

MD-in-a-Box v2 — User Guide

Interactive Simulations of Binary Atom Mixtures

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Demo Mode (default at startup, press B in Manual mode)

The device cycles automatically through all mixture settings, each following a standard temperature protocol. The simulation loops continuously.

- A** Cycle display info
- X** Skip forward to next setting
- Y** Skip backward to previous setting
- B** Switch to **Manual mode** (keeps current state)
- A+B** Shutdown

Info display (button A cycles):

- View 1 T_{sp} : Setpoint temperature
- View 2 Lennard Jones parameters:
 - ϵ_{AB} AB interaction strength (ϵ_{AB})
 $\epsilon_{AB} > 1$ AB attraction is stronger than AA and BB attraction
 - r_{NB} Fraction of B particles (N_B/N_{total})
 - r_{sizeB} Size ratio between B and A particles d_B/d_A
- View 3 $gravity$: Total gravity, and x,y components

A color-gradient bar at the top of the screen shows progress

Manual Mode (press B in Demo mode)

The simulation continues from the current demo state. Use **A** to select a parameter, then **X/Y** to adjust it.

- A** Cycle selected parameter
- X** Increase selected parameter
- Y** Decrease selected parameter
*(at $T_{sp} = 0$: first **Y** arms quench prompt, second **Y** within 2s zeroes all velocities)*
- B** Return to Demo mode (T-ramp resumes, Lennard Jones parameters kept)
- A+B** Shutdown

Adjustable parameters:

- T_{sp} Target (setpoint) temperature
- Gravity Gravity strength
- Pause Freeze/unfreeze the simulation (also shows the calibration status of the accelerometer)
- Coupling Langevin thermostat coupling strength
- r_{NB} Fraction of type-B particles (N_B/N)
- r_{sizeB} Size ratio of particle B relative to particle A
- ϵ_{AB} A–B cross-interaction strength (ϵ_{AB})
($\epsilon_{AA} = \epsilon_{BB} = 1$)

Standard Temperature Protocol

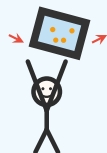
Every setting follows the same 8-phase protocol. The thermostat ramps *linearly* between temperatures over 45 000 MD steps (≈ 90 s):

| Phase | T | Description |
|-------|-----------|---------------------------------------|
| 1 | 5.0 | Hot gas, (Mixing initial structure) |
| 2 | 5.0 – 0.8 | Cooling |
| 3 | 0.8 | Liquid like |
| 4 | 0.8 – 0.1 | Cooling and Crystallizing |
| 5 | 0.1 | Crystal or glass |
| 6 | — | Hard quench: Velocities zeroed |
| 7 | 0.0 | Crystal or glass |
| 8 | 0.0 – 2.0 | Heating / Melting |

Full cycle ≈ 12 min.

Physical Interaction (accelerometer)

- Tilt the device Gravity direction follows
- Shake it Box walls push atoms, causing heating.



Demo Settings Overview

All settings use 100 atoms and the same temperature protocol.

| Setting | N_B/N | d_B/d_A | ϵ_{AB} |
|--|---------|-----------|-----------------|
| Monoatomic system | 0 | — | — |
| Symmetric mixture | 0.5 | 1.0 | 1.0 |
| Equal size, AB interactions disfavoured | 0.5 | 1.0 | 0.1 |
| Equal size, AB interactions favoured | 0.5 | 1.0 | 2.0 |
| Large & small, AB interactions disfavoured | 0.3 | 1.5 | 0.5 |
| Large & small, AB interactions favoured | 0.3 | 1.5 | 2.0 |
| Few large, AB interactions favoured | 0.1 | 1.3 | 2.0 |
| Few small, AB interactions favoured | 0.1 | 0.6 | 2.0 |

N_B/N : fraction of **B** (blue) atoms.

d_B/d_A : diameter ratio.

$\epsilon_{AB} < 1$: A/B tends to phase separate;

$\epsilon_{AB} > 1$: enhanced A–B attraction.

References & Info

- ❖ “MD in a Box” code: [boj.dk/md-in-a-box](https://github.com/boj.dk/md-in-a-box)
- ❖ Browser based MD program: [urp.dk/md](https://github.com/urp.dk/md)
- ❖ ulab: <https://github.com/v923z/micropython-ulab>
- ❖ Hardware:
 - Raspberry Pi Pico 2 (RP2350)
 - Pico Display Pack 2.0 by Pimoroni
 - Fermion: BNO055 Intelligent 9-axis Sensor (Breakout) by DFRobot
 - Box for the device: “Pimoroni Display Pack 2 Case” by JeffCurless