MD-in-a-Box v2 — User Guide

Interactive Simulations of Binary Atom Mixtures

Bo Jakobsen *IMFUFA · Department of Science and Environment (INM) · Roskilde University (RUC)*

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	`Tsp` : Setpoint temperature	
View 2	Lennard Jones parameters:	
	`epsilon_AB`	AB interaction strength (ε_{AB}) $\varepsilon_{AB} > 1$ 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

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
Shake it

Gravity direction follows
Box walls push atoms, causing heating.

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 2 s 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
`epsilon_AB`	A–B cross-interaction strength (ε_{AB}) ($\varepsilon_{AA} = \varepsilon_{BB} = 1$)

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.
$\varepsilon_{AB} < 1$: A/B tends to phase separate;
$\varepsilon_{AB} > 1$: enhanced A–B attraction.

References & Info

- "MD in a Box" code: `boj.dk/md-in-a-box`
- Browser based MD program: `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