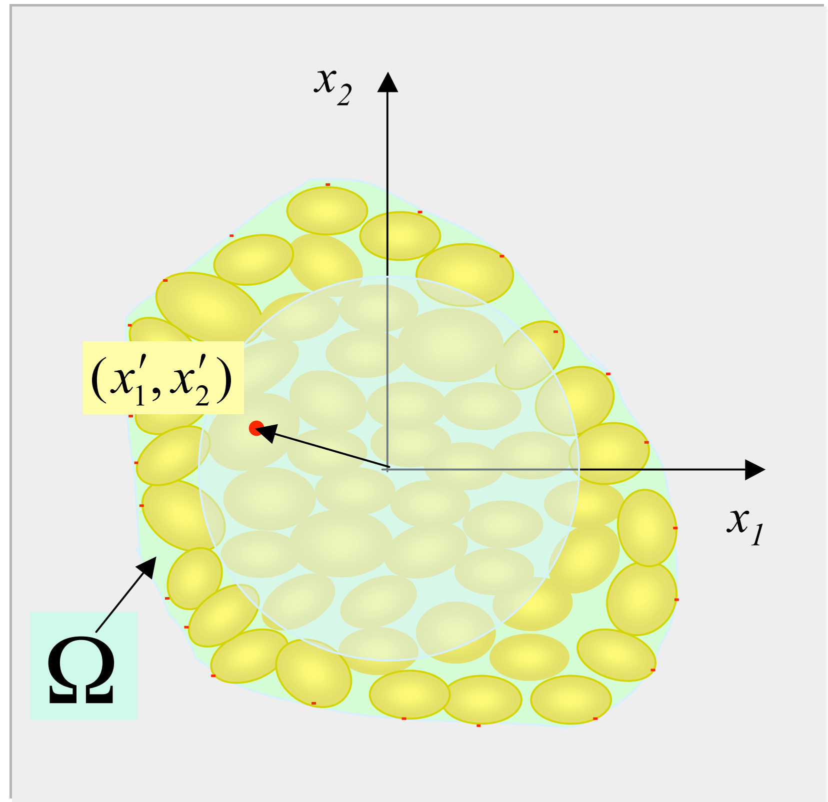
Continuumization

Map quantities from discrete to continuous media:

- Mapping based on smoothing function
- Mapping of *conserved* quantity

$$\bar{f}(x_i) = \int_{\Omega} \phi(x_i - x_i') f(x_i') dx_i'$$

$$\int_{\Omega} \phi(x_i - x_i') dx_i' = 1$$



US Army Corps of Engineers

Conservation Equations for Particle

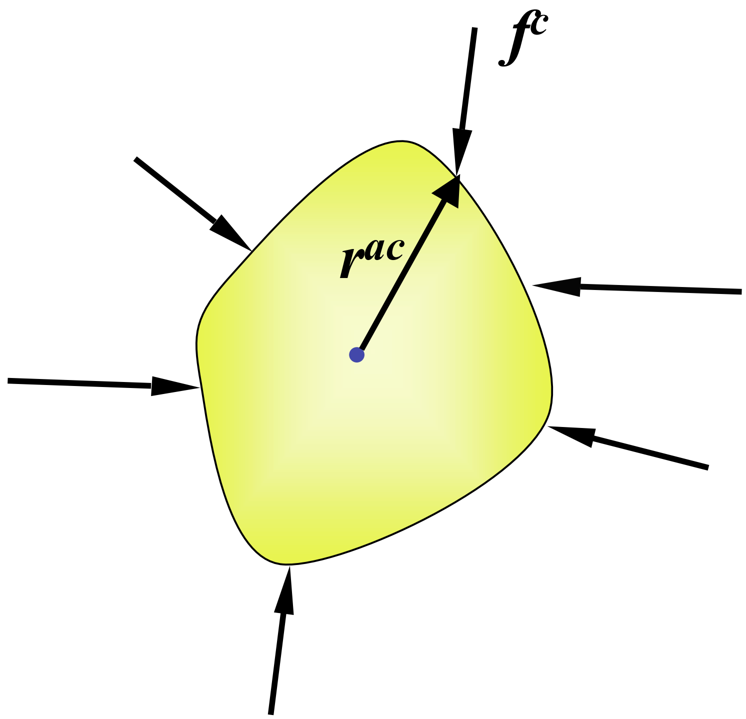
Mechanical quantities to be conserved for each particle:

- Linear Momentum

$$\sum_{c}^{N_c^p} f_i^c - V^p \rho^s a_i^p = 0$$

- Rotational Momentum

$$\sum_{c}^{N_c^p} e_{ijk} r_j^c f_i^c - \rho^s I \omega_k^p = 0$$



Approximate Integration Over Particle

The integration becomes summation of particle quantities:

- Linear Momentum

$$\sum_{p}^{N^p} \phi^p \left(\sum_{c}^{N_c^p} f_i^c - V^p \rho^s a_i^p \right) = 0$$

- Rotational Momentum

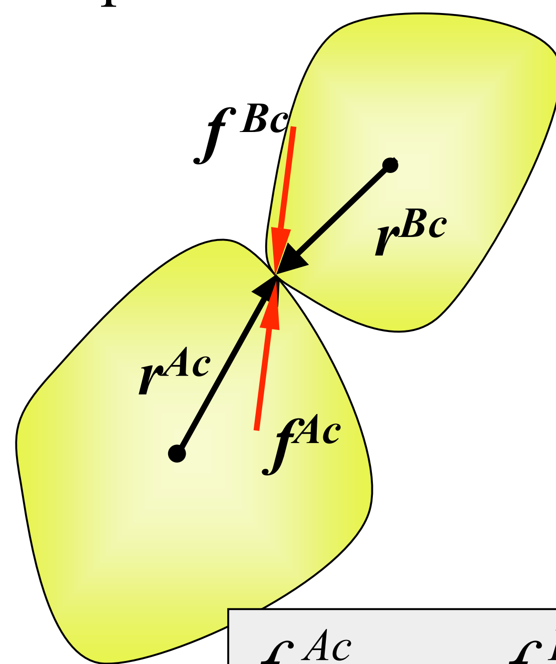
$$\sum_{p}^{N^p} \phi^p \left(\sum_{c}^{N_c^p} e_{ijk} r_j^c f_i^c - \rho^s I \omega_k^p \right) = 0$$

Contact Quantities

Renumber in terms of contacts pairs rather than particles:

- Linear Momentum

$$\sum_{c}^{N^c} (\phi^A - \phi^B) f_i^c = \sum_{p}^{N^p} V^p \rho^s a_i^p$$



$$f_i^{Ac} = -f_i^{Bc}$$

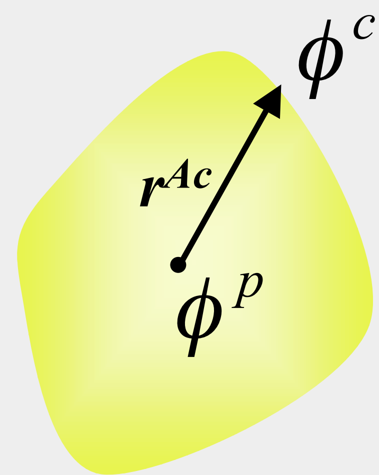
- Rotational Momentum

$$\sum_{c}^{N^c} (\phi^A r_j^{Ac} - \phi^B r_j^{Bc}) f_i^c e_{ijk} = \sum_{p}^{N^p} \rho^s I \omega_k^p$$

Conversion of Difference Term

$$\phi^p(x_i^p) \approx \phi^c(x_i^c) - r_i^{Ac}\nabla_i\phi(x_i^c)$$

$$\nabla_i\phi = \frac{\partial\phi}{\partial x_i}$$



Write summation in terms of contacts

$$\sum_c^{N^c}(\phi^A - \phi^B)f_i^c = \sum_p^{N^p} V^p\rho^s a_i^p$$

$$\Downarrow$$

$$\sum_c^{N^c}\nabla_j\phi^A(r_j^{Ac} - r_j^{Bc})f_i^c = \sum_p^{N^p} V^p\rho^s a_i^p$$

Smoothed Conservation of Linear Momentum

$$\sum_{c}^{N^c} \nabla_j \phi^c (r_j^{Ac} - r_j^{Bc}) f_i^c = \sum_{p}^{N^p} V^p \rho^s a_i^p$$

$$\Downarrow$$

$$\nabla_j \overline{\sigma}_{ij} = \overline{\rho a}_i$$

$$\boxed{\overline{\sigma}_{ij} = \sum_{c}^{N^c} \phi^c (r_j^{Ac} - r_j^{Bc}) f_i^c}$$

Smoothed Conservation of Rotational Momentum

$$\sum_{c}^{N^c} \nabla_l \phi^c e_{ijk} (r_l^{Ac} r_j^{Ac} - r_l^{Bc} r_j^{Bc}) f_i^c$$

$$+ \sum_{c}^{N^c} \phi^c e_{ijk} (r_j^{Ac} - r_j^{Bc}) f_i^c = \sum_{p}^{N^p} V^p \rho^s a_i^p$$

$$\Downarrow$$

$$\nabla_j \overline{\mu}_{ij} + e_{ijk} \overline{\sigma}_{ij} = \overline{\rho I \omega_k}$$

$$\overline{\mu}_{kl} = \sum_{c}^{N^c} \phi^c e_{ijk} (r_l^{Ac} r_j^{Ac} - r_l^{Bc} r_j^{Bc}) f_i^c$$

Equilibrium in Cosserat Media

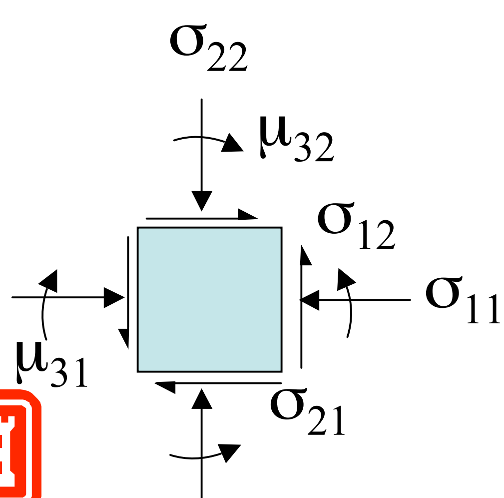
$$\frac{\partial \sigma_{ij}}{\partial x_j} = 0$$

$$\frac{\partial \mu_{ij}}{\partial x_j} + e_{ikl}\sigma_{kl} = 0$$

$$\frac{\partial \sigma_{11}}{\partial x_1} + \frac{\partial \sigma_{12}}{\partial x_2} = 0$$

$$\frac{\partial \sigma_{21}}{\partial x_1} + \frac{\partial \sigma_{22}}{\partial x_2} = 0$$

$$\frac{\partial \mu_{31}}{\partial x_1} + \frac{\partial \mu_{32}}{\partial x_2} + (\sigma_{12} - \sigma_{21}) = 0$$



$\sigma_{12} \neq \sigma_{21}$ in presence of gradient in μ_{3j}.

Remarks on Conservation Equations

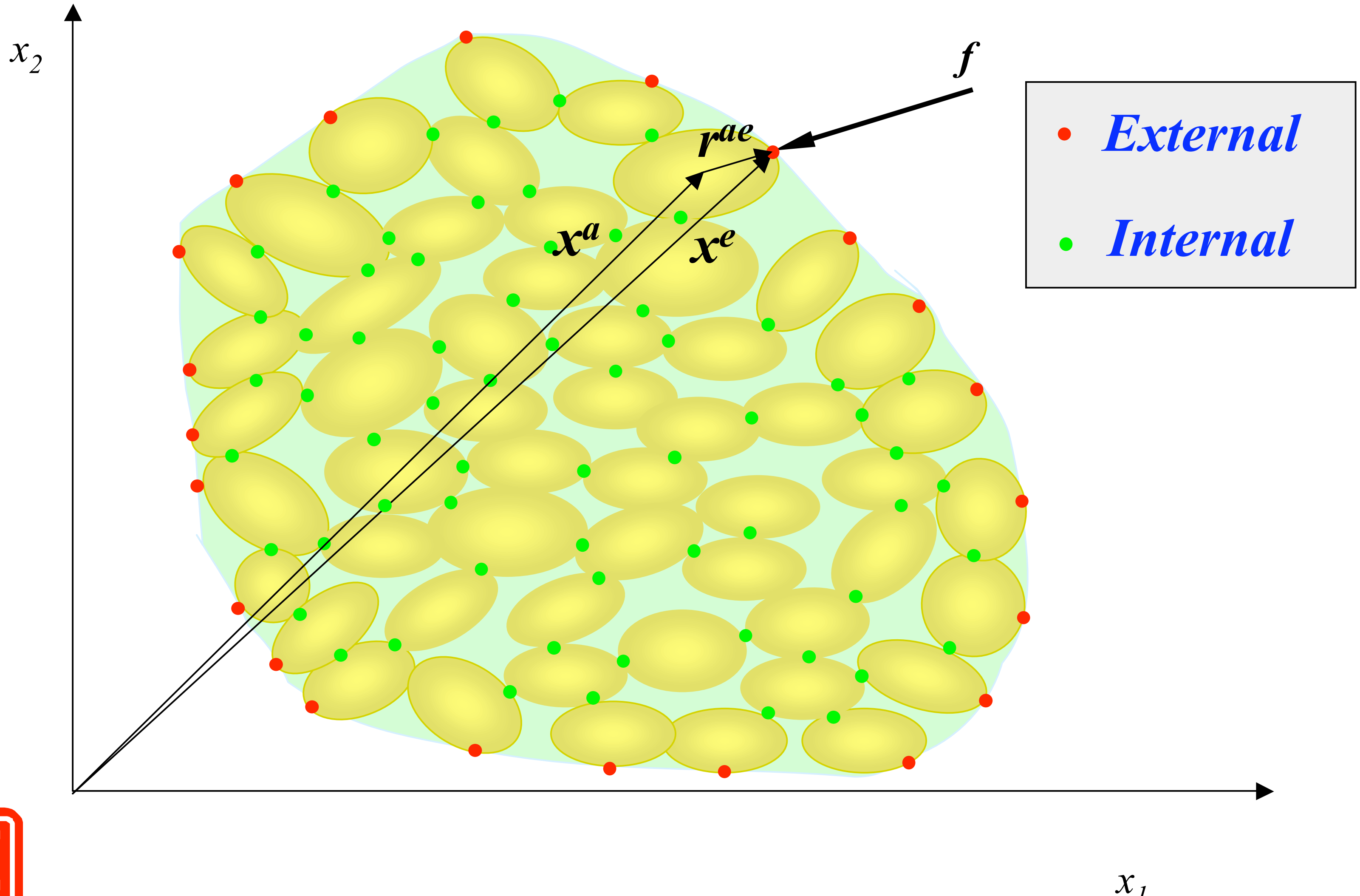
- Coupled stress comes from averaging discrete system
- Smoothed equations are those of Cosserat medium

$$\overline{\sigma}_{ij} \neq \overline{\sigma}_{ji} \Leftrightarrow \nabla_l \overline{\mu}_{kl} \neq 0$$

- Significance of μ_{kl} depends of order of particle radius

$$\overline{\mu}_{kl} = \sum_{c}^{N^c} \phi^c e_{ijk} (r_l^{Ac} r_j^{Ac} - r_l^{Bc} r_j^{Bc}) f_i^c$$

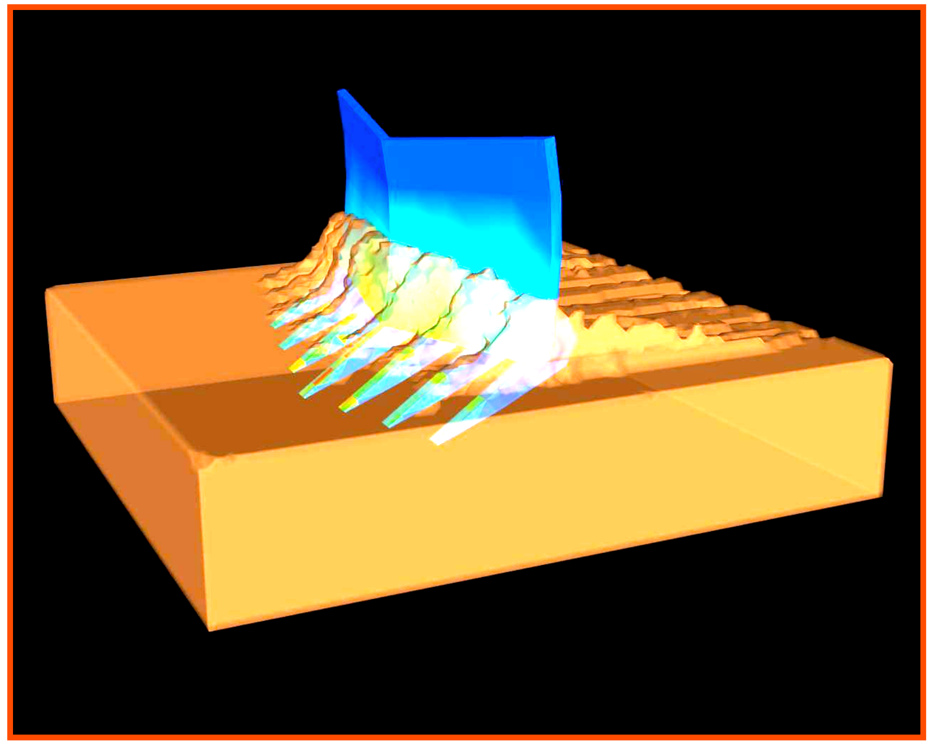
The Granular Domain of Bardet and Vardoulakis



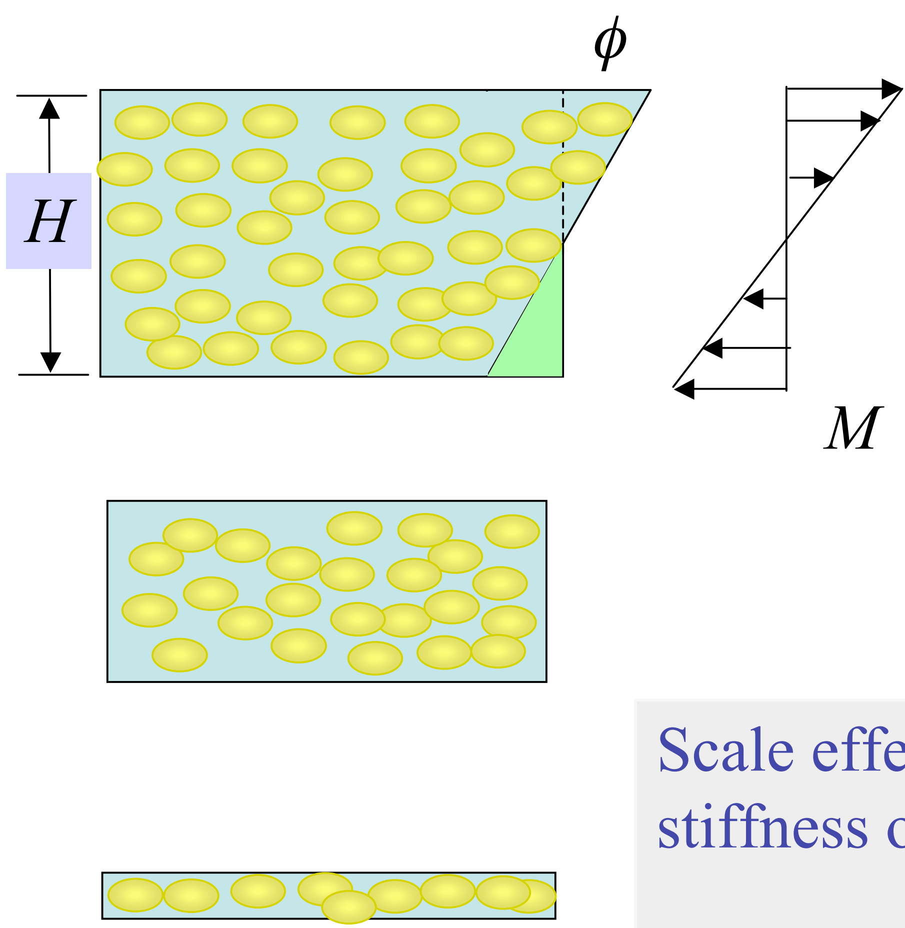
Influence of Problem Type

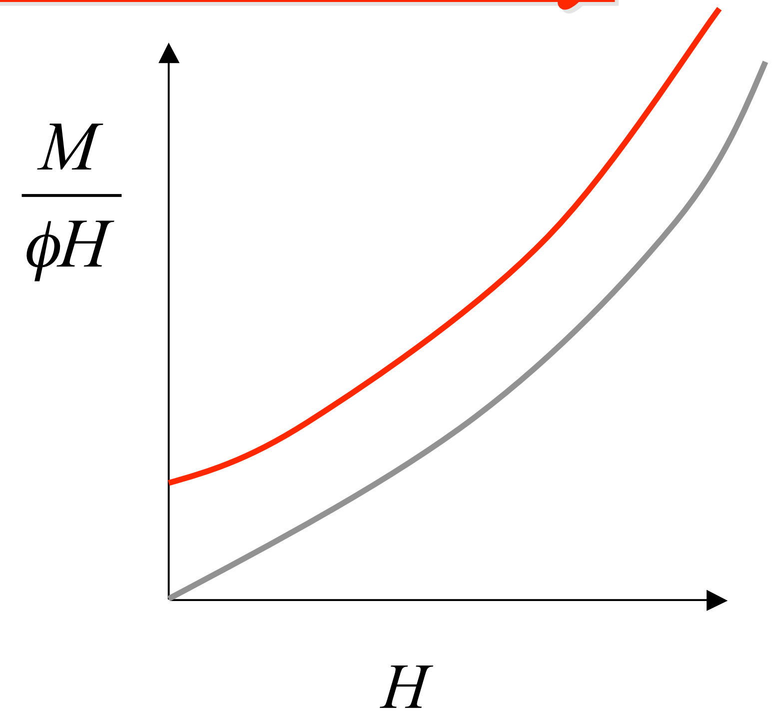
$$\overline{\sigma}_{ij} = \sum_{c}^{N^c} \phi^c (r_j^{Ac} - r_j^{Bc}) f_i^c$$

- Strain is dimensionless
- Some problems not affected by scale



Scale Effect in Coupled Stress Theory





Scale effect results from *intrinsic* flexure stiffness of material.

Similarly, wave propagation is dispersive.

Conclusions

Conclusions . . .

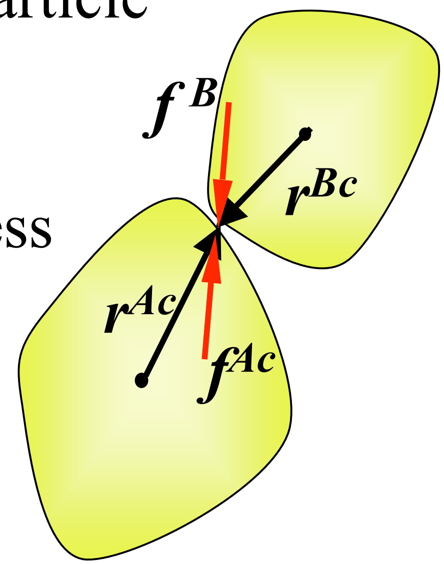
- Any continuumization (homogenization) of momentum conservation equations in discrete media will include couples with asymmetric Cauchy stress tensor.

- This conclusion does not involve consideration of boundaries, and is true irrespective of averaging volume.

✓ **Effects that are small in the *actual soil* can dominate the *simulation* because of particle size. *Particle size is not a simple issue of accuracy but of representing the correct physics.***

. . . and more Conclusions

Scaled-up constitutive equations for DEM based on particle pairs might not be appropriate.



- Interactions might involve particle groups (to suppress particle chains)
- Particle rotations might be suppressed
- Shear bands and boundary layers represented as distinct features in simulations

Thank You