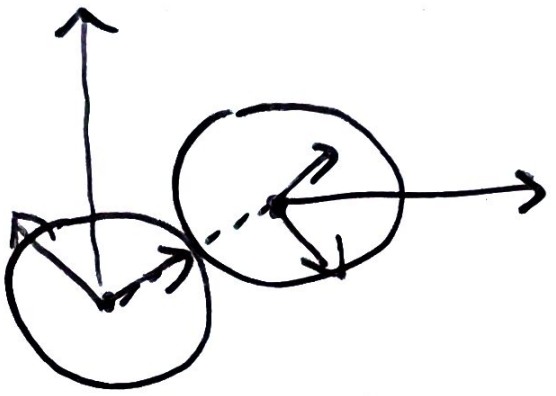
Project Gas Simulator

① Detect collision in a time iteration



② If collision detected :

a. ~~Go back~~ For next time itr, mark particles which had collided

b. In next iteration, resolve x and y velocities along line of collision and ⊥ to it

c. Do momentum conserv. and calculate new velocities

d. Update x and y coordinates

⇒ Detect collision by particle dist. less than sum of radii

⇒ Make the position discretization very small (low vel.) and have high vel. in animation

° Functionalities to have

① Heat conduction
- wall temperature (or region)

② Diffusion

③ Fluid flow
- Custom walls and obstacles
- fluid dynamics (like nozzle flow)

④ Chemical reaction
- vibrational relaxation
- unimolecular reactions

- Next steps

→ ✓ Add varying particle sizes

→ ✓ Add colored particles

→ ✓ Add inside walls

→ Add heater walls and space

→ ✓ Add gravity

→ ✓ Add association reactions

→ Check physics

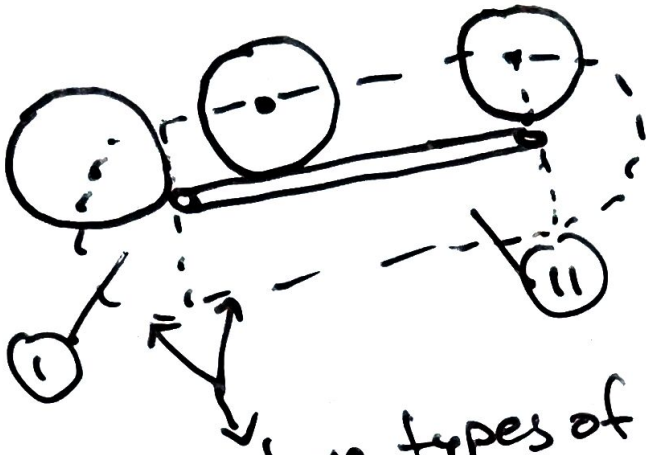
- Side Notes

→ Use in polygon function to gen. random pts. enclosed in a polygon region

→ ✓ Find faster method to detect inter-particle collision (to remove 2 nested for loops)

The wall collision issue

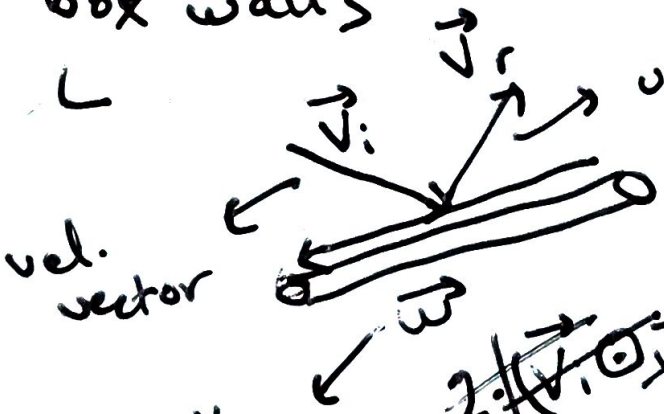
→



two types of bounding boxes (for wall collision detection)

→ Treat (1) by considering fixed wall edge point (reuttle || velocity)

→ Treat (11) by a similar method as in box walls



use householder reflection

$2 \cdot (\vec{v}_i \odot \vec{w})\vec{w} - \vec{v}_i$

$= \vec{v}_r$

The wall collision jitter issue

→ ✓ Create another wall collision flag matrix

Issues to solve

① ~~Find~~ faster method to detect inter-particle collision ✓

② ~~Solve~~ issue of changing discretization of speed (high speed particle pass through wall) → speed up animation at low speeds ✓

The reactive gas

→ Make an array is Molecule to store info on atoms constituting a specific molecule

ex.: [0, 0, 1, 0, 0, 1, 0, 2, 2, 0 ..]

Mol. A Mol. B

→ When rel. vel. along C-O-C is greater than threshold : identify molecule formation

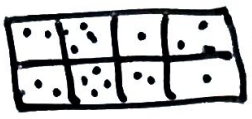
↳ keep switching vel. directions & mag. of 11 vel. vectors of atoms betw^n ○○ and ○○ events

[swap betw^n vel. state of particles before and after collision]

→ Initially, wait till all particles are in a separated position

The wind tunnel mode ~~mode~~ Fix mode

[Also see hash grid!! : divide and rule]

↳  ← → ${}^6C_2$ vs. ${}^3C_2 \times 2$

[Fix quantum tunnelling problem!]

↳ decrease time step: a simple soln.

[Fix molecule dissociation issue]

↳ ① use hash only for non-reactive gas

↳ ② increase range of neighbouring cells while collision checking

(1→2) (1→3)

Fix: quantum tunneling when gas is reactive of molecules

↳ inside wall collision force should be transmitted to both atoms of a molecule if they are in contact

↳ add x and y update like box wall

Hash grid implementation [v16]

→ Cell size :

↳ [works better than 2 for loops for large no. of particles]

cell_nos ~~size~~ = floor(L / part_dia)

cell_size = L / cell_nos

→ nPart = 1000
size = 2
box_xmax = box_ymax = 100
time = 1000

Existing : 9.52 sec.
Hash grid : 2.33 sec. !!

→ See how to implement hash grid with 2 particles with diff. sizes

↳ Take cell size to be = max particle dia

↳ Create 3D lookup:

→ stacks particles

↳ create 2D ctr array to store and update indices for 3D lookup as particles fill in

Fluid flow feature

→ Fix jitter: Off when inside wall active

↳ jitter matrix conflicting with X/Y update of inside wall