Granular-matter project options — adapted to course methods (ENGLISH)

Below you find three fleshed-out project options (the three you liked, in that order) adapted to use methods from the course textbook 'Simulation of Complex Systems' (16 methods / chapters). For each project I list: - scientific question, - recommended method(s) from the book (chapter names), - why those methods fit, - concrete simulation plan (parameters & experiments), - mandatory figures and required outputs that match the course report template.

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? Recommended course methods (from the textbook) - Molecular dynamics / particle simulations (Chapter 1): use as a DEM-like particle integrator for grains. - Brownian dynamics / stochastic integration (Chapter 5): optional if you add stochastic driving or thermal-like noise. - Cellular automata / rule-based CA (Chapter 4): to implement a complementary simple grid-based model for quick parameter sweeps. Why these methods? 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. The CA variant (e.g., a lattice flow or rule-184 style traffic CA) is computationally cheap and useful to explore large parameter ranges and to illustrate mechanisms (clog/no-clog) with clear visual outputs. Concrete simulation plan - 2D rectangular silo geometry with a bottom central orifice. Particles: soft disks with radius drawn from a distribution (monodisperse and polydisperse cases). - Integrator: velocity-Verlet or leapfrog (as in Chapter 1). Include gravity, normal repulsive contact using a soft potential, and tangential frictional force (simplified Coulomb friction). - Observables: • discharge time for fixed initial fill height (run many realizations for each orifice size). • fraction of runs that clog within a time cutoff → clogging probability vs orifice / particle size ratio. • geometry of arches (snapshots) and contact-force maps. - Parameter sweep: orifice diameters D = [2.0, 2.5, 3.0, 4.0] × mean particle diameter; friction μ = [0.0, 0.3, 0.6]; polydispersity levels. - CA alternate model: lattice where grains fall with simple local rules; include probabilistic unblock (vibration) parameter. Figures & report outputs (to match template) - Fig.1 Method schematic (silo geometry + particle/CA rules). - Fig.2 Example simulation snapshots showing arch formation (sequence). - Fig.3 Clogging probability vs orifice size for different μ. - Fig.4 Histogram of discharge times (log scale) and sample force-chain image. - Table comparing MD-based DEM vs CA (Overview table). Notes on reproducibility & code - Use the textbook's MD recipes for integrator selection and timestep guidance. See Chapter 1 for leapfrog/Verlet integrators and implementation notes.

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)? Recommended course methods (from the textbook) - Forest-fire / sandpile / self-organized criticality ideas (Chapter 3): sandpile and SOC models provide a direct template for avalanche statistics. - Cellular automata / Game of Life-style CA (Chapter 4): for a discrete height/toppling sandpile model. - Molecular dynamics (Chapter 1): for a more physical particle-based pile to measure angle and local stresses. Why these methods? The sandpile/forest-fire chapters explain self-organized critical models and toppling rules that directly model avalanche distributions. A lattice sandpile CA is perfect to get power-law avalanche statistics quickly. A particle MD model complements the CA with more realistic pile geometry and angle-of-repose measurement. Concrete simulation plan - CA sandpile: implement Abelian sandpile or Bak–Tang–Wiesenfeld rules on a matrix, toppling threshold, drive by adding grains at the apex until relaxation. Record avalanche sizes and durations. - Particle MD pile:

drop particles one-by-one onto a base, allow them to settle; slowly increase slope (or add grains) until avalanches occur; measure angle of repose after relaxation. - Observables: • angle of repose vs friction parameter. • avalanche size distribution (power-law fit) and cut-off dependence on system size. • avalanche frequency vs driving rate. - Parameter sweep: friction-like parameter, particle polydispersity, driving rate (slow vs faster). Figures & report outputs - Fig.1 Method schematic (CA rules and MD pile). - Fig.2 CA avalanche size distribution (log–log) with fitted slope. - Fig.3 Sequence of MD pile snapshots showing avalanche onset. - Fig.4 Angle-of-repose vs friction coefficient plot. - Table comparing CA sandpile vs MD particle pile (advantages / disadvantages). Notes Chapter 3 (forest fires & SOC) contains discussion and code references for sandpile-like models and how to analyze power-law behavior. Use that for data-analysis methods and finite-size considerations.

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? Recommended course methods (from the textbook) - Molecular dynamics / particle simulations (Chapter 1): simulate collisions, gravity, and vibrating boundary. - Brownian dynamics / stochastic terms (Chapter 5): for adding noisy, stochastic forcing if modelling small-scale agitation. - Sugarscape / agent-based ideas for segregation (Chapter 16): use Sugarscape as inspiration for rule-based agent movement and segregation metrics. Why these methods? A particle-resolved MD simulation naturally captures per-collision dynamics and percolation of small particles beneath larger ones. If you want a complementary, simpler model, Sugarscape-like agent rules (agents with sizes and local movement rules) let you test hypotheses faster and compute segregation indices (Gini-like metrics) as in socio-spatial segregation problems. Concrete simulation plan - MD particle box with a vibrating base (vertical sinusoidal motion). Two species: small and large particles; vary size ratio s = R_large / R_small and density ratio. - Observables: • vertical concentration profiles vs time. • segregation index (e.g., fraction of large particles in top layer) vs time. • segregation timescale as function of vibration acceleration Γ = A (2πf)^2 / g. - Parameter sweep: size ratio, density ratio, vibration amplitude/frequency. - Agent-based complementary model: agents move stochastically upward or downward with local rules biased by neighbor packing — measure macroscopic segregation metrics. Figures & report outputs - Fig.1 Method schematic (vibrating box + particle species). - Fig.2 Time evolution of vertical concentration profiles. - Fig.3 Segregation index vs time for different Γ and size ratios. - Fig.4 Comparison table: MD vs agent-based (Sugarscape-inspired) rules. Notes Chapter 16 includes exercises and models of segregation (Schelling-like) that help design segregation metrics and agent-based rules. Chapter 1 gives MD implementation details for collision and boundary handling; Chapter 5 explains stochastic forcing which can be useful to model small perturbations.

Practicalities — how these adapt to the course report template

- Team size & pages: all three projects are suitable for a 2-person team (9 pages). - References: include the relevant textbook chapters and key literature (Zuriguel, Jaeger, Bak–Tang–Wiesenfeld, Schelling). - Figures: each project supplies at least 5 figures (method schematic, example snapshot(s), plots, histograms). - Methods Overview table: compare for each project 2–3 methods (MD, CA, Agent-based) with features/advantages/limits. - Method figure: a mandatory illustration (Fig.1) showing geometry and algorithm flow for reproducibility. Book chapters used as method references in these adaptations: - Molecular dynamics (Chapter 1). [see book]. - Forest fires / sandpile / SOC (Chapter 3). [see book]. - The Game of Life / cellular automata (Chapter 4). [see book]. - Brownian dynamics (Chapter 5). [see book]. - Sugarscape / segregation and agent-based ideas (Chapter 16). [see book]. If you want, I can: 1) produce a ready-to-submit LaTeX skeleton that follows exactly your PDF template (sections, figure/table placeholders, bib file entries), or 2) generate an English PDF summary of these three adapted project options (formatted for emailing your partner).