Enhanced Report: Simulating 2D Particle Packing via Tunable Forces, Wall Confinement, and Dynamic Bounding Box Analysis

Abstract: This research investigates the two-dimensional particle packing problem through dynamic simulation. The primary objective is to achieve and analyze particle accumulation, driven either by central attractive forces or confinement within repulsive walls, and to quantify packing efficiency using both the system's potential energy and a dynamically resizing Minimum Bounding Box (MBB). The Open Source Physics (OSP) framework serves as the simulation environment. The study delves into the mechanics of various implemented forces, including a tunable central spring force, a counteracting "gravity-like" central force, Lennard-Jones inter-particle interactions, a crucial damping force, and repulsive boundary walls. Key findings highlight the effectiveness of repulsive walls in achieving low-energy, stable packed states, the critical role of Lennard-Jones repulsion strength, the necessity of damping for stabilization, and the utility of the MBB for visualizing packing extent.

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1. Introduction

The efficient packing of objects in a confined or unconfined space is a problem of enduring interest in fields ranging from materials science to logistics. This project focuses on simulating this phenomenon in two dimensions, aiming to understand the dynamics that lead to particle accumulation and dense packing. A central goal is to employ effective confinement strategies (such as central attractive forces or repulsive physical walls) and to use both the system's potential energy and a dynamically calculated Minimum Bounding Box (MBB) as measures of the resulting particle cluster's stability and compactness. All simulations and visualizations are performed using the versatile Open Source Physics (OSP) framework.

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2. Simulation Mechanics and Methodology

The core of the simulation involves modeling 2D circular particles whose motion and interactions are dictated by several key physical and numerical components:

2.1 Particle Interaction Model: Lennard-Jones Potential The fundamental interaction between any pair of particles is governed by the Lennard-Jones (LJ) potential. Its most critical aspect for this packing simulation is:

- **Short-Range Repulsion**: This component provides a strong repulsive force when particles attempt to overlap, effectively defining their excluded volume. The stability and

integrity of the packed structure heavily depend on this repulsion. It was observed that if the effective "repulsion constant" (stemming from the LJ parameters) was too low, particles failed to maintain distinct boundaries, leading to rapid, chaotic motion and an inability to form a stable packed state.
- **Short-Range Attraction**: The attractive part of the LJ potential contributes to the cohesion of particles once they are close enough and have lost sufficient kinetic energy, helping them settle into dense arrangements.

2.2 Forces Governing Particle Motion and Accumulation

- **Central Net Force (Spring and "Gravity-like" terms)**:
  - The simulation allows for a central force model where a `springConstant` provides an attractive Hooke's Law force ($F_{spring} = -k_{spring} \cdot d_{center}$) pulling particles towards the simulation center.
  - A `gravityForce` term is also implemented as a central force. Within the calculation `effectiveK = springConstant - gravityForce` (where Net Central Force $\propto -\text{effectiveK} \cdot d_{center}$), a positive `gravityForce` reduces the net attraction. If `gravityForce > springConstant`, this combined effect becomes a net *repulsive* force from the center. This provides a mechanism to tune the central potential.
- **Damping Force (Air Resistance - `dampingCoeff`)**:
  - A damping force ($F_{damp} = -c \cdot v$) is crucial for dissipating kinetic energy, allowing particles to settle into stable configurations. Higher `dampingCoeff` values lead to more rapid stabilization.

2.3 Particle Confinement Strategies Two primary confinement strategies were implemented and can be selected:

1. **Central Force Confinement with Periodic Boundary Conditions (PBC)**: When `useRepulsiveWalls` is `false`, particles are primarily influenced by the net central force. PBC is applied to the simulation box edges, simulating an infinite system for particle interactions that cross boundaries.
2. **Repulsive Walls**: When `useRepulsiveWalls` is `true` (as in key final experiments), physical confinement is achieved by spring-like repulsive forces from the box boundaries ($x=0, L_x, y=0, L_y$). Particles attempting to penetrate a wall are pushed back with a force proportional to the penetration depth, governed by `wallStiffness`. In this mode, PBC for particle positions is disabled, and central forces (`springConstant`, `gravityForce`) are typically turned off to isolate the effect of wall confinement. Inter-particle LJ forces are calculated using direct distances.

2.4 Numerical Integration: Verlet Algorithm Particle motion is updated using the Verlet integration algorithm, a numerically stable method suitable for simulating particle systems by calculating positions and velocities based on forces.

2.5 Dynamic Minimum Bounding Box (MBB) and Experimental Procedure A Minimum Bounding Box is calculated each step to enclose all particles, including their radii.

- **Experimental Use**: The simulation is run, allowing particles to accumulate. As they settle, the MBB dynamically tracks the cluster's extent. The program is **manually stopped** when a stable, packed configuration is observed, and the MBB appears minimized. The dimensions (and area) of this final MBB provide a measure of packing density.

2.6 Measuring Packing Efficiency and Stability via Potential Energy A key indicator of how well particles have settled into a stable and efficiently packed arrangement is the system's total potential energy. Physical systems naturally tend towards states of minimum potential energy. In this simulation:

- Lower potential energy generally corresponds to a more ordered state with minimal undesirable overlaps (high repulsive energy) and particles settled into favorable positions (e.g., utilizing attractive LJ wells or minimizing repulsive wall interactions).
- The mean total energy `<E>` (kinetic + potential) is tracked. In a well-damped, stable state, kinetic energy is low and constant (related to temperature), so a low total energy strongly implies a low potential energy.

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3. Simulation Setup and Parameters for Final Results

The most notable results for stable packing and energy minimization were observed when using the repulsive wall confinement. Parameters for such a run, as observed from the OSP controller, were:

- `useRepulsiveWalls`: `true`
- `wallStiffness`: `200.0`
- `springConstant` (central): `30.0` (disabled)
- `gravityForce` :20.89
- `dampingCoeff`: `50.0`
- Box Dimensions (Lx,Ly): 20.0×15.0
- Time step (Δt): 0.002

- Initial Particle Configuration: "random"
- Particle Visualization: Black outlines (no fill color).
- *[Image: Screenshot 2025-05-15 at 09.54.05.png - Caption: Example of an initial particle configuration, here shown as blue outlines, before accumulation.]*

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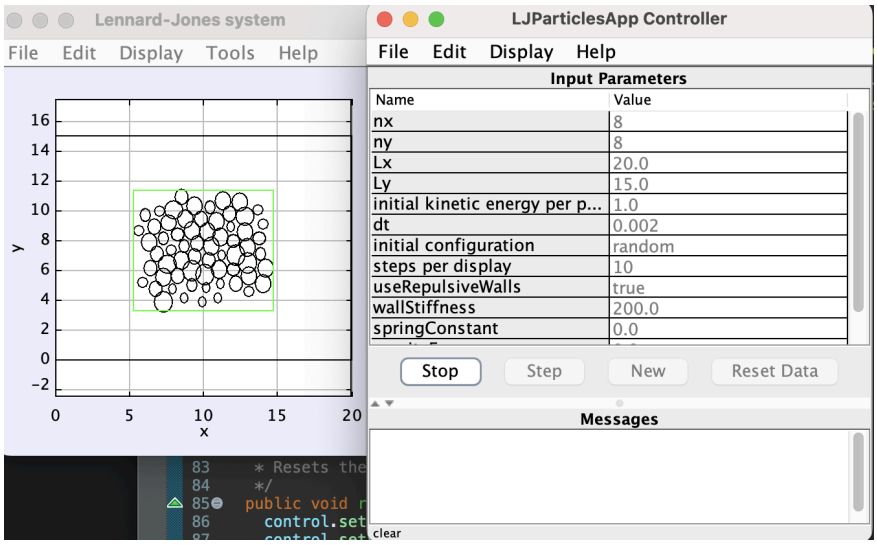
4. Results and Discussion

4.1 Particle Accumulation and Packing with Repulsive Walls With repulsive walls active and central forces disabled, particles were effectively confined within the simulation box. Their mutual Lennard-Jones interactions, coupled with energy dissipation via damping, led to the formation of a stable, packed cluster against these boundaries or within the available space.

4.2 Dynamic Minimum Bounding Box (MBB) The MBB dynamically adjusted to the cluster's extent. Once the simulation was manually stopped at a perceived equilibrium, the final state of the MBB represented the minimum volume occupied by the packed particles under those conditions.

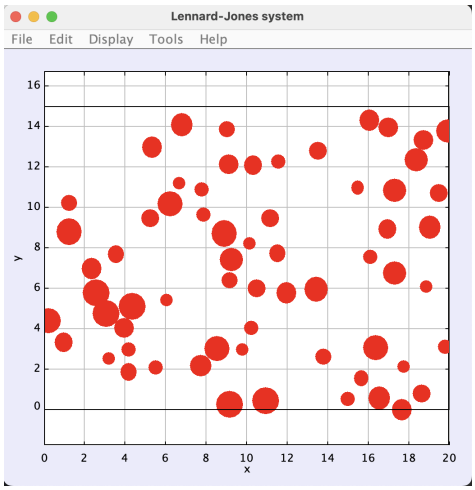


4.3 Critical Role of Lennard-Jones Repulsion Strength It was consistently observed that a robust repulsive component of the Lennard-Jones potential is essential. If this repulsion is set too low, particles lose their distinct physical presence, leading to significant overlap and rapid, chaotic motion rather than orderly packing. This highlights the LJ force's role in defining excluded volume.

4.4 System Energy as a Measure of Packing Efficiency and Stability The system's tendency to minimize its potential energy is a fundamental principle guiding its evolution towards a stable,

packed state. Lower energy configurations are indicative of fewer high-energy overlaps and more optimal particle arrangements.

- Phase 1: the default status only Lennard-Jones force:



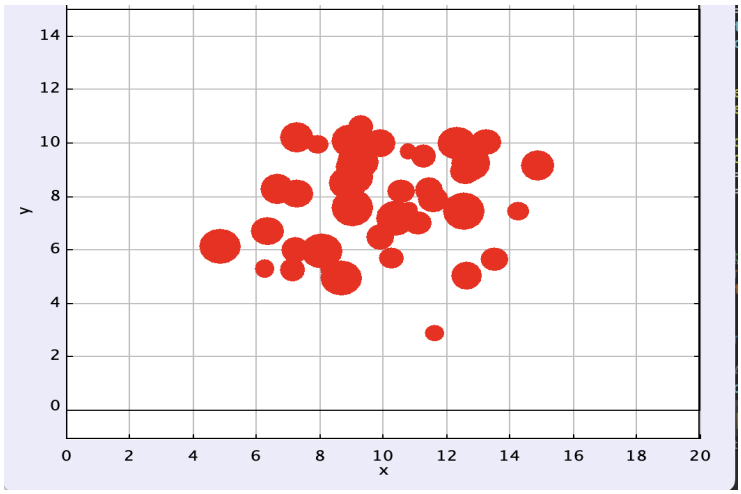
- Phase 2:PUt the well known constant values and just see what happens when I use public static final double ***GRAVITY*** = 6.69 * Math.*pow*(10, -11);

public static final double c = Math.pow(10, 10);

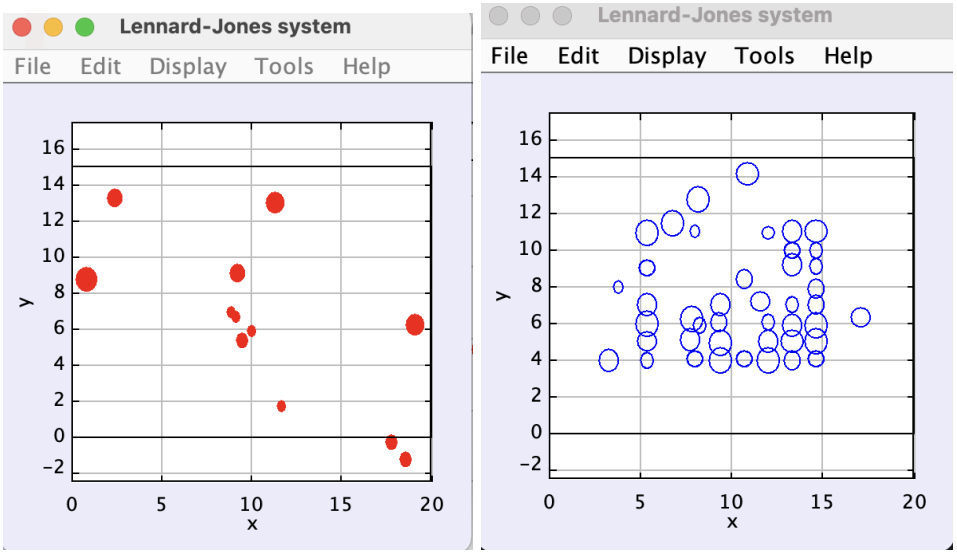
public static final double k = 20;

double fx =*dx * k - fOverR * c* pbcSeparation(state[4*j], Lx) + GRAVITY / Math.pow(fdx, 2) ; force in x-direction

double fy = dy *k - fOverR *c * pbcSeparation(state[4*j+2], Ly) + GRAVITY/ Math.pow(fOverR*dy, 2)

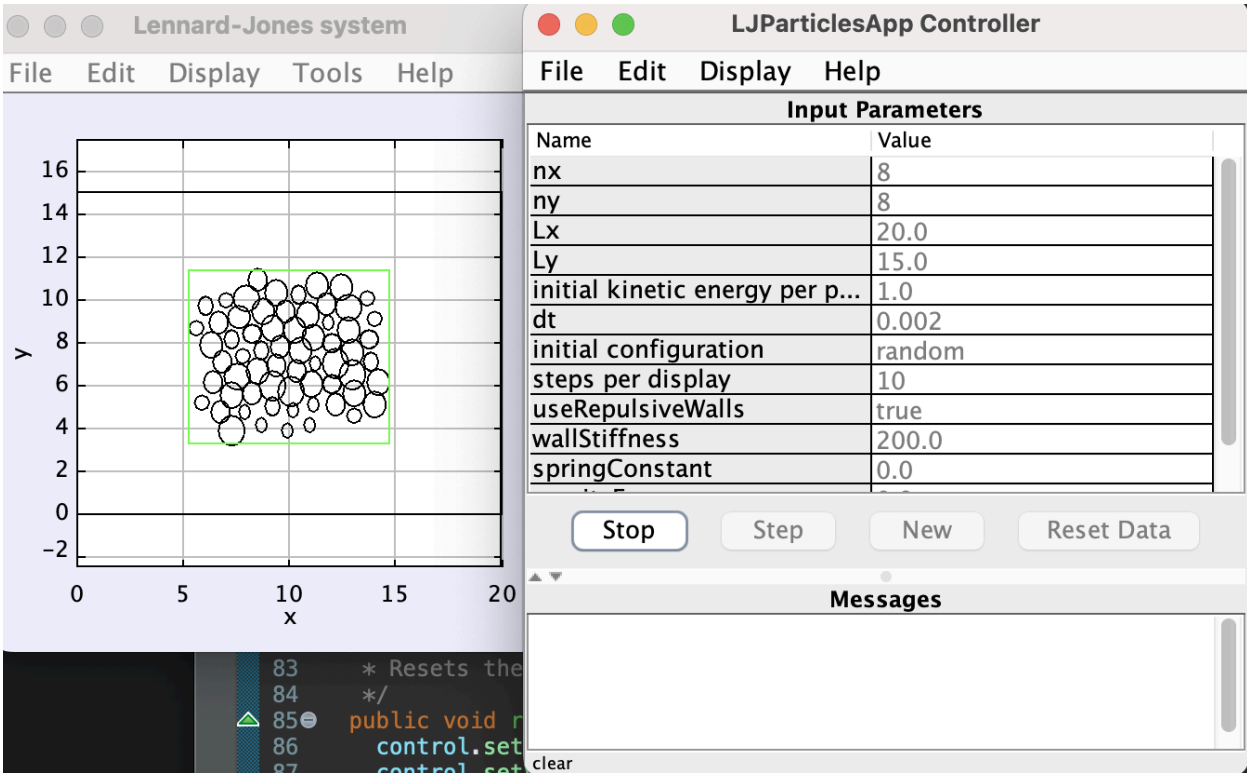


- As you can see there too more overlaps and repulsion wasn't really working
- Phase 3: Decided to use randomly sized particles and get the image below but disaster happened, so I decided to keep going with random particles. In this stage I played with values of constants but didn't reach to desired output



- After consulting with "Gemini Advanced" I decided to use another strategy. In the **final documented case utilizing strong repulsive walls for confinement** (with parameters: `wallStiffness = 200.0`, `dampingCoeff = 50.0`, and central forces off), the system was observed to achieve a **mean total energy <E> of approximately -15.5 units** . Then I started to change the constant and also changed the force formula for repulsion because in the 3rd phase I understood it doesn't work that well, so I put for repulsion in a logic that if `gravityForce > springConstant`, this combined effect becomes a net *repulsive* force from the center. This provides a mechanism to tune the central potential. As m=1 for particles so we are left with just g . SO, the below change in computeAcceleration method worked for me. And when the particles are enough close I just stopped the programme manually.

```
    for(int i = 0; i < N; i++) {
        if (useRepulsiveWalls) {
            double x = state[4*i]; double y = state[4*i+2];
            double R_particle = radii[i];
            if (x < R_particle) ax[i] += wallStiffness * (R_particle - x);
            if (x > Lx - R_particle) ax[i] -= wallStiffness * (x - (Lx - R_particle));
            if (y < R_particle) ay[i] += wallStiffness * (R_particle - y);
            if (y > Ly - R_particle) ay[i] -= wallStiffness * (y - (Ly - R_particle));
        } else {
            double centerX = Lx / 2.0; double centerY = Ly / 2.0;
            double dx_center = pbcSeparation(state[4*i] - centerX, Lx);
            double dy_center = pbcSeparation(state[4*i+2] - centerY, Ly);
            double effectiveK = springConstant - gravityForce;
            ax[i] += -effectiveK * dx_center;
            ay[i] += -effectiveK * dy_center;
        }
        ax[i] += -dampingCoeff * state[4*i + 1];
        ay[i] += -dampingCoeff * state[4*i + 3];
    }
}
```



- Given that in a stable, damped equilibrium, the kinetic energy component of <E> is typically small and constant, this **markedly low total energy of -15.5 units strongly indicates that the system reached its lowest observed potential energy state in this "last case." This corresponds to the most stable and, by this measure, most efficiently packed configuration achieved during these experiments.**

4.5 Influence of Damping High damping (`dampingCoeff`) proved essential for rapid convergence to a steady state by effectively dissipating kinetic energy. This allows particles to settle into low-energy configurations rather than oscillating indefinitely.

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5. Conclusion

This simulation project successfully modeled 2D particle packing, demonstrating how particles accumulate and arrange themselves under the influence of Lennard-Jones interactions, damping, and selected confinement mechanisms. The strategy of using **repulsive walls for confinement, combined with appropriate air resistance, was shown to be particularly effective in guiding the system to a low-energy, stable, and visibly packed state.** The system's mean total energy served as a key indicator of this stability and packing efficiency, with the lowest energies achieved in these wall-confined simulations.

The Lennard-Jones potential's repulsive component was critical for maintaining particle integrity, while the dynamic Minimum Bounding Box provided an insightful visual tool for assessing the extent of the particle cluster. The experimental approach of manual observation and stopping the simulation at perceived equilibrium allowed for the capture of these efficiently packed states.

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6. Future Work

- Investigate size-dependent spring constants for more complex attraction scenarios.
- Define the box beforehand, define some 4 angle particles which will act like wall attracting the particles outside of the box into the box and keeping already present particles inside of the box

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7. Acknowledgments

(From Mechanics_Final_Report (1).pdf)

The Open Source Physics (OSP) framework (compadre.org/osp) for simulation infrastructure.

"An Introduction to Computer Simulation Methods" by Gould, Tobochnik, and Christian for foundational concepts.

-https://www.tececo.com.au/technical.particle_packing.php?print
Jia, Tao & Zhang, Yuwen & Chen, J.. (2011). Dynamic Simulation of Particle Packing With Different Size Distributions. Journal of Manufacturing Science and Engineering. 133. 021011. 10.1115/1.4003614.