
Granular Project Options Adapted to Course Methods

1) Clogging in granular flow through a bottleneck

❓ Scientific Question

- Can we quantify how the probability of clogging (arching) and the discharge statistics depend on (a) the orifice diameter, (b) the grain size distribution, and (c) the particle-wall friction? [3]

🛠️ Recommended Course Methods

- **Molecular dynamics / particle simulations (Chapter 1):** Use as a DEM-like particle integrator for grains[4].
  - **Why it fits:** Molecular-dynamics-style particle simulation is the closest analogue to a discrete-element method (DEM) and will let you reproduce realistic arch formation and contact forces[5].
- **Cellular automata / rule-based CA (Chapter 4):** To implement a complementary simple grid-based model for quick parameter sweeps[6].
  - **Why it fits:** The CA variant is computationally cheap and useful to explore large parameter ranges and to illustrate mechanisms (clog/no-clog) with clear visual outputs[7].
- **Brownian dynamics / stochastic integration (Chapter 5):** Optional if you add stochastic driving or thermal-like noise[8].

⚙️ Concrete Simulation Plan

- **Geometry:** 2D rectangular silo geometry with a bottom central orifice[9].
- **Particles:** Soft disks with radius drawn from a distribution (monodisperse and polydisperse cases)[10].
- **Integrator:** Velocity-Verlet or leapfrog (as in Chapter 1)[11].
  - Include gravity, normal repulsive contact using a soft potential, and tangential frictional force (simplified Coulomb friction)[12].
- **Observables:**
  - Discharge time for fixed initial fill height (run many realizations for each orifice size)[13].
  - Fraction of runs that clog within a time cutoff $\rightarrow$ clogging probability vs orifice / particle size ratio[14].
  - Geometry of arches (snapshots) and contact-force maps[15].
- **Parameter Sweep:**

    - Orifice diameters $D = [2.0, 2.5, 3.0, 4.0] \times$ mean particle diameter[16].
    - Friction $\mu = [0.0, 0.3, 0.6]$[17].
    - Polydispersity levels[18].
- **CA Alternate Model:** Lattice where grains fall with simple local rules; include probabilistic unblock (vibration) parameter[19].
- **Notes:** Use the textbook's MD recipes for integrator selection and timestep guidance (See Chapter 1)[20].

📊 Figures & Report Outputs (Mandatory)

- Fig. 1: Method schematic (silo geometry + particle/CA rules)[21].
- Fig. 2: Example simulation snapshots showing arch formation (sequence)[22].
- Fig. 3: Clogging probability vs orifice size for different μ[23].
- Fig. 4: Histogram of discharge times (log scale) and sample force-chain image[24].
- **Table:** Comparing MD-based DEM vs CA (Overview table)[25].

2) Avalanches and angle of repose in granular piles

❓ Scientific Question

- How do grain friction and shape (approximated via effective friction) affect the angle of repose and the statistics of avalanches (size distribution and frequency)? [26]

🛠️ Recommended Course Methods

- **Forest-fire / sandpile / self-organized criticality ideas (Chapter 3):** Sandpile and SOC models provide a direct template for avalanche statistics[27].
  - **Why it fits:** The sandpile/forest-fire chapters explain self-organized critical models and toppling rules that directly model avalanche distributions[28].
- **Cellular automata / Game of Life-style CA (Chapter 4):** For a discrete height/toppling sandpile model[29].
  - **Why it fits:** A lattice sandpile CA is perfect to get power-law avalanche statistics quickly[30].
- **Molecular dynamics (Chapter 1):** For a more physical particle-based pile to measure angle and local stresses[31].
  - **Why it fits:** A particle MD model complements the CA with more realistic pile geometry and angle-of-repose measurement[32].

⚙️ Concrete Simulation Plan

- **CA Sandpile:**
  - Implement Abelian sandpile or Bak-Tang-Wiesenfeld rules on a matrix, toppling threshold[33].
  - Drive by adding grains at the apex until relaxation[34].
  - Record avalanche sizes and durations[35].
- **Particle MD Pile:**
  - Drop particles one-by-one onto a base, allow them to settle[36].
  - Slowly increase slope (or add grains) until avalanches occur[37].
  - Measure angle of repose after relaxation[38].
- **Observables:**
  - Angle of repose vs friction parameter[39].
  - Avalanche size distribution (power-law fit) and cut-off dependence on system size[40].

    - Avalanche frequency vs driving rate[41].
- **Parameter Sweep:** Friction-like parameter, particle polydispersity, driving rate (slow vs faster)[42].
- **Notes:** Chapter 3 (forest fires & SOC) contains discussion and code references for sandpile-like models and how to analyze power-law behavior (Use for data-analysis methods and finite-size considerations)[43].

📊 Figures & Report Outputs (Mandatory)

- Fig. 1: Method schematic (CA rules and MD pile)[44].
- Fig. 2: CA avalanche size distribution (log-log) with fitted slope[45].
- Fig. 3: Sequence of MD pile snapshots showing avalanche onset[46].
- Fig. 4: Angle-of-repose vs friction coefficient plot[47].
- **Table:** Comparing CA sandpile vs MD particle pile (advantages / disadvantages)[48].

3) Granular segregation (the Brazil-nut effect)

❓ Scientific Question

- Under vertical vibration, how do particle size ratio, density contrast, and vibration amplitude/frequency determine segregation timescales and the steady-state vertical profile? [49]

🛠️ Recommended Course Methods

- **Molecular dynamics / particle simulations (Chapter 1):** Simulate collisions, gravity, and vibrating boundary[50].
  - **Why it fits:** A particle-resolved MD simulation naturally captures per-collision dynamics and percolation of small particles beneath larger ones[51].
- **Sugarscape/agent-based ideas for segregation (Chapter 16):** Use Sugarscape as inspiration for rule-based agent movement and segregation metrics[52].
  - **Why it fits:** Sugarscape-like agent rules let you test hypotheses faster and compute segregation indices (Gini-like metrics)[53].
- **Brownian dynamics / stochastic terms (Chapter 5):** For adding noisy, stochastic forcing if modelling small-scale agitation[54].

⚙️ Concrete Simulation Plan

- **MD Particle Box:**
  - Particle box with a vibrating base (vertical sinusoidal motion)[55].
  - Two species: small and large particles[56].
  - Vary size ratio $s=R\_large/R\_small$ and density ratio[57].
- **Observables:**
  - Vertical concentration profiles vs time[58].
  - Segregation index (e.g., fraction of large particles in top layer) vs time[59].
  - Segregation timescale as function of vibration acceleration $\Gamma=A(2\pi f)^2/g$[60].
- **Parameter Sweep:** Size ratio, density ratio, vibration amplitude/frequency[61].
- **Agent-based Complementary Model:** Agents move stochastically upward or downward with local rules biased by neighbor packing - measure macroscopic segregation metrics[62].

- **Notes:** Chapter 16 helps design segregation metrics and agent-based rules[63]; Chapter 1 gives MD implementation details[64]; Chapter 5 explains stochastic forcing[65].

📊 Figures & Report Outputs (Mandatory)

- Fig. 1: Method schematic (vibrating box + particle species)[66].
- Fig. 2: Time evolution of vertical concentration profiles[67].
- Fig. 3: Segregation index vs time for different Γ and size ratios[68].
- Fig. 4: Comparison table: MD vs agent-based (Sugarscape-inspired) rules[69].

📝 Practicalities and Report Requirements (General)

- **Team Size & Pages:** All three projects are suitable for a 2-person team (9 pages)[70].
- **References:** Include the relevant textbook chapters and key literature (Zuriguel, Jaeger, Bak-Tang-Wiesenfeld, Schelling)[71].
- **Figures:** Each project supplies at least 5 figures (method schematic, example snapshot(s), plots, histograms)[72].
- **Methods Overview Table:** Compare for each project 2-3 methods (MD, CA, Agent-based) with features/advantages/limits[73].
- **Method Figure (Mandatory):** A mandatory illustration (Fig. 1) showing geometry and algorithm flow for reproducibility[74].
