An Optimal Analysis on Collision-Pair Search Algorithm in Lagrangian Particle Tracking Method

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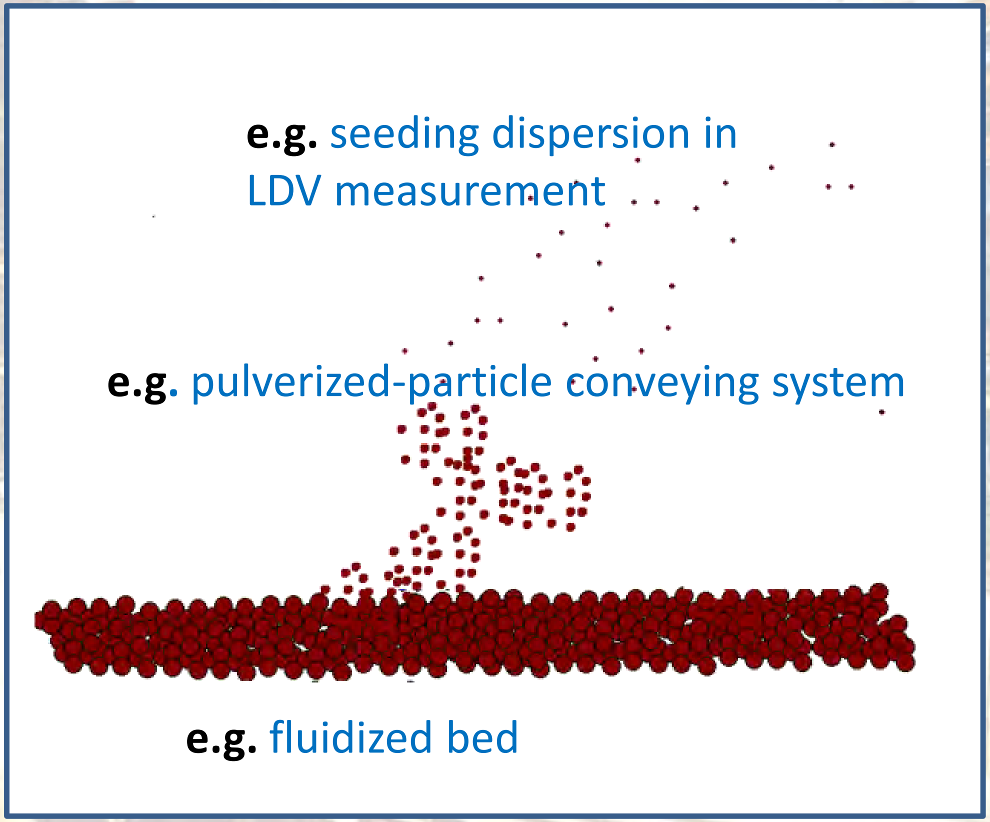
Introduction

Classification of particle-laden flows

- **Dilute**
  - collision free
- **Dense**
  - Collision dominated
  - Contact dominated



Crowe, C. T., Sommerfeld, M., & Tsuji, Y., 1998. *Multiphase Flow with Droplets and particles*. CRC Press.

Simulation of particle-laden flows

- Carrier fluid: Eulerian framework
  - Eddy viscosity model
    - Low-Reynolds-number k-ε turbulence model
    - RSM turbulence model
- Dispersed particles: Lagrangian framework
  - Particle tracking methods
    - deterministic
    - stochastic
  - Particle-fluid interactions
    - Particle source in cells : PSI-cell method
  - Particle collision model
    - Hard-sphere model
    - Soft-sphere model

Equation of motion of particles

- Translation:

$$m_p \frac{d\mathbf{U_p}}{dt} = \mathbf{F_D} + \mathbf{F_S} + \mathbf{F_M} + \mathbf{F_G}$$

- Rotation:

$$I_p \frac{d\mathbf{\Omega_p}}{dt} = \mathbf{T_v}$$

I_p : momentum of inertia

$\mathbf{\Omega_p}$: rotational velocity

$\mathbf{F_D}$ = quasi-steady drag

$\mathbf{F_S}$ = Saffman lift

$\mathbf{F_M}$ = Magnus lift

$\mathbf{F_G}$ = gravitatonal force

$$\mathbf{F_D} = \frac{\pi}{8}\rho_g C_D d_p^2 \left|\mathbf{U_g} - \mathbf{U_p}\right|\left(\mathbf{U_g} - \mathbf{U_p}\right)$$

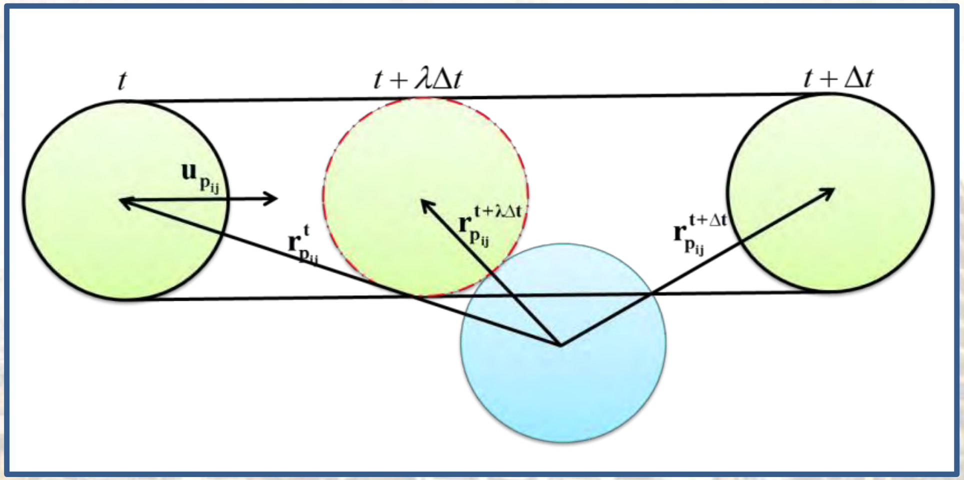
$$C_D = \frac{24}{\mathrm{Re}_p}\left(1 + 0.15\,\mathrm{Re}_p^{0.687}\right) \qquad \mathrm{Re}_p = \frac{\rho_g d_p \left|\mathbf{U_g} - \mathbf{U_p}\right|}{\mu}$$

$$\mathbf{F_S} = 1.61 \cdot f_s \cdot d_p^2 \left(\rho_g \mu\right)^{\frac{1}{2}} \left|\mathbf{\Omega_g}\right|^{-\frac{1}{2}} \left[\left(\mathbf{U_g} - \mathbf{U_p}\right) \times \mathbf{\Omega_g}\right]$$

$$\mathbf{F_M} = \frac{\pi}{8}\rho_g \left|\mathbf{U_g} - \mathbf{U_p}\right| C_{LR} d_p^2 \left[\frac{\left(\mathbf{U_g} - \mathbf{U_p}\right) \times \left(\mathbf{\Omega_p} - 0.5\mathbf{\Omega_g}\right)}{\left(\mathbf{\Omega_p} - 0.5\mathbf{\Omega_g}\right)}\right]$$

$$\mathbf{T_v} = -C_{T_v} \frac{\rho_g}{2}\left(\frac{d_p}{2}\right)^5 \left|\mathbf{\Omega_p} - \mathbf{0.5\Omega_g}\right|\left(\mathbf{\Omega_p} - \mathbf{0.5\Omega_g}\right)$$

Detection of inter-particle collision



$if\,(\mathbf{U_{ij}} \cdot \mathbf{r_t} < 0)$

{

$$d_{\min} = \left| \mathbf{r_t} + \frac{\mathbf{U_{ij}}}{|\mathbf{U_{ij}}|} \cdot \mathbf{r_t} \right|$$

$if\,(d_{\min} < \frac{1}{2}(d_i + d_j))$

{

$$d_{\mathrm{collision}} = |\mathbf{U_{ij}}|\Delta t - \sqrt{\left[\frac{1}{2}(d_i + d_j)\right]^2 - d_{\min}{}^2}$$

$$\lambda = \frac{d_{\mathrm{collision}}}{|\mathbf{U_{ij}}|\Delta t}$$

$if\,(\lambda < 1)$

occurence of collision

}

}

Determination of Post-collision Conditions by Hard-sphere Collision Model

- Impulse equation
  - Translation

$$\mathbf{U}^*_{\mathbf{p_i}} = \mathbf{U}_{\mathbf{p_i}} + \frac{\mathbf{J}}{m_{p_i}}$$

$$\mathbf{U}^*_{\mathbf{p_j}} = \mathbf{U}_{\mathbf{p_j}} - \frac{\mathbf{J}}{m_{p_j}}$$

$$\mathbf{J} = J_n \mathbf{e_n} + J_t \mathbf{e_t}$$

$$J_t = \begin{cases} -\dfrac{2}{7}\dfrac{m_{p_i} m_{p_j}}{m_{p_i} + m_{p_j}} \left|(\mathbf{U_{ct}})_{\mathbf{ij}}\right| & \text{for } J_t < f \cdot J_n \\ -f J_n & J_t \geq f \cdot J_n \end{cases}$$

$$J_n = -\frac{m_{p_i} m_{p_j}}{m_{p_i} + m_{p_j}} (1 + e) (\mathbf{U_{ij}} \cdot \mathbf{e_n})$$

  - Rotation

$$\mathbf{\Omega}^*_{\mathbf{p_i}} = \mathbf{\Omega}_{\mathbf{p_i}} + \frac{d_i}{2I_p} \mathbf{e_n} \times \mathbf{J}$$

$$\mathbf{\Omega}^*_{\mathbf{p_j}} = \mathbf{\Omega}_{\mathbf{p_j}} + \frac{d_j}{2I_p} \mathbf{e_n} \times \mathbf{J}$$

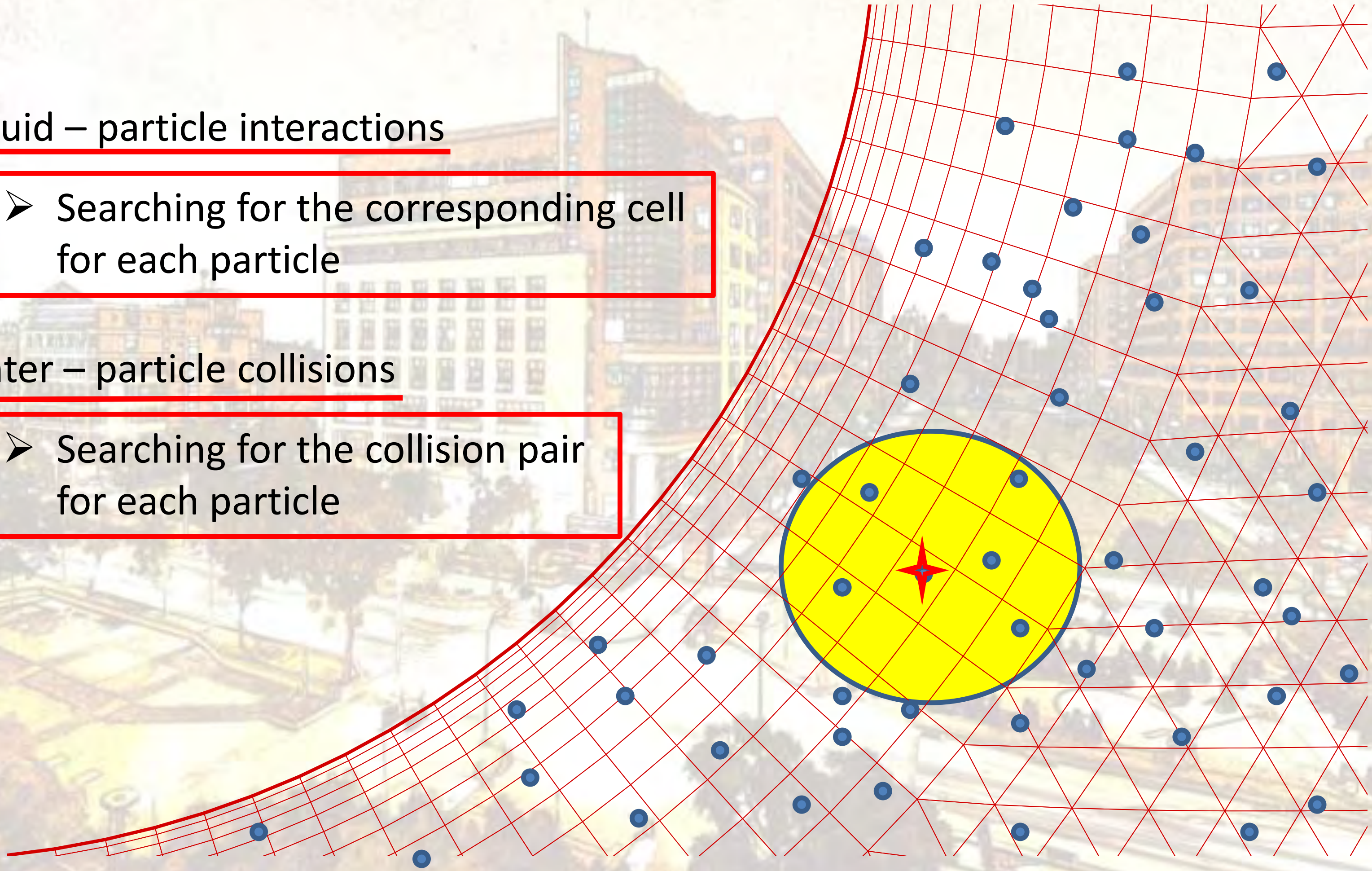
$$(\mathbf{U_{ct}})_{\mathbf{ij}} = \mathbf{U}_{\mathbf{p_i}} - \mathbf{U}_{\mathbf{p_j}} + \frac{d_i}{2} \mathbf{\Omega}_{\mathbf{p_i}} \times \mathbf{e_n} + \frac{d_j}{2} \mathbf{\Omega}_{\mathbf{p_j}} \times \mathbf{e_n}$$

$$\mathbf{e_n} = -\frac{\mathbf{r_{t+\lambda_1 \Delta t}}}{\left|\mathbf{r_{t+\lambda_1 \Delta t}}\right|} \qquad \mathbf{e_t} = -\frac{(\mathbf{U_{ij}})_{\mathbf{ct}}}{\left|(\mathbf{U_{ij}})_{\mathbf{ct}}\right|}$$

$$\mathbf{r_t} = \mathbf{r_{j,t}} - \mathbf{r_{i,t}}$$

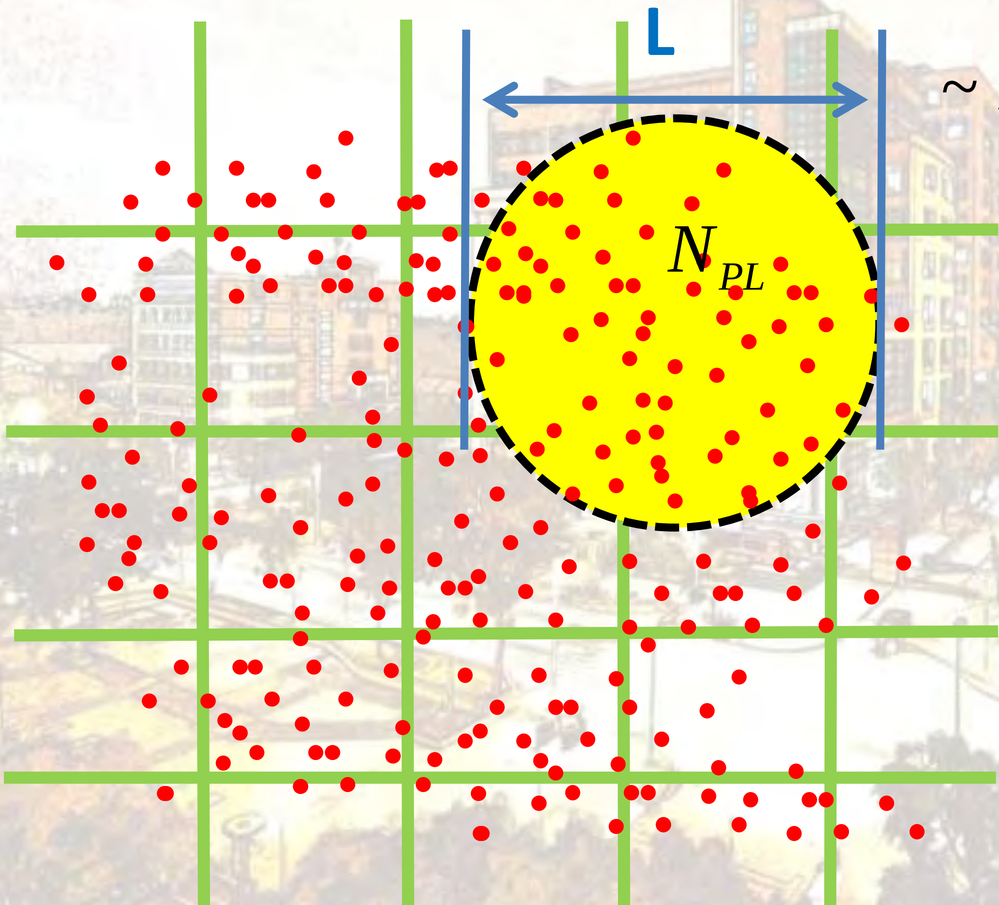
Cost-effective algorithms for Lagrangian particle tracking method

- Fluid – particle interactions
  - Searching for the corresponding cell for each particle
- Inter – particle collisions
  - Searching for the collision pair for each particle



Sub-region for searching collision pairs of particles

Grid Meshes

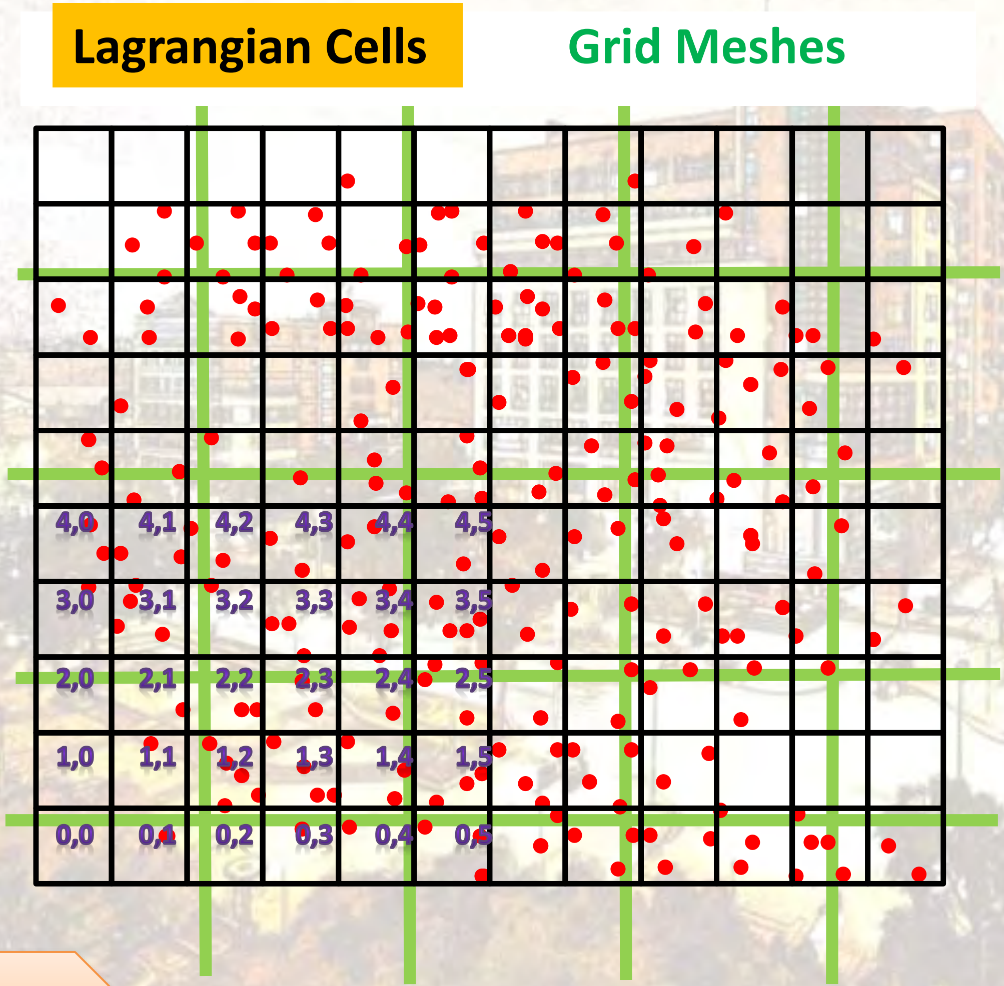


$$\sim N_{PL} \times \left(N_{PL} - 1 \right)$$

```
for (i=0; i< NOP; i++)
{
   for (j=i+1; j < NOP; j++)
   {
      DIST = POP[i] –POP[j]
      if  ( dot_product[DIST, DIST]| < L)
         CALL  collision_check(i,j)
   }
}
```

B. P. B. Hoomans, J. A. M. Kuipers, W. J. Briels and W. P. M. van Swaaij, "Discrete particle simulation of bubble and slug formation in a two-dimensional gas-fluidized bed: a hard-sphere approach", *Chemical Engineering science*, **55**, 99-118 (1996)

Link-list approach for searching collision pairs of particle



Link-list method (Allenm and Tildesly, 1986)

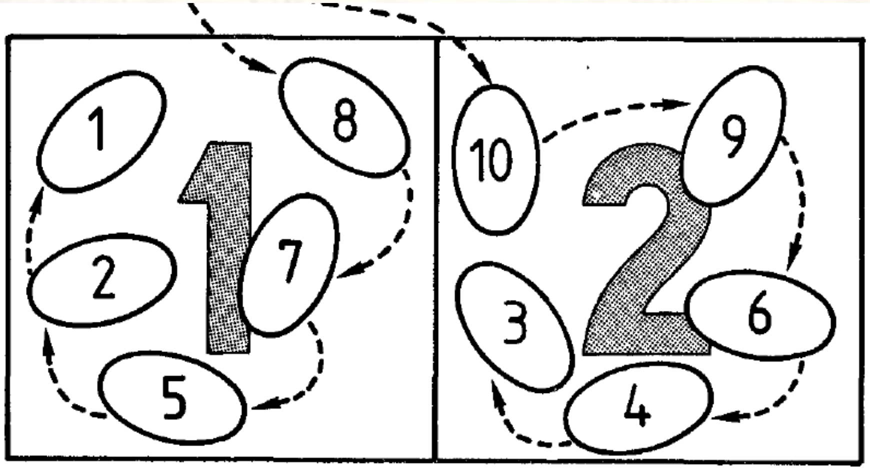


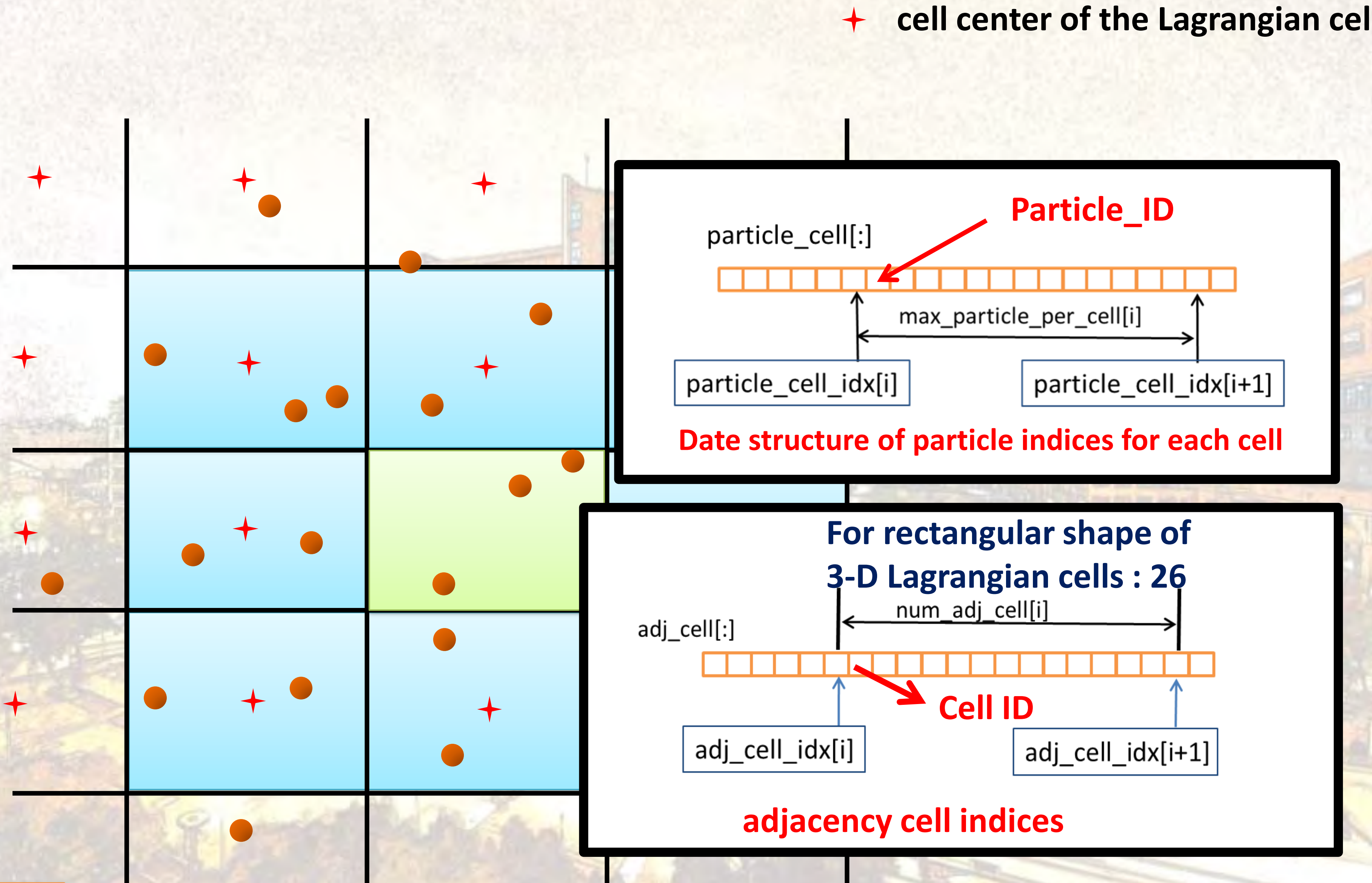
Fig. 5.5 The cell method in two dimensions. (a) The central box is divided into $M \times M$ cells ($M = 5$). (b) A close-up of cells 1 and 2, showing the molecules and the link-list structure.

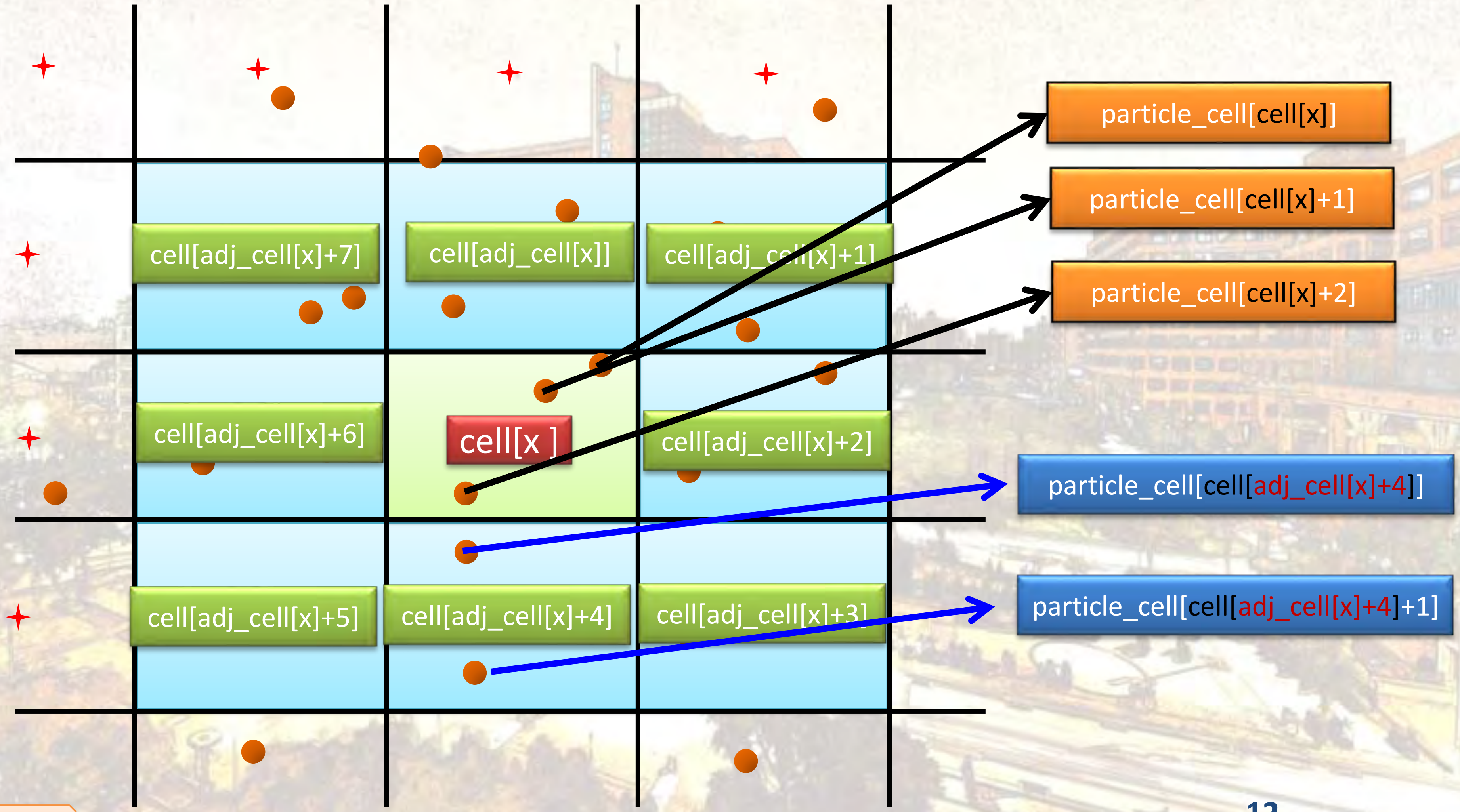
position:	1	2	3	4	5	6	7	8	9	10
HEAD:	8	10								
LIST:	0	1	0	3	2	4	5	7	6	9

Sequential processes

➔ hard to parallelize

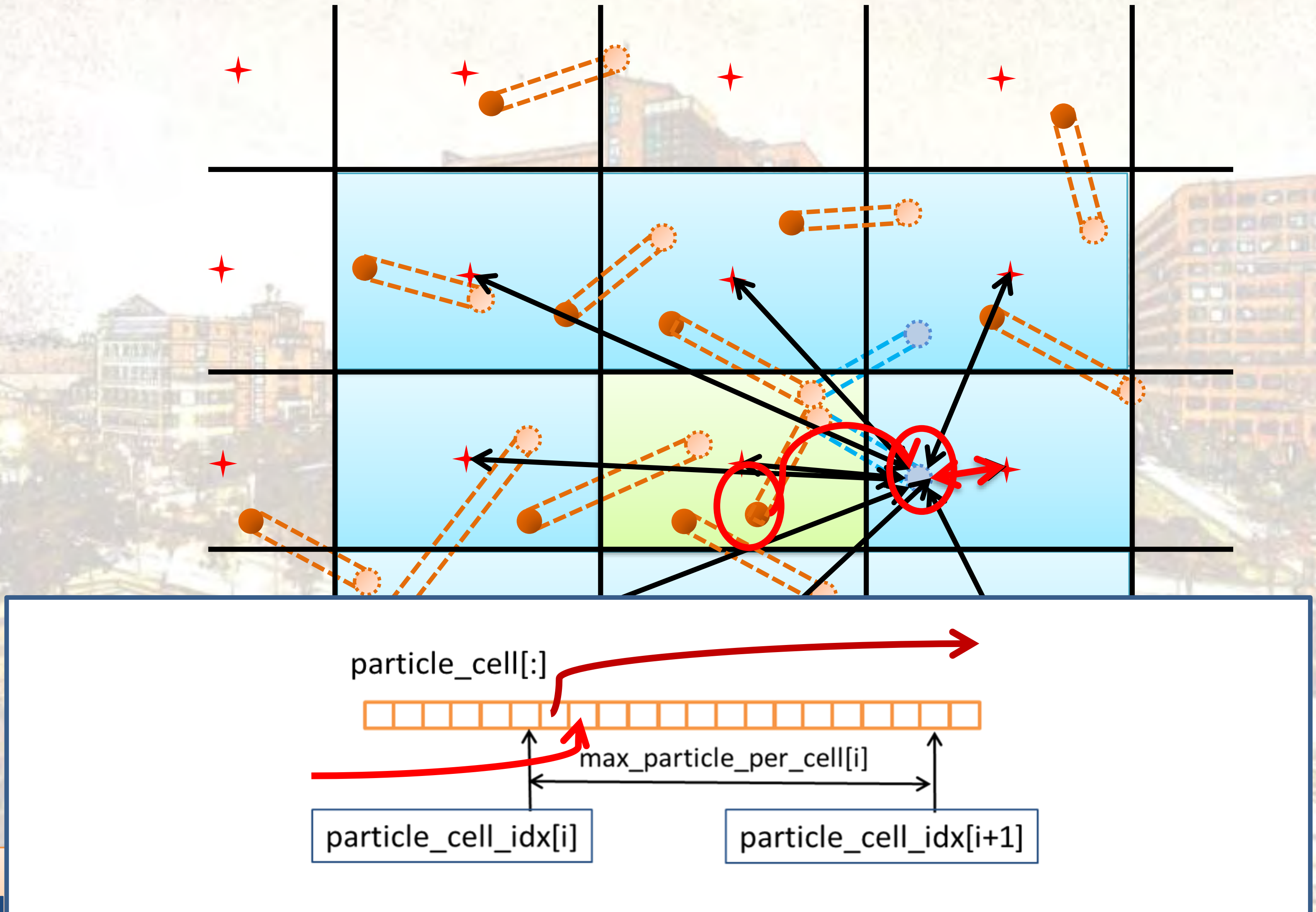
Allenm, M. P., and Tildesly, D. J., 1986, Computer Simulation of Liquids, Oxford Science Publication.


cell center of the Lagrangian cell
Particle_ID
particle_cell[:]
max_particle_per_cell[i]
particle_cell_idx[i]
particle_cell_idx[i+1]
Date structure of particle indices for each cell
For rectangular shape of
3-D Lagrangian cells : 26
num_adj_cell[i]
adj_cell[:]
Cell ID
adj_cell_idx[i]
adj_cell_idx[i+1]
adjacency cell indices

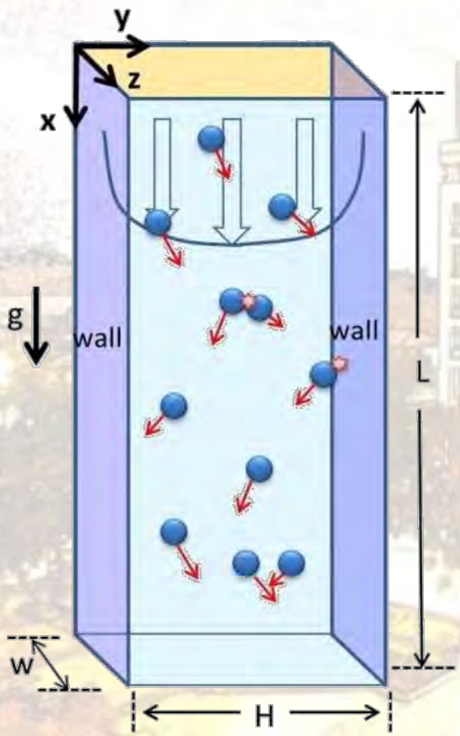


cell[adj_cell[x]+7]
cell[adj_cell[x]]
cell[adj_cell[x]+1]
cell[adj_cell[x]+6]
cell[x]
cell[adj_cell[x]+2]
cell[adj_cell[x]+5]
cell[adj_cell[x]+4]
cell[adj_cell[x]+3]
particle_cell[cell[x]]
particle_cell[cell[x]+1]
particle_cell[cell[x]+2]
particle_cell[cell[adj_cell[x]+4]]
particle_cell[cell[adj_cell[x]+4]+1]

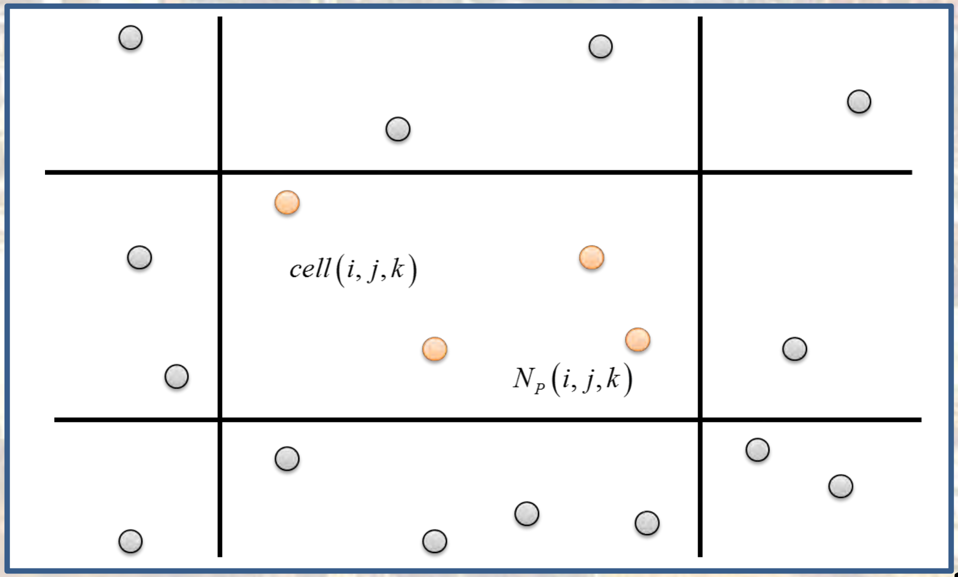
Re-allocated of particle indices for each cell



Benchmark problem for computational efficiency test



- Particle number : 1,000 ~ 20,000,000
- Number of Lagrangian cell : 80,000, 640,000, 5,120,000
- Particle density : 8800 kg/m^3
- Particle diameter : 10 µm
- Carrier-fluid : air



CPU TIME of Lagrangian Particle tracking

$$\mathrm{LCPU} = C_1 (N_{CELL}) + C_2 \times N_{PT} + C_3 \times (N_{SL})(N_{SL} - 1)$$

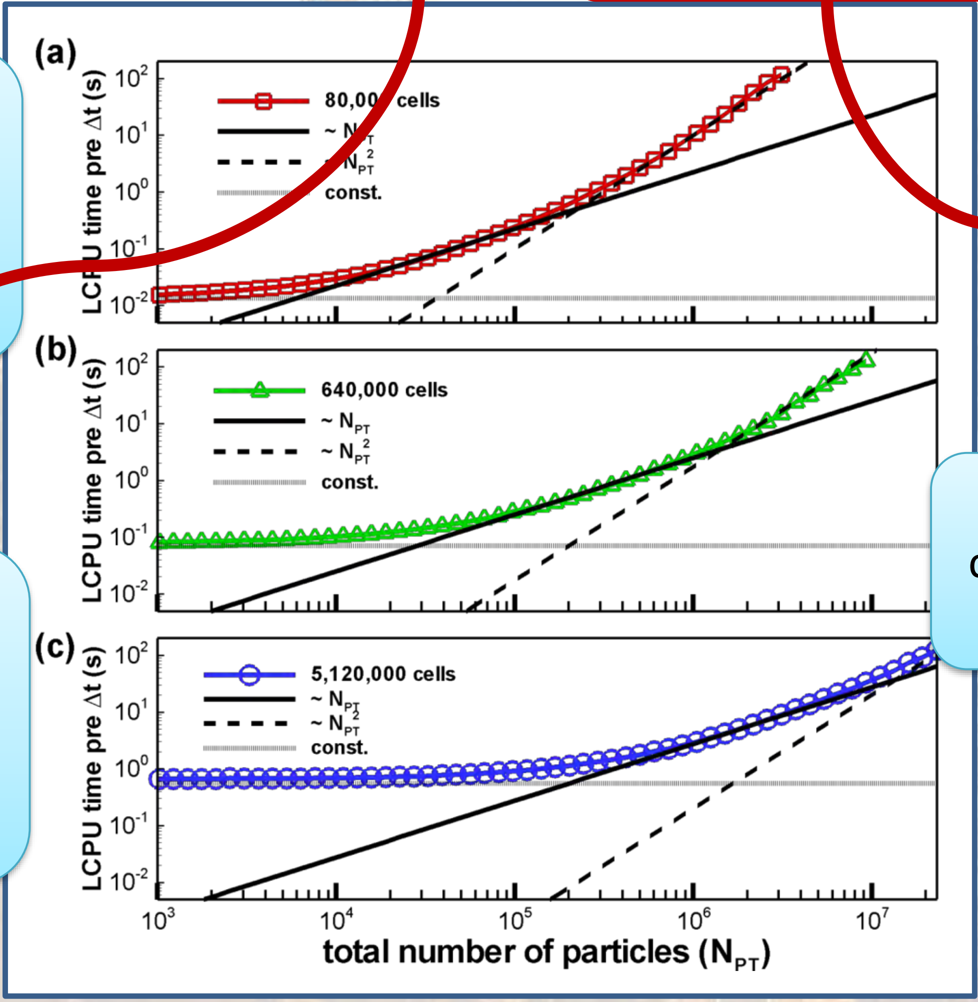
$$N_{SL} \approx 27 \frac{N_{PT}}{N_{CELL}}$$

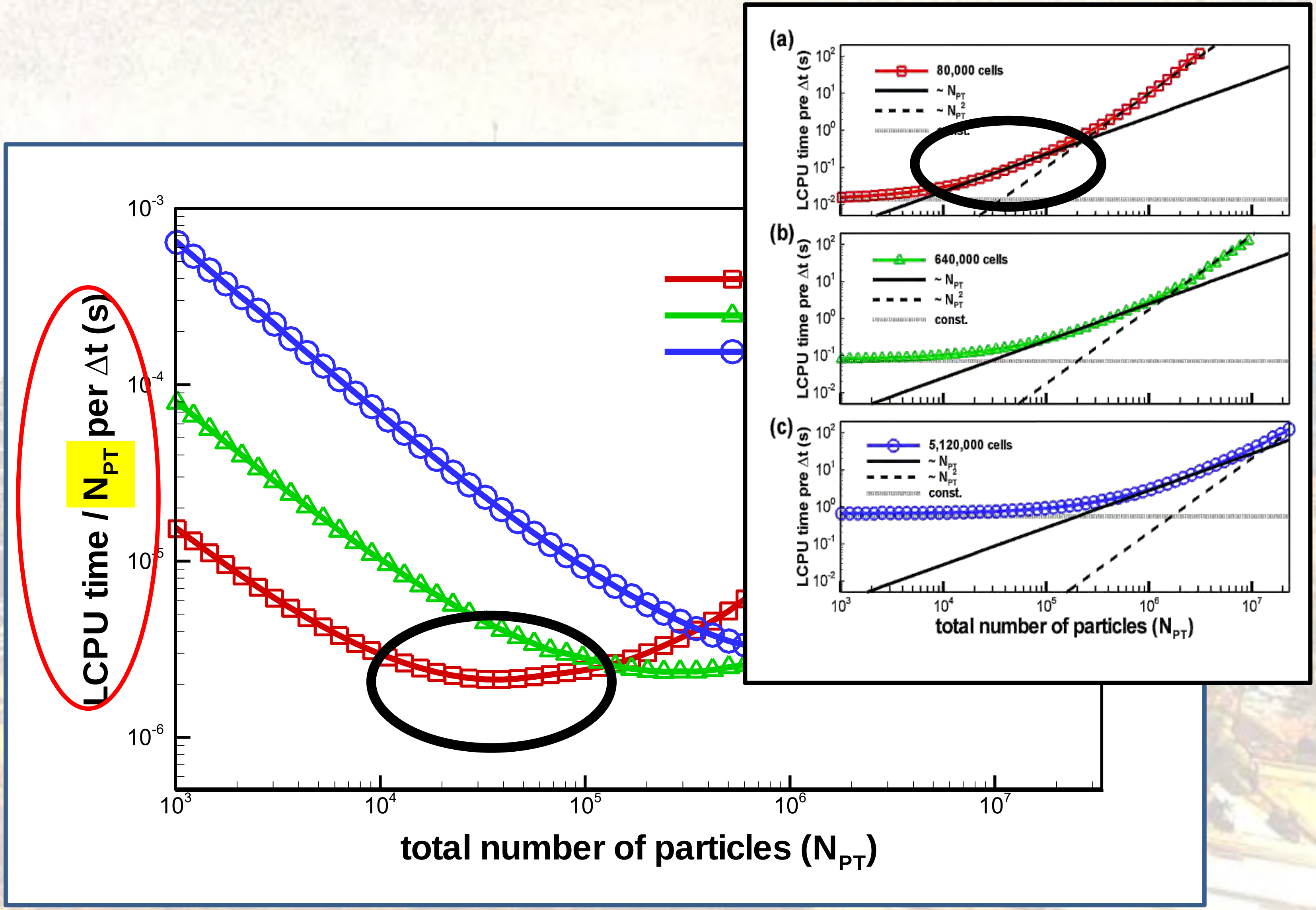
$$\sim N_{PT}^2$$

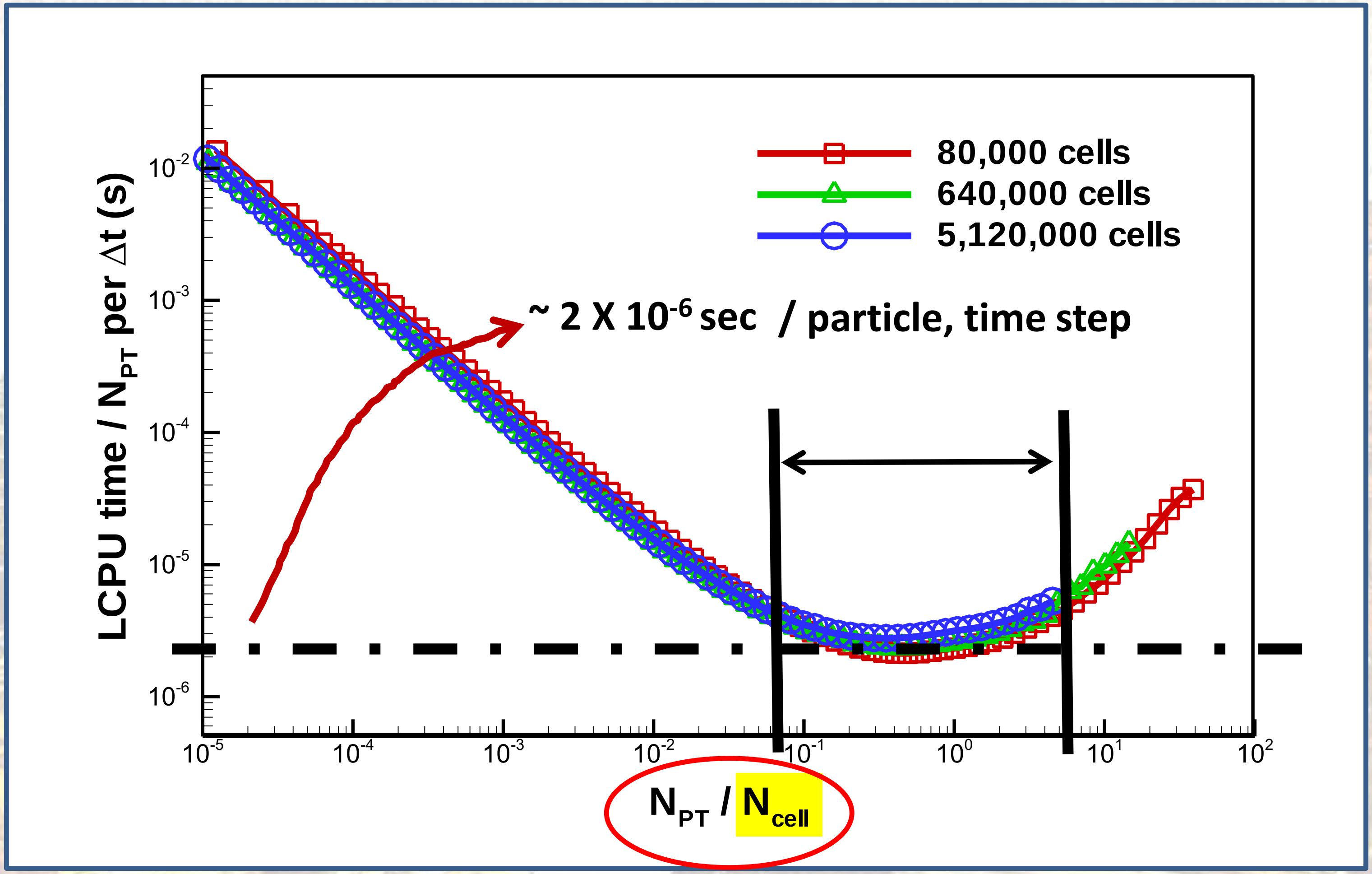
updating the carrier flow properties for each Lagrangian cell

solving the equations of motion for each particle & re-allocating the particles' indices in each Lagrangian cell

searching for the collision pairs in each Lagrangian cell




LCPU time / N_{PT} per Δt (s)
total number of particles (N_{PT})
(a)
80,000 cells
~ N_{PT}
~ N_{PT}^2
const.
(b)
640,000 cells
(c)
5,120,000 cells
LCPU time pre Δt (s)

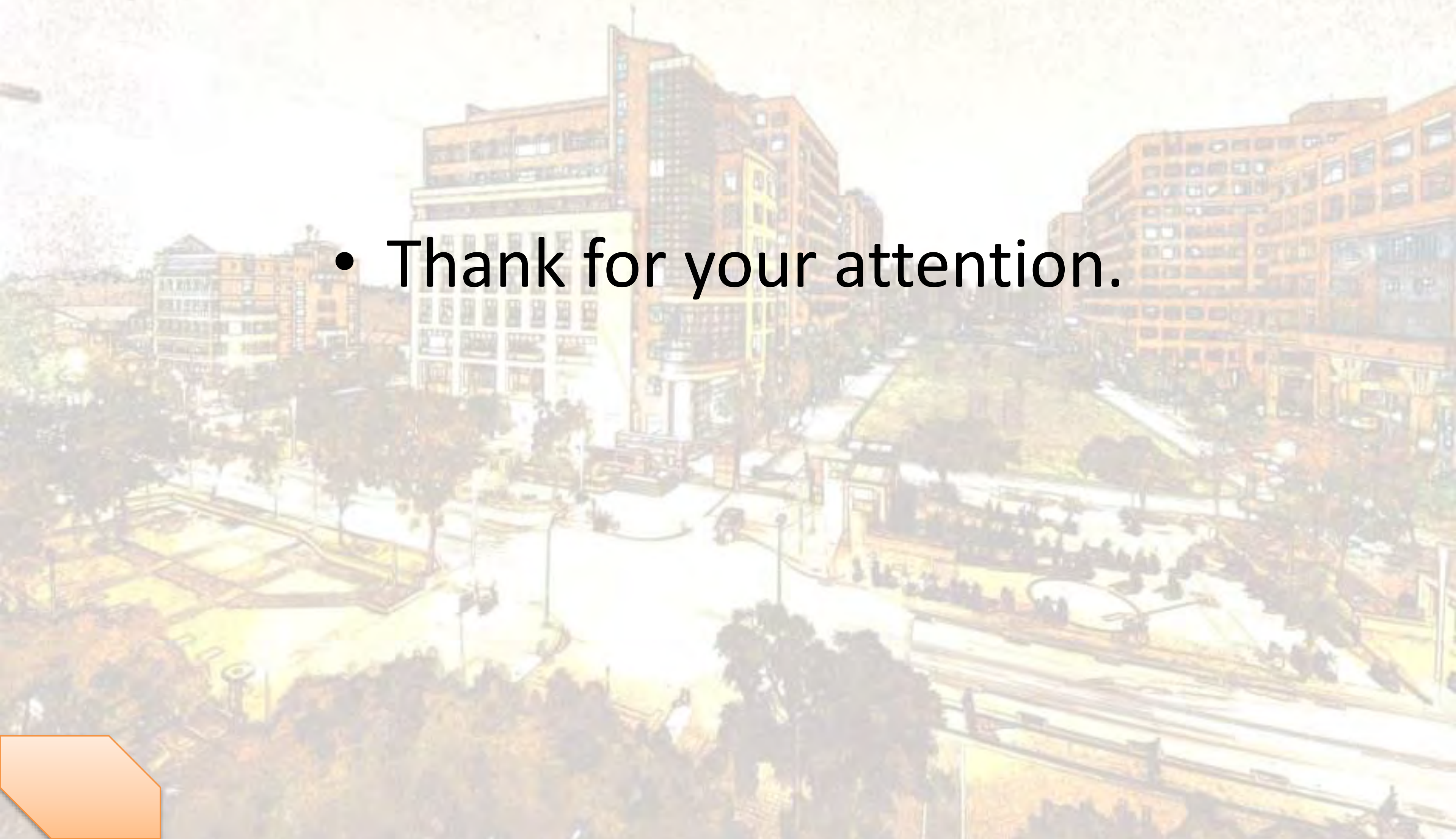


LCPU time / N_PT per Δt (s)
10^-2
10^-3
10^-4
10^-5
10^-6
80,000 cells
640,000 cells
5,120,000 cells
~ 2 X 10^-6 sec / particle, time step
10^-5
10^-4
10^-3
10^-2
10^-1
10^0
10^1
10^2
N_PT / N_cell

Concluding Remarks

- A cost-effective "link-list" algorithm which takes into account the search of inter-particle collisions in the particle tracking process is employed.

- Optimal computational efficiency in solving particles' motion together with inter-particle collisions can be obtained by generating the Lagrangian - cell system based on the criterion of $N_{PT} / N_{CELL} = O(10^0)$.



- Thank for your attention.