DEM Modeling: Lecture 01

Introduction

Sample Previous Projects

- Soft-particle DEM simulations of 2-D granular flow in a high-shear mixer
- A review of continuum hydrodynamics using molecular dynamics
- A 3-D analytical geometry based contact detection procedure for sphero-cylinder shaped bodies
- An algorithm for contact detection of cylindrical bodies
- Polygonal collision detection for DEM
- Discrete element modeling of a ball on a rotating plate
- A discrete element model for simulating fracture in solids

Project Report Outline

- Introduction
- Background
- Theory/Algorithm Description
- Implementation
- Results
- Conclusions
- References
- Tables
- Figures
- Appendices (derivations, codes, etc.)

Questions to Address

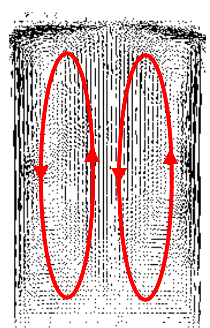
- Why use computational models?
- What is DEM?
- How is DEM different from other methods such as CFD and FEM?
- What are DEM’s strengths and weaknesses?
- What will be discussed in this course?

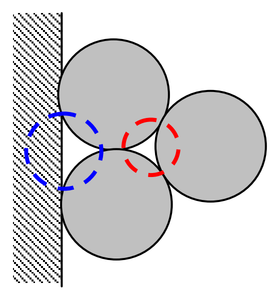
Motivation for Computational Modeling

- Experimental measurements of particulate flows are often difficult or expensive to make
  - can’t easily investigate internal structure
    - PEPT (Stewart *et al*., 2001)
    - x-rays (Baxter *et al*., 1989)
    - nuclear magnetic resonance (NMR) / magnetic resonance imaging (MRI) (Nakagawa *et al*., 1993)
    - γ-ray tomography (Langston *et al*., 1997)
    - radio pill (Dave *et al*., 1998)
    - radioactive tracers (Larachi *et al*., 1995)
    - intrusive probes
    - “freezing” the system (Brone and Muzzio, 2000)

Motivation for Computational Modeling…

- Experimental measurements of particulate flows are often difficult or expensive to make…
  - observations at boundaries
    - behavior at boundaries isn't necessarily the same as the internal behavior, *e.g.* side-wall convection (video), packing structure





  - some quantities are difficult to measure
    - *e.g.* inter-particle forces, coordination number, particle orientation and rotational speed

Motivation for Computational Modeling…

- Some environments and properties are difficult to investigate experimentally
  - *e.g.*, inter-particle friction, modified gravity

- Computer models can be used to overcome these difficulties; however, care must be taken to address the following
  - proper modeling of the physics
  - computational issues such as:
    - stability, accuracy, duration, storage
  - validation

Motivation for Computational Modeling…

- reduce the number of experiments
- optimize design and operating conditions; allow for more creative design
- computational models are well suited for parametric studies

⇒ "A case study of the economic benefit of the application of CFD in one chemical and engineered-material company over a six-year period conservatively estimated that the application of CFD generated approximately a six-fold return on the total investment in CFD." (Davidson, 2001)

Modeling Approaches

- Two broad classes of approaches for modeling particulate materials
  - continuum
  - discrete

Modeling Approaches…

- Continuum Approach
  - treat as a continuous substance, ignore individual particles
  - assumes the length scale of importance >> particle length scale
  - apply conservation of mass, momentum, and energy to small regions of the material
  - also need constitutive relations that define a particular substance, *e.g.* how stress and strain (or strain rate) are related for that substance
    - *e.g.* Newtonian fluid behavior
    - constitutive laws for particulate materials are not widely agreed upon, hundreds have been proposed, most are phenomenological (for dense flows in particular) (Cundall, 2001)
    - several constitutive laws may be required to describe different regions of the flow
  - solve the resulting equations numerically using methods such as finite differences, finite volumes, or finite elements

Modeling Approaches…

- Continuum Approach…
  - not well suited to investigate phenomena occurring at the length scale of a particle diameter
  - some particulate system phenomena are highly dependent on particle level behavior, *e.g*. shear bands
  - best suited to investigate large scale systems, *e.g.* at the unit operation scale

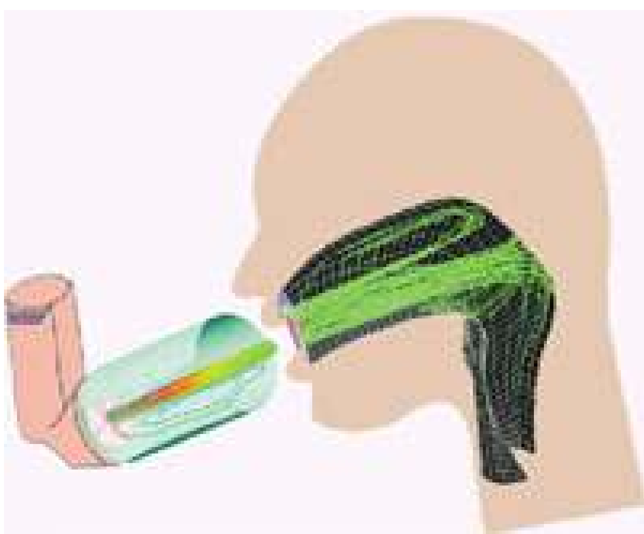
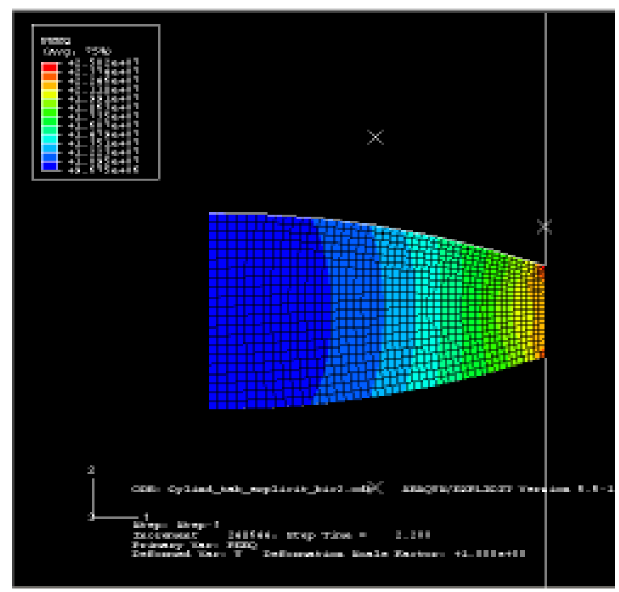


Figure 1. Computational fluid dynamics (CFD) simulation of a freely bubbling gas-fluidized bed showing the growth in bubble size with height in the bed. Red indicates regions where the solids fraction approaches maximum packing; blue indicates regions with no solids.

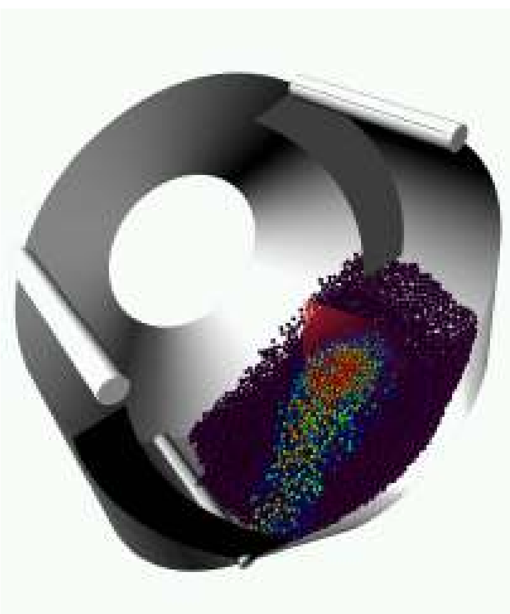


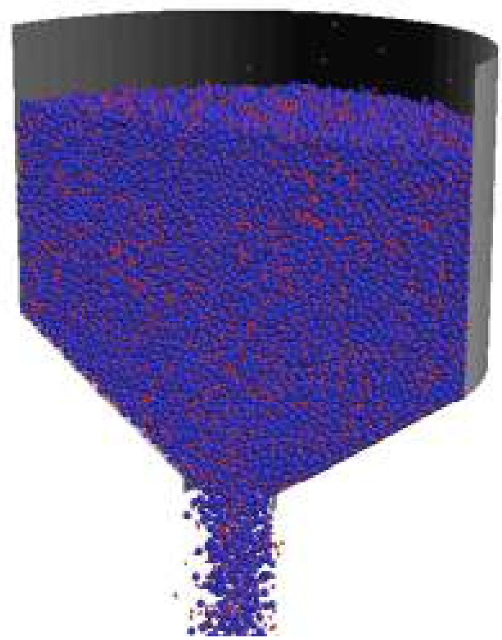
Modeling Approaches…

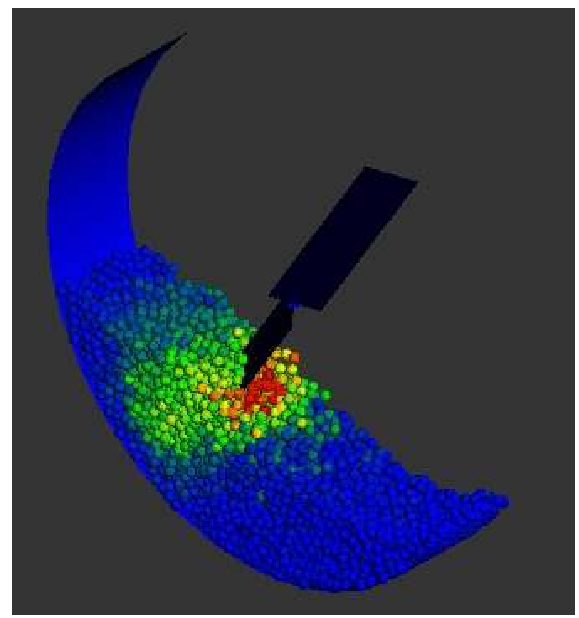
- Discrete Approach
  - *e.g.*, the discrete element method (DEM)
  - models the behavior of individual particles
  - overall system behavior the result of individual interactions
  - examples include:
    - cellular automata (Baxter and Behringer, 1991)
    - Monte Carlo methods (Rosato *et al.*, 1986)
    - hard-particle methods (Campbell and Brennen, 1982; Luding, 1995)
    - soft-particle methods (Cundall and Strack, 1979; Walton and Braun, 1986)
  - these methods are used in fields other than granular flows
    - traffic simulations, astronomy, computer networks, crowd dynamics, biosystems interactions, roller bearing dynamics

Modeling Approaches…

- Discrete Approach…
  - very good for investigating phenomena occurring at the length scale of a particle diameter
  - not well suited for modeling larger scale systems exactly
    - *e.g.* V_{system} = 1 L, d = 100 μm $\Rightarrow$ ~10^8 particles
    - however, can use DEM to approximate system behavior and gain insight
  - need information at the particle scale, e.g. particle shape, particle-particle friction, particle mechanical properties, etc.







Issues to Consider

- Make sure the physical model is a good one
  - 2D/3D, viscous/inviscid, compressible/incompressible, laminar/turbulent, frictional/non-frictional, deformable/rigid, etc.
  - CFD/FEM: continuum methods – not suited for phenomena occurring at a particle length scale
  - DEM: force models, particle shape, degree of deformation, number of particles
  - appropriate constitutive laws
  - appropriate boundary conditions
- Make sure the computational model is a good one
  - grid/element quality (discretization errors)
  - convergence criteria
  - time step / stiffness / model parameters
- Model validation

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