Modelling Dust Interactions Using a Fully Kinetic Numerical Framework

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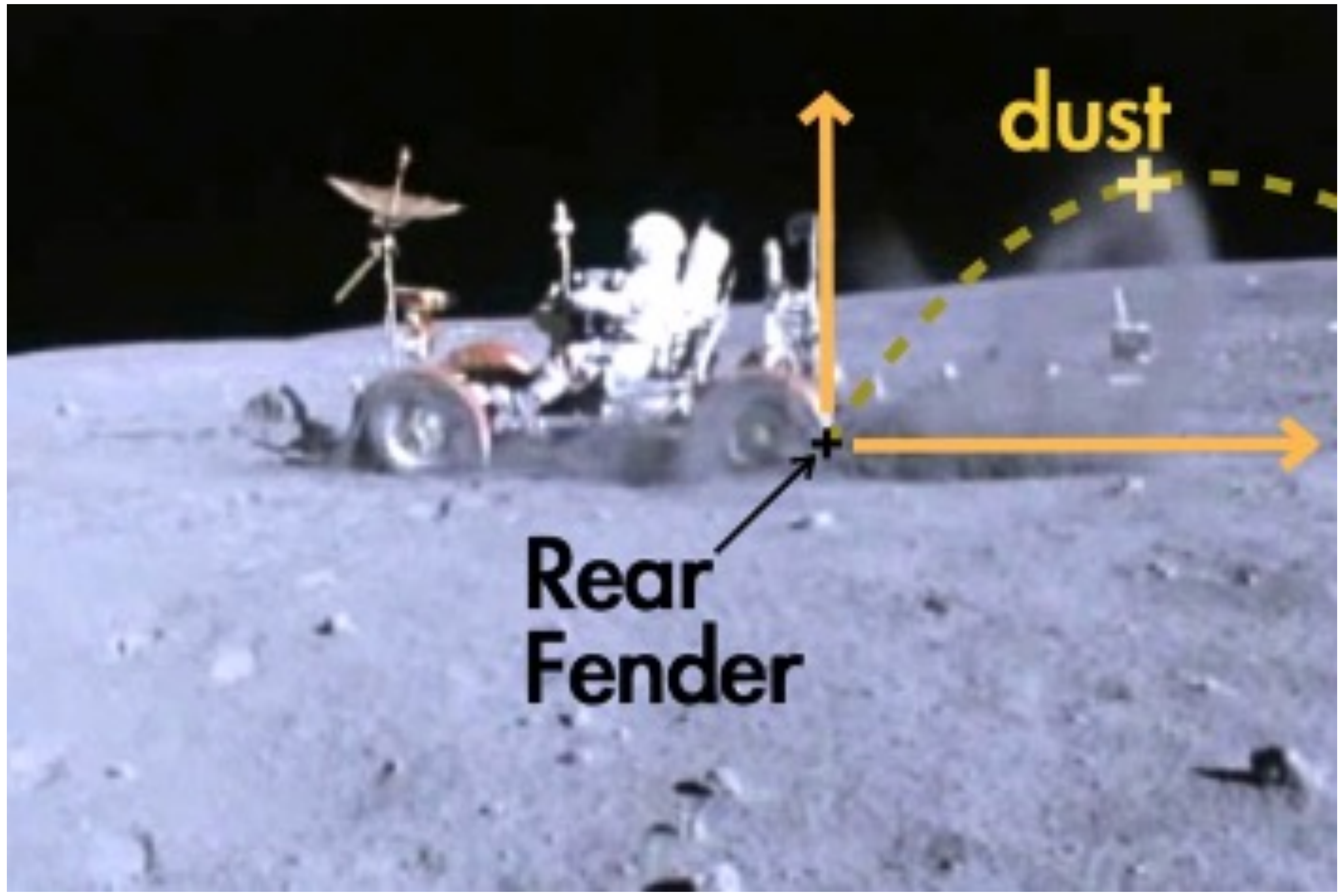
Dust Transport.

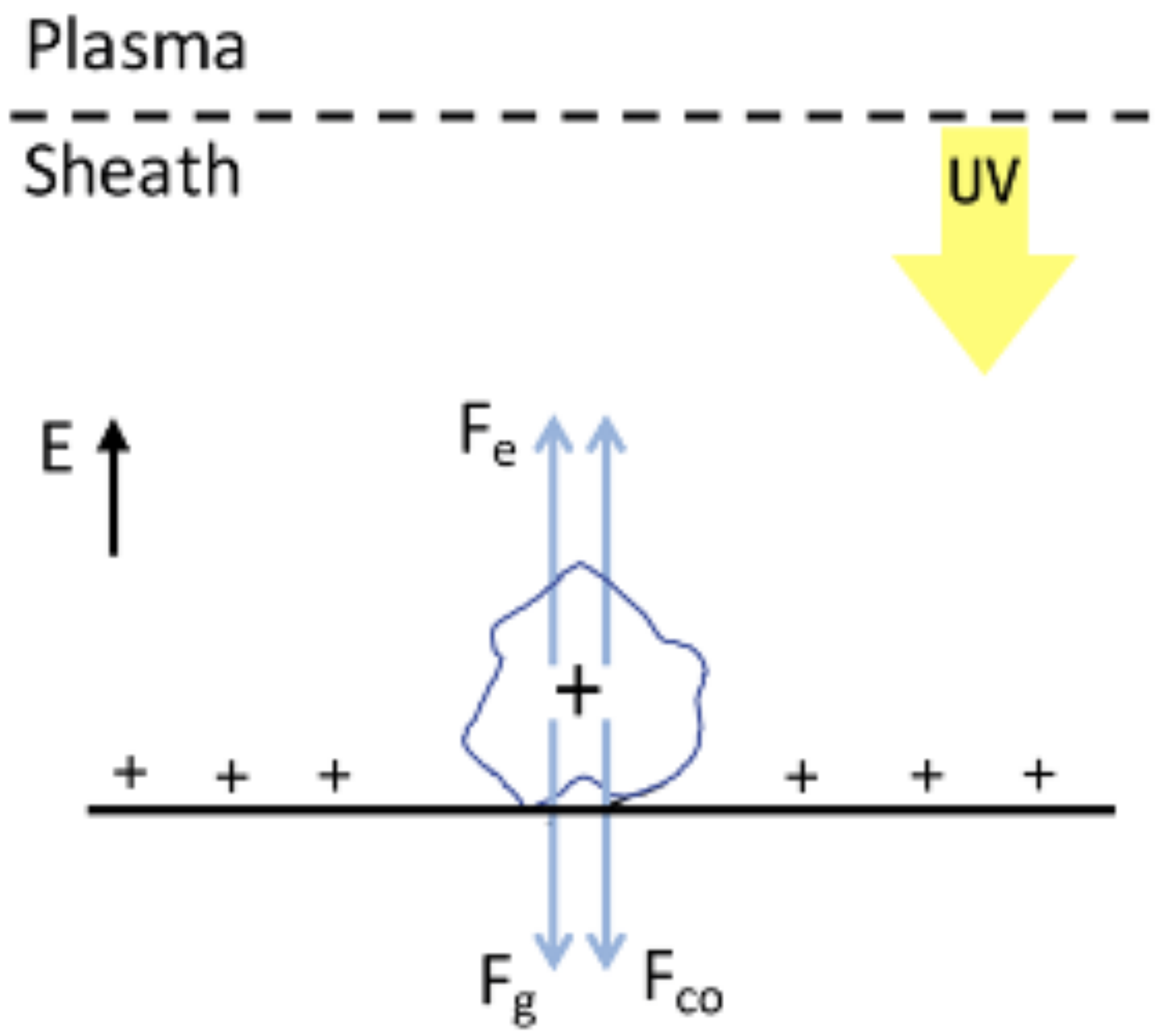
- Dust transport - driven by impacts, exposure to solar wind plasma and ultraviolet radiation - shapes the properties of the lunar regolith.
- Dust is also mobilised by human activities, representing both a technical and a health hazard.



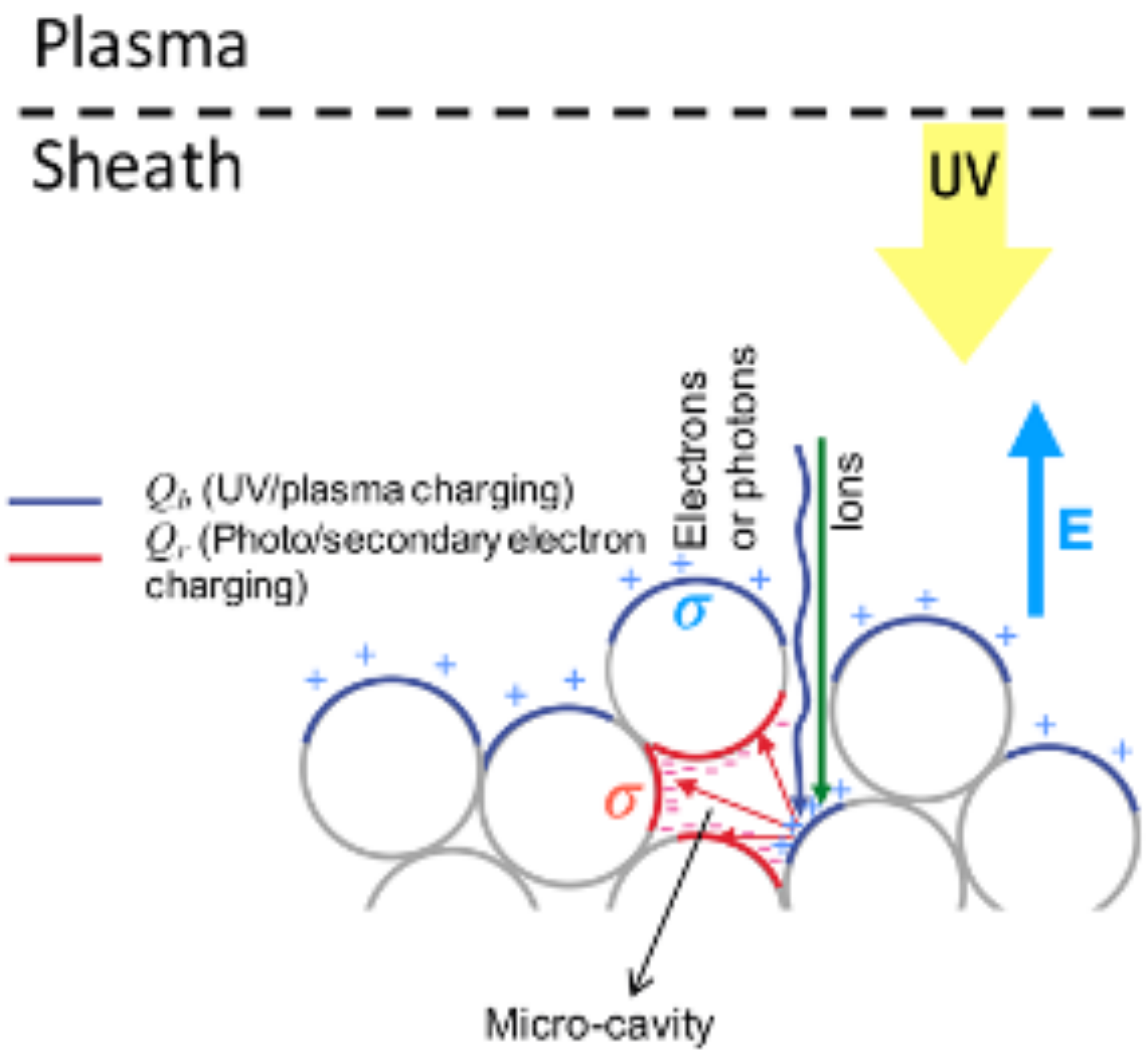
[Dust particles in the LRV trails; Hsu & Horányi 2012]

[Lunar Horizon Glow; Criswell 1973]

Grain Charging on a Surface.



Conventional view



Patched Charge Model
[Wang et al. 2016; Schwan et al., 2017]

Lofting Criterium: $Q_dE = F_e + F_c > F_g + F_{co}$

Modeling Dust Dynamics.

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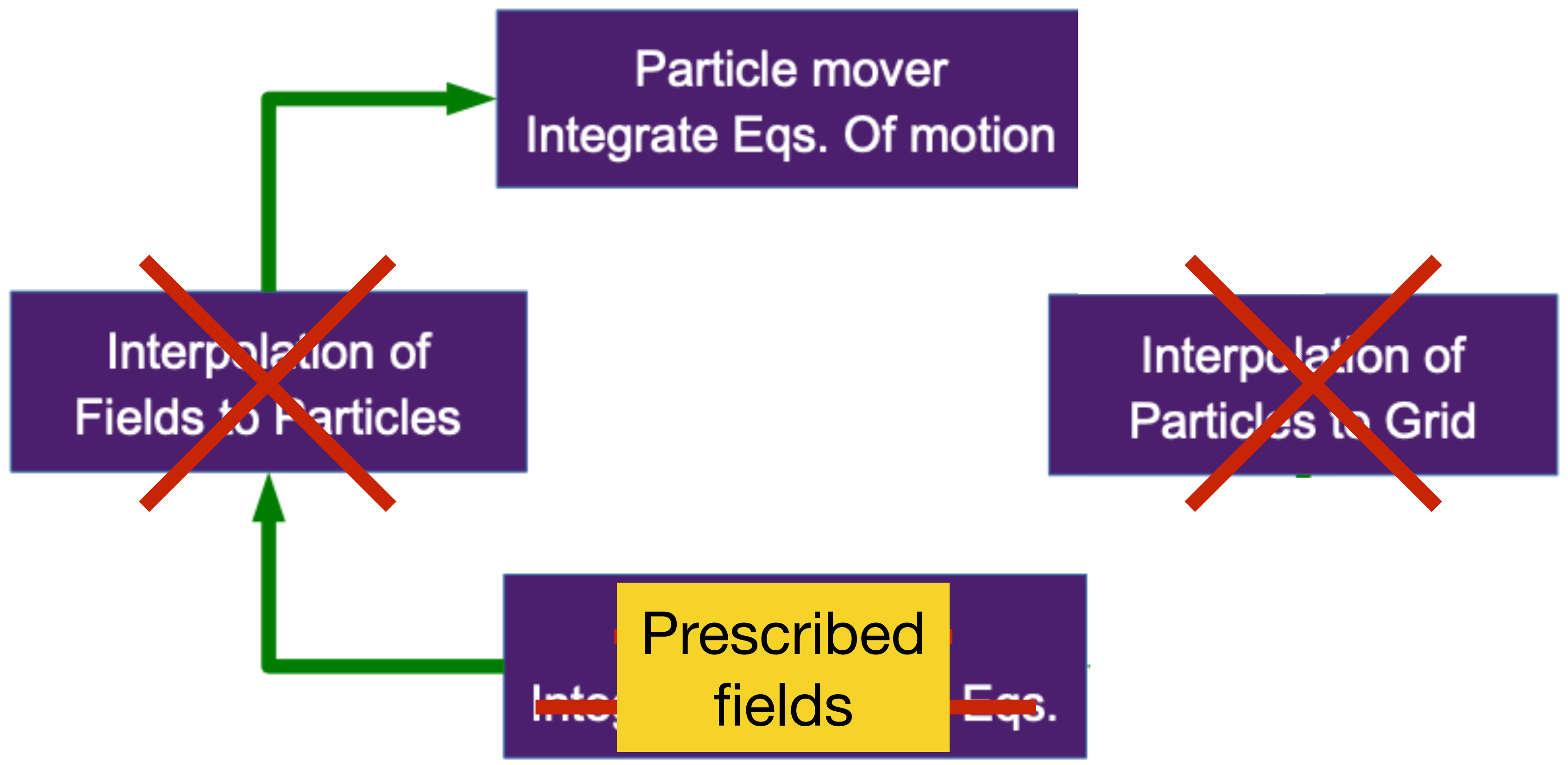
- *From a numerical/modelling point of view*, the current capabilities to study the dynamics of grain-scale charging processes and their interactions are limited due to the need to *self-consistently* merge several orders of magnitude in length and time scales.
    - **Test-particle models**.

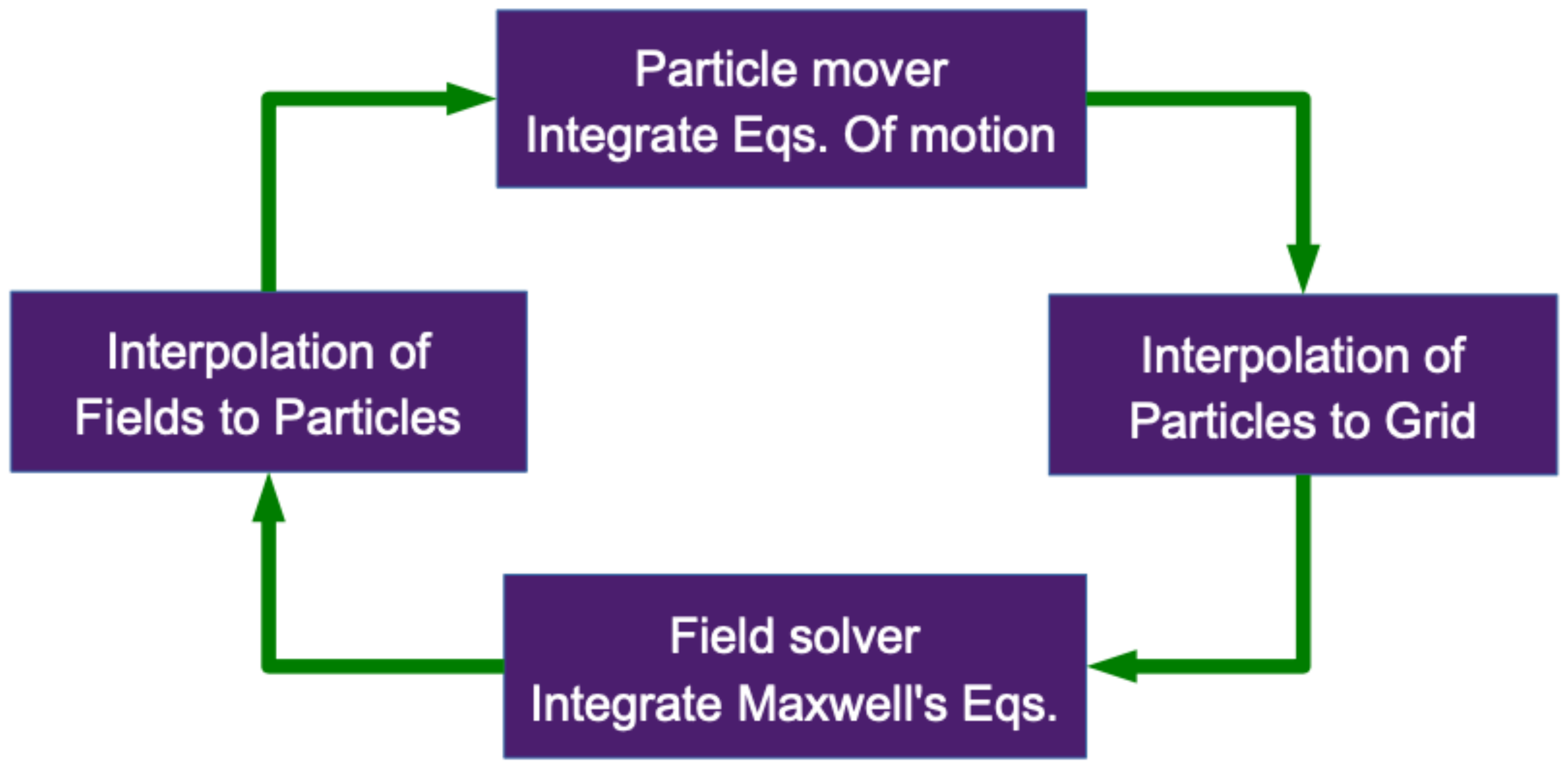
    (Major drawback: no feedback mechanism is implemented between the particle-generated and the external electromagnetic fields.)

    - **Particle-in-cell models**.

    (Major drawback: needed computational resources skyrocket quickly due to the need to resolve Debye scales.)



Test-particle approach



Particle-in-cell approach

Modeling Dust Dynamics.

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- *From a numerical/modelling point of view*, the current capabilities to study the dynamics of grain-scale charging processes and their interactions are limited due to the need to self-consistently merge several orders of magnitude in length and time scales.
  - **Test-particle models**.

  (Major drawback: no feedback mechanism is implemented between the particle-generated and the external electromagnetic fields.)
  - **Particle-in-cell models**.

  (Major drawback: needed computational resources skyrocket quickly due to the need to resolve Debye scales.)

- *No framework currently exists that provide a clear path from the grain-scale mechanism responsible for lofting/ removing a dust particle from a regolith surface to an operational environment to develop and test the effectiveness of dust mitigation techniques.*

Theory and Simulation.

- **Objective**

  Develop a framework of numerical models that couple the microphysics of grain-scaled processes with the self-consistent solution of the near-surface plasma environment.

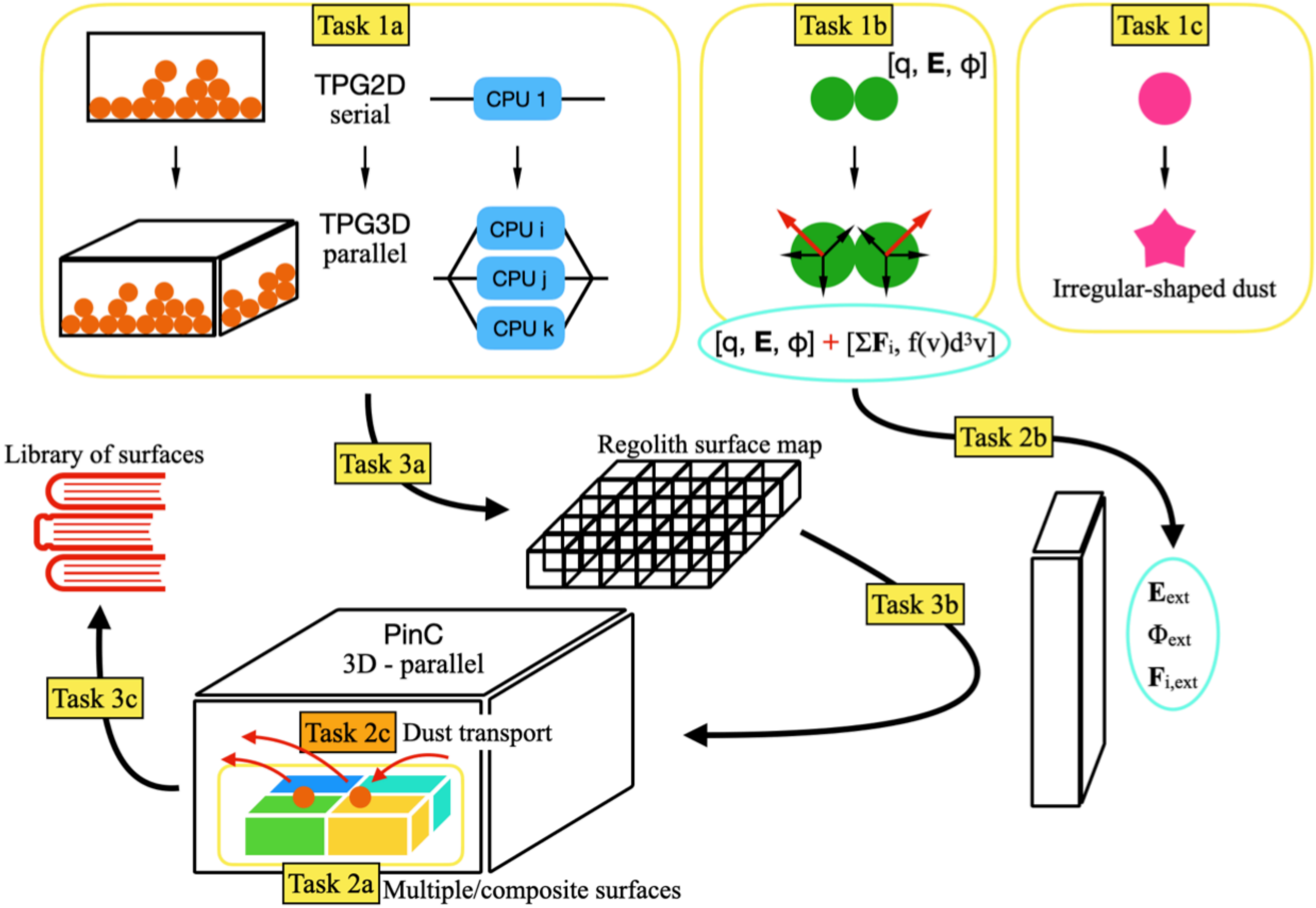
- **Impact/Innovation**

  The proposed framework will be used to merge the qualitative understanding of the microscopic processes to the macroscopic behaviour of the lunar regolith, providing a much-needed tool to advance the effectiveness of dust mitigation techniques.

- **Approach**

  We equip a basic particle-particle and a particle-in-cell code with a comprehensive multi-physics model and the necessary code-coupling mechanisms.

Modelling Approach.



Modelling Approach.

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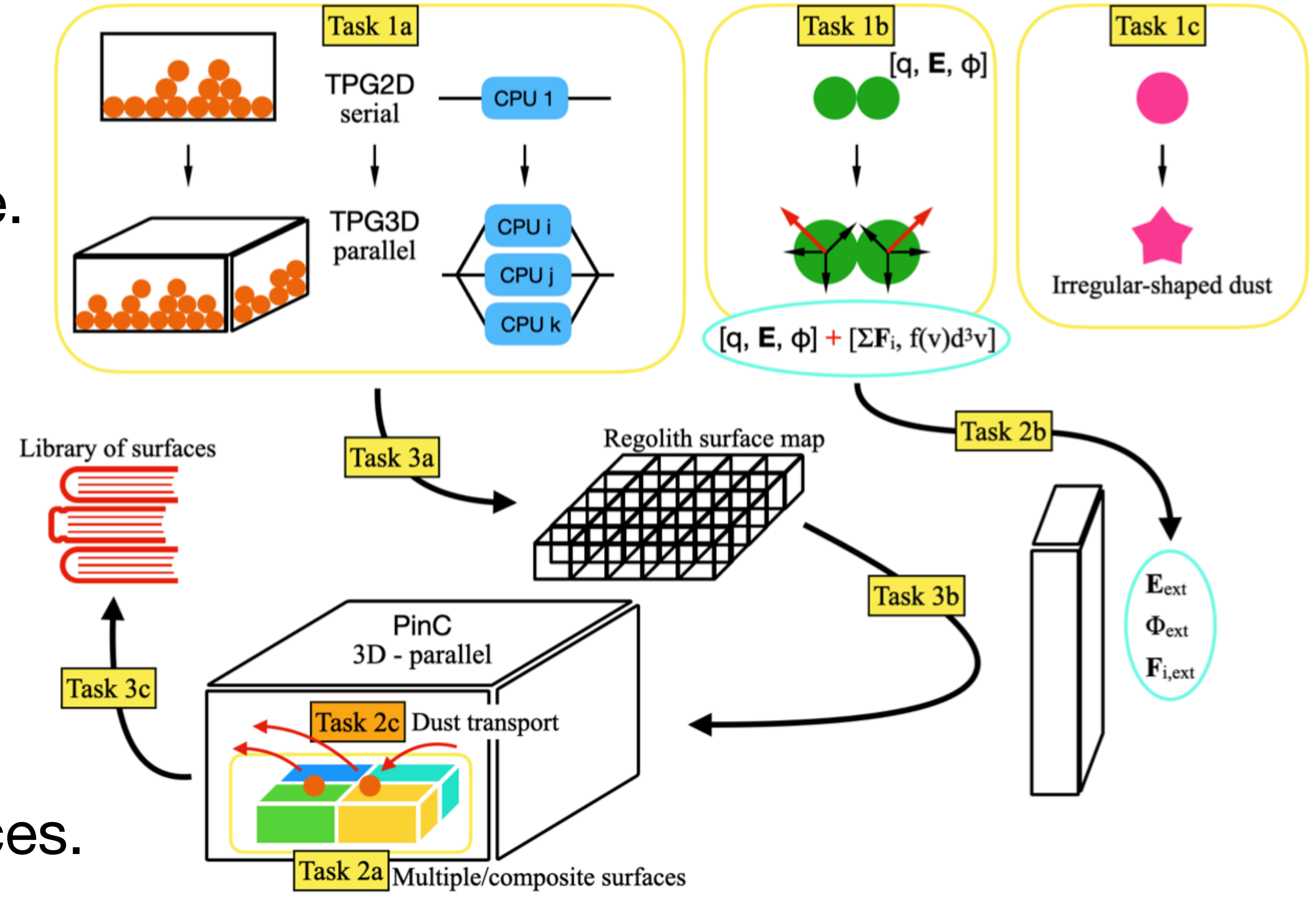
- Task 1 (TPG2D→TPG3D):
  a. Expand the numerical model from 2D to 3D and parallelise the code.
  b. Develop a force-balance model, including cohesion, adhesion, and microgravity effects.
  c. Develop the option to include non-spherical, irregular-shaped dust particles.
- Task 2 (PinC):
  a. Expand the model to include multiple and composite objects/surfaces.
  b. Develop the option for prescribed electromagnetic fields and secondary particle effects.
  c. Develop a dust-kinetic model to evaluate dust transport phenomena.
- Task 3 (Code coupling):
  a. Provide a mapping structure that merges the TPG3D components into a surface.
  b. Develop the code structure in PinC to load TPG3D regolith mapping structures.
  c. Build a library of realistic regolith surfaces.



TPG3D.

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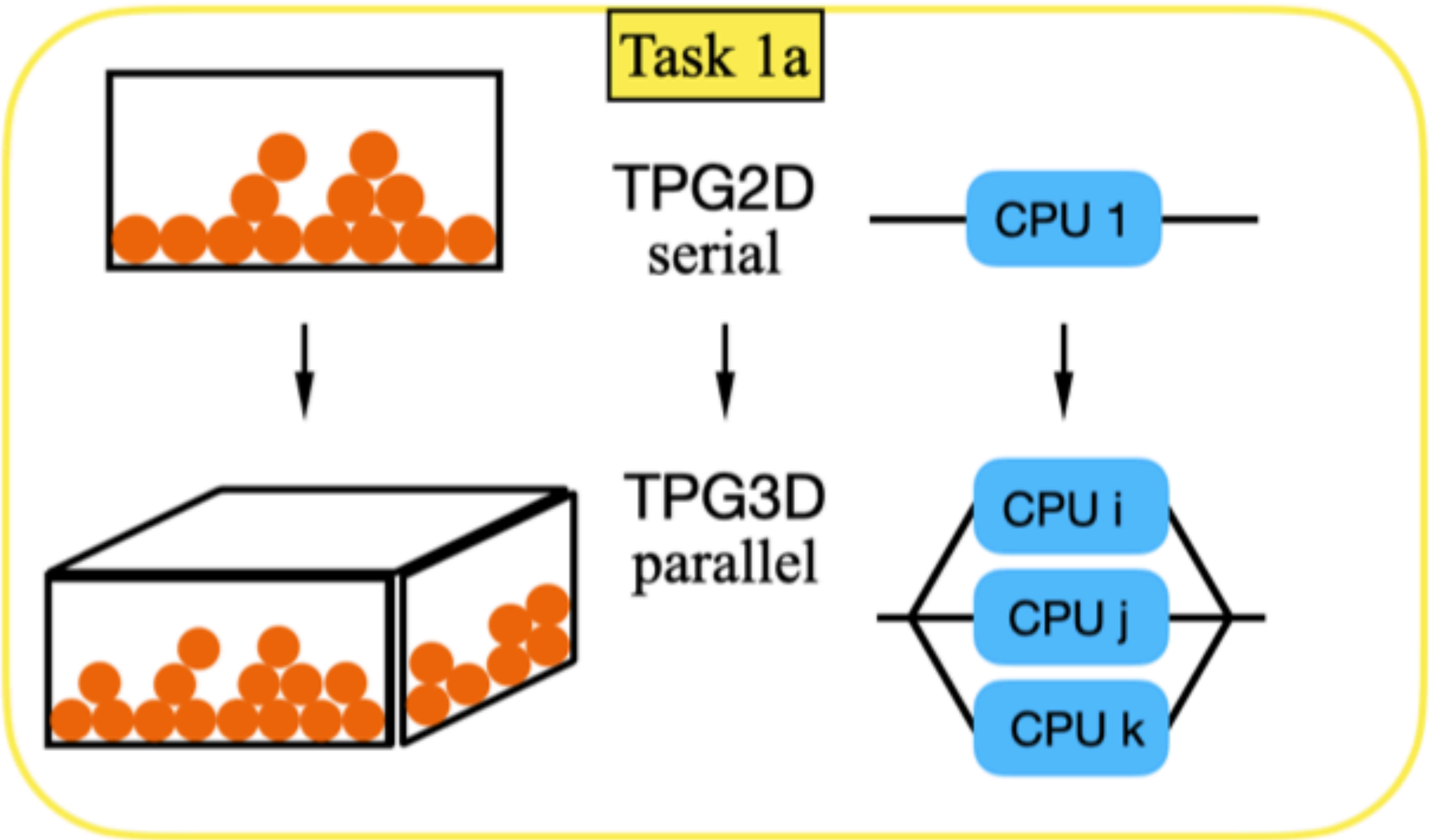
- Parallelisation.
  - OpenMP approach (shared memory).
    - No major redesign needed.
    - Limits the code to run within one computing node.
  - MPI approach (distributed memory).
    - Major redesign needed.
    - No limit on the amount of computing power that can be used. (apart from overhead considerations).



- **Major hurdle:** TPG's computational cycle implements the Barnes-Hut tree algorithm (i.e., a reduction operation). Parallelisation is therefore not efficient at the root level.

Barnes-Hut tree algorithm.

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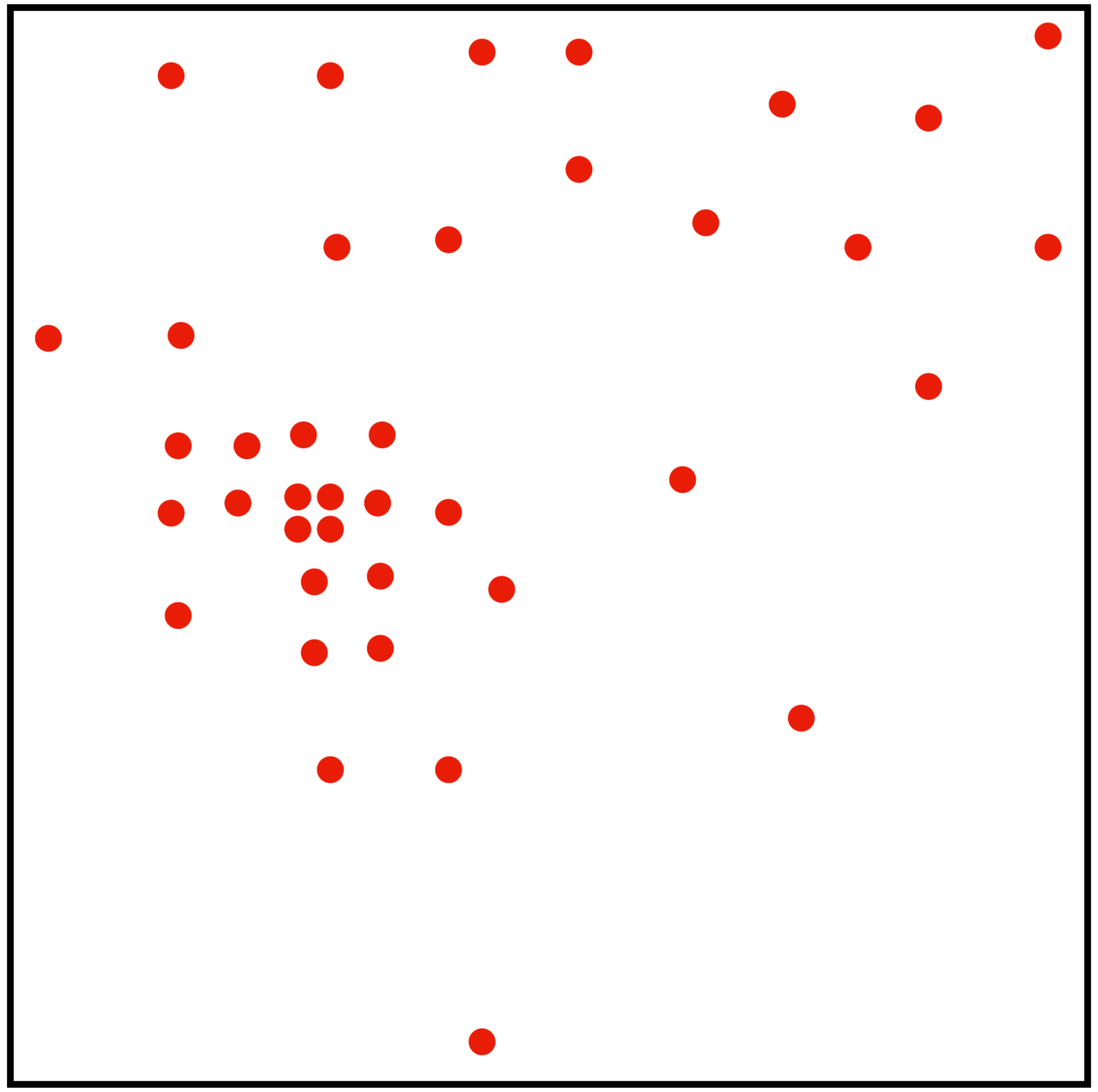
- Approximation algorithm designed for n-body simulations.
  - No fixed grid, so not bound by CFL constraints.



Barnes-Hut tree algorithm.

- Approximation algorithm designed for n-body simulations.
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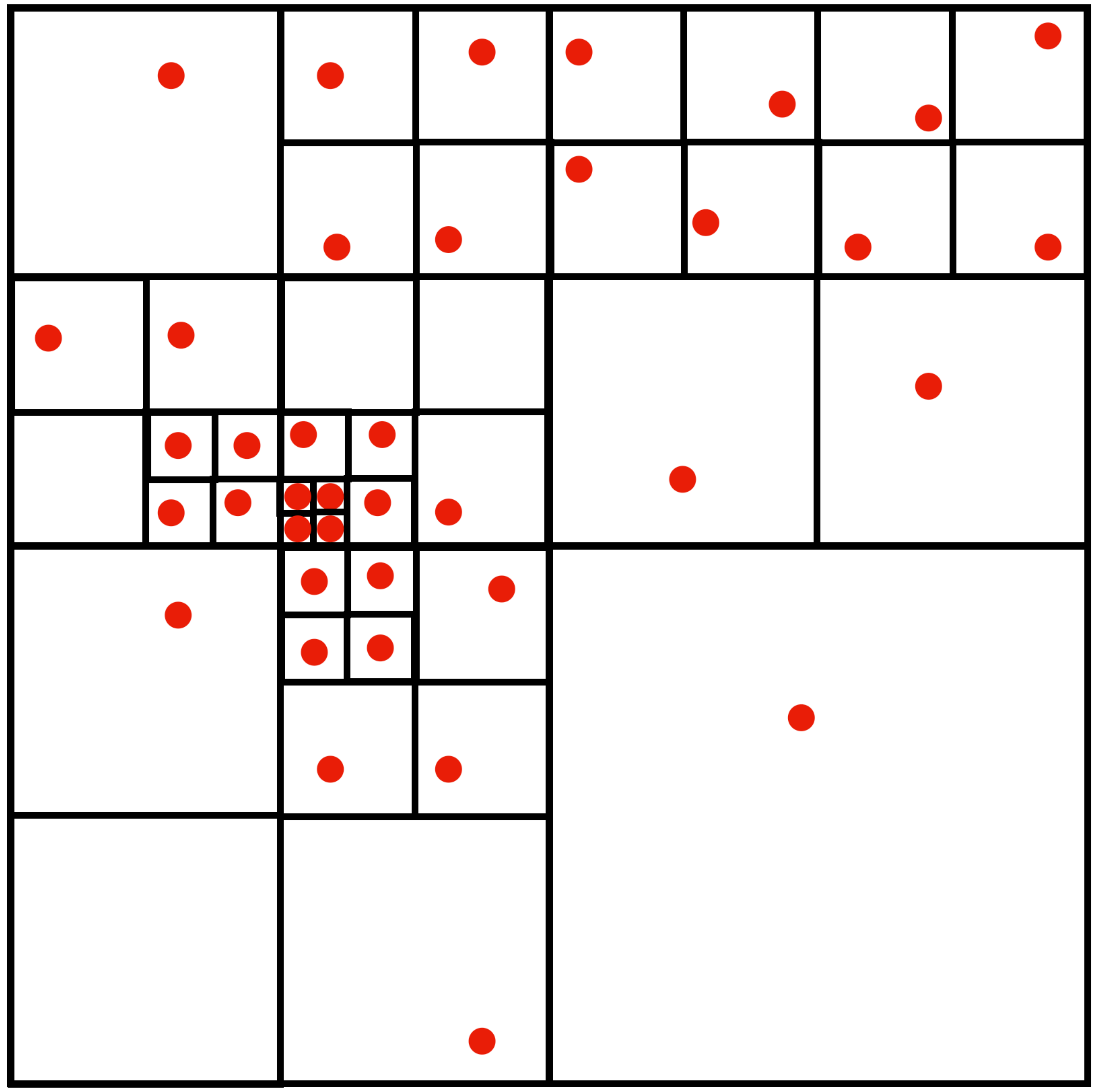
  - Divisions are constructed depending on particle/surface segment density.



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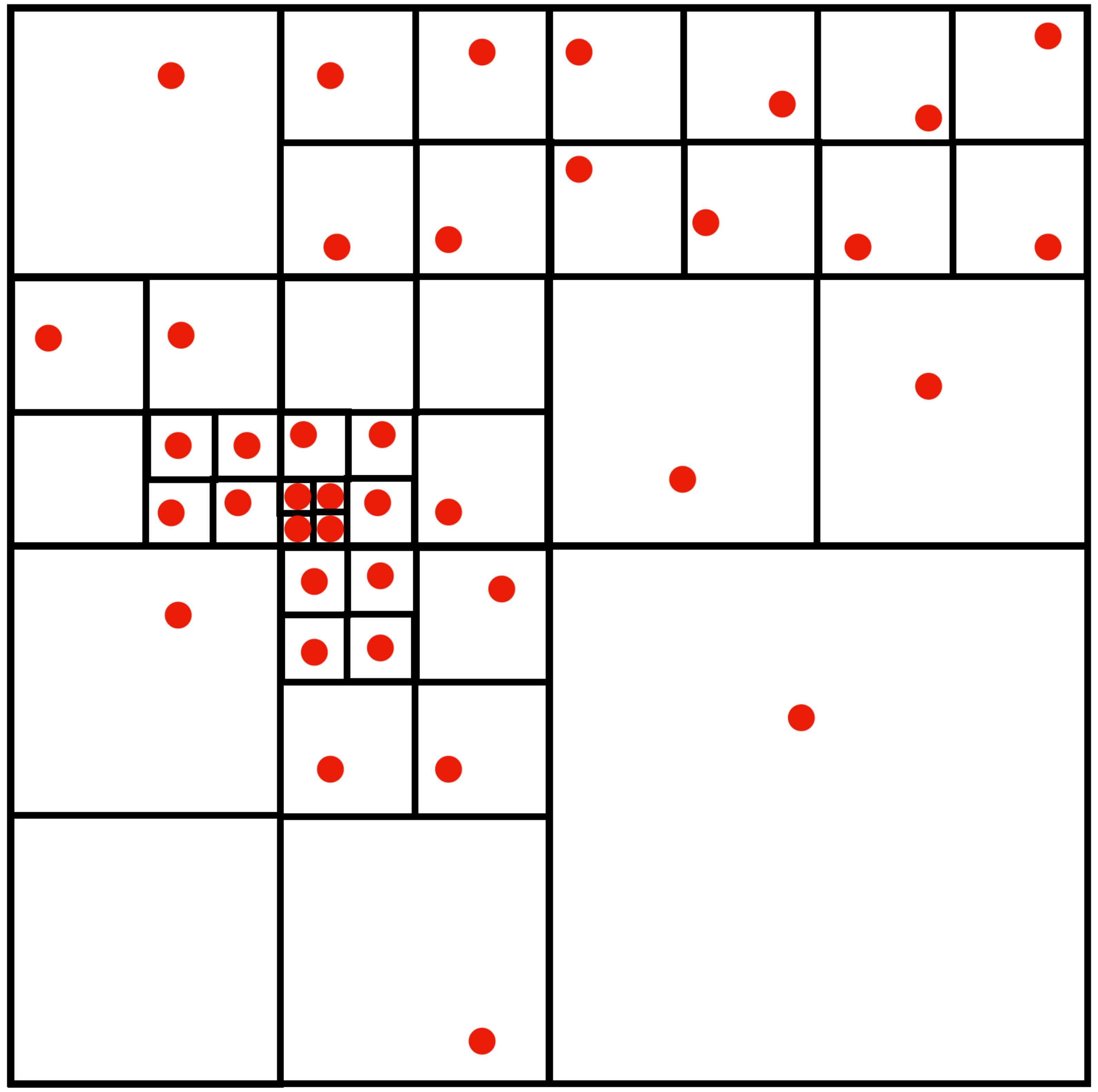

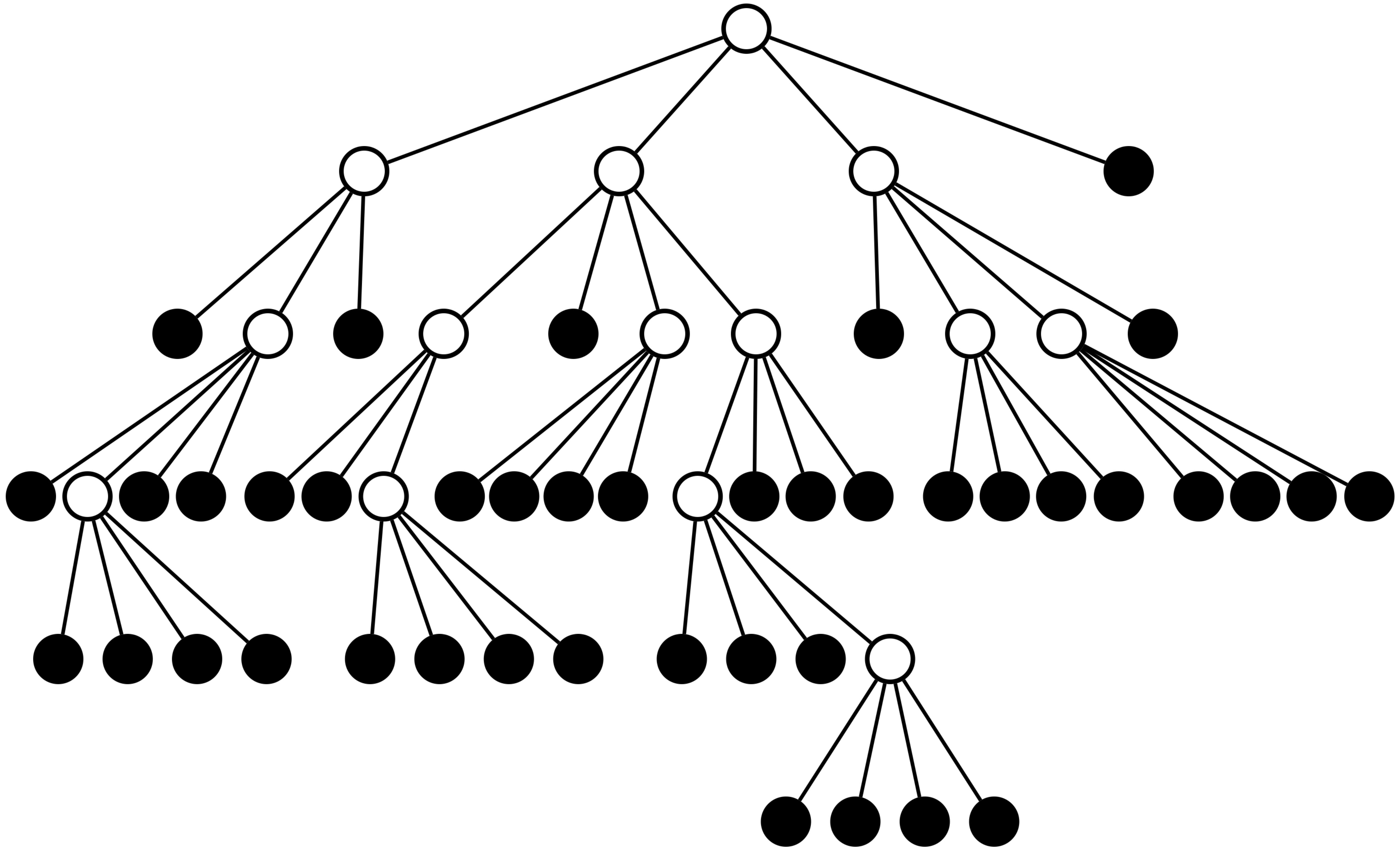

Barnes-Hut tree algorithm.

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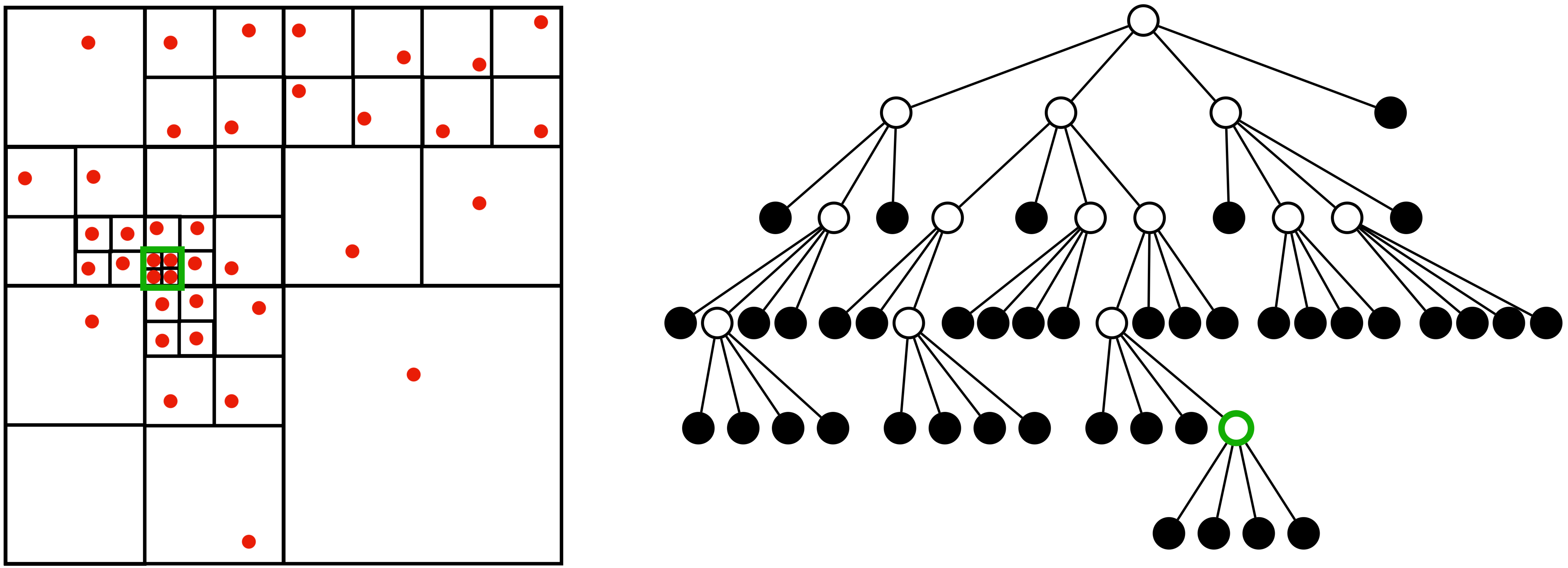
- Approximation algorithm designed for n-body simulations.
  - Divisions are constructed depending on particle/surface segment density.
  - Short range interactions, use brute force, i.e., Coulomb's Law.



Barnes-Hut tree algorithm.

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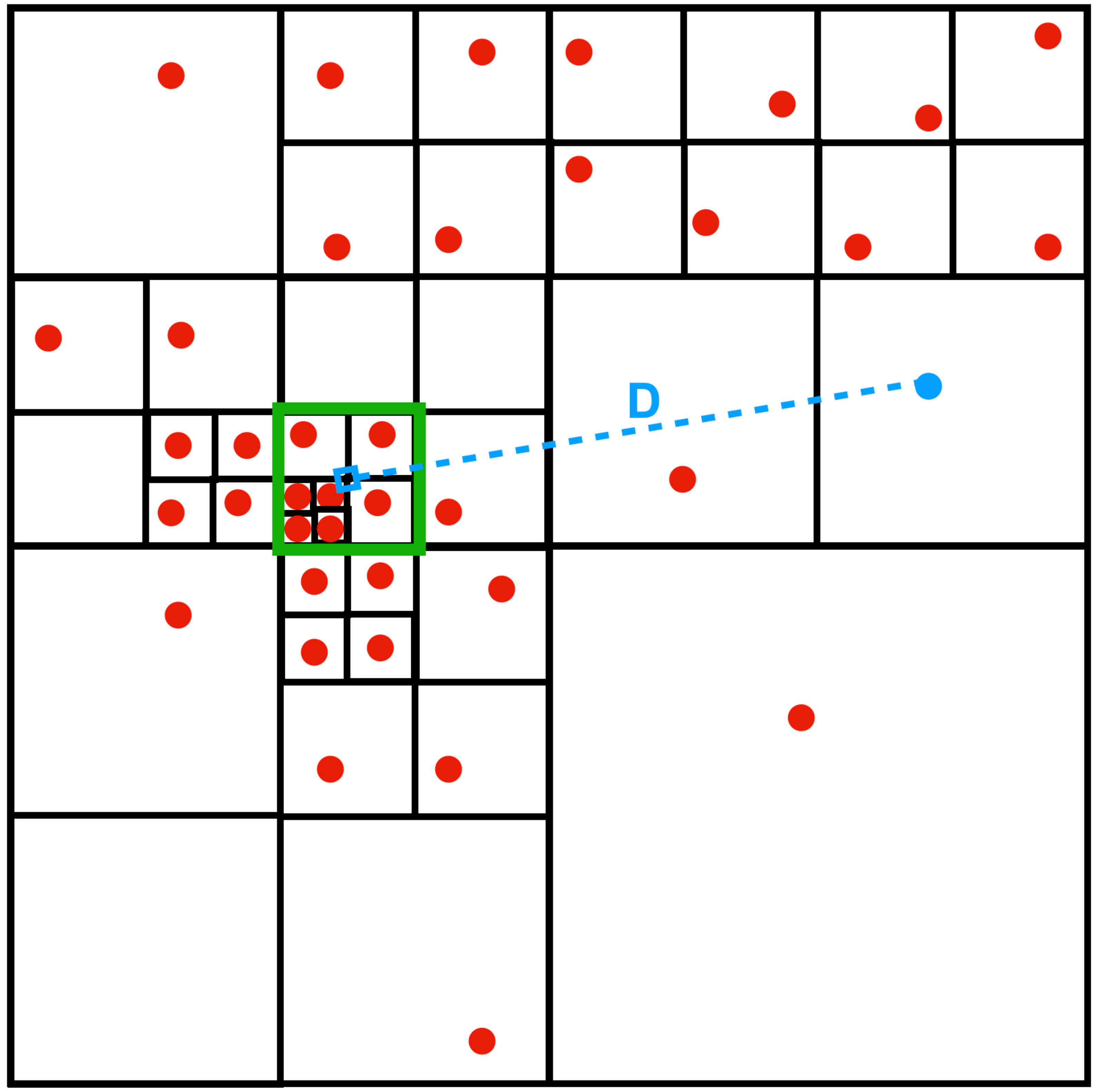
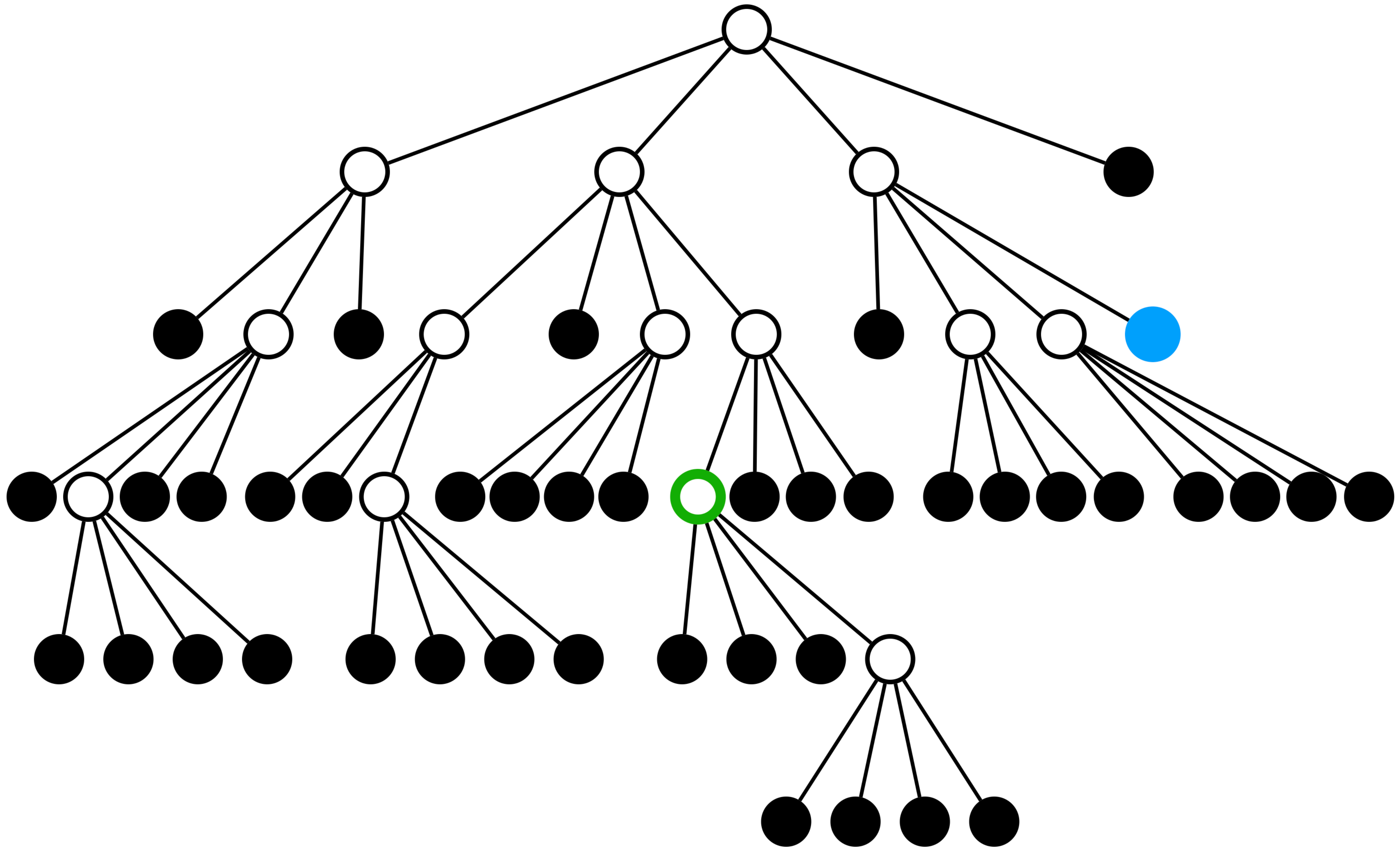
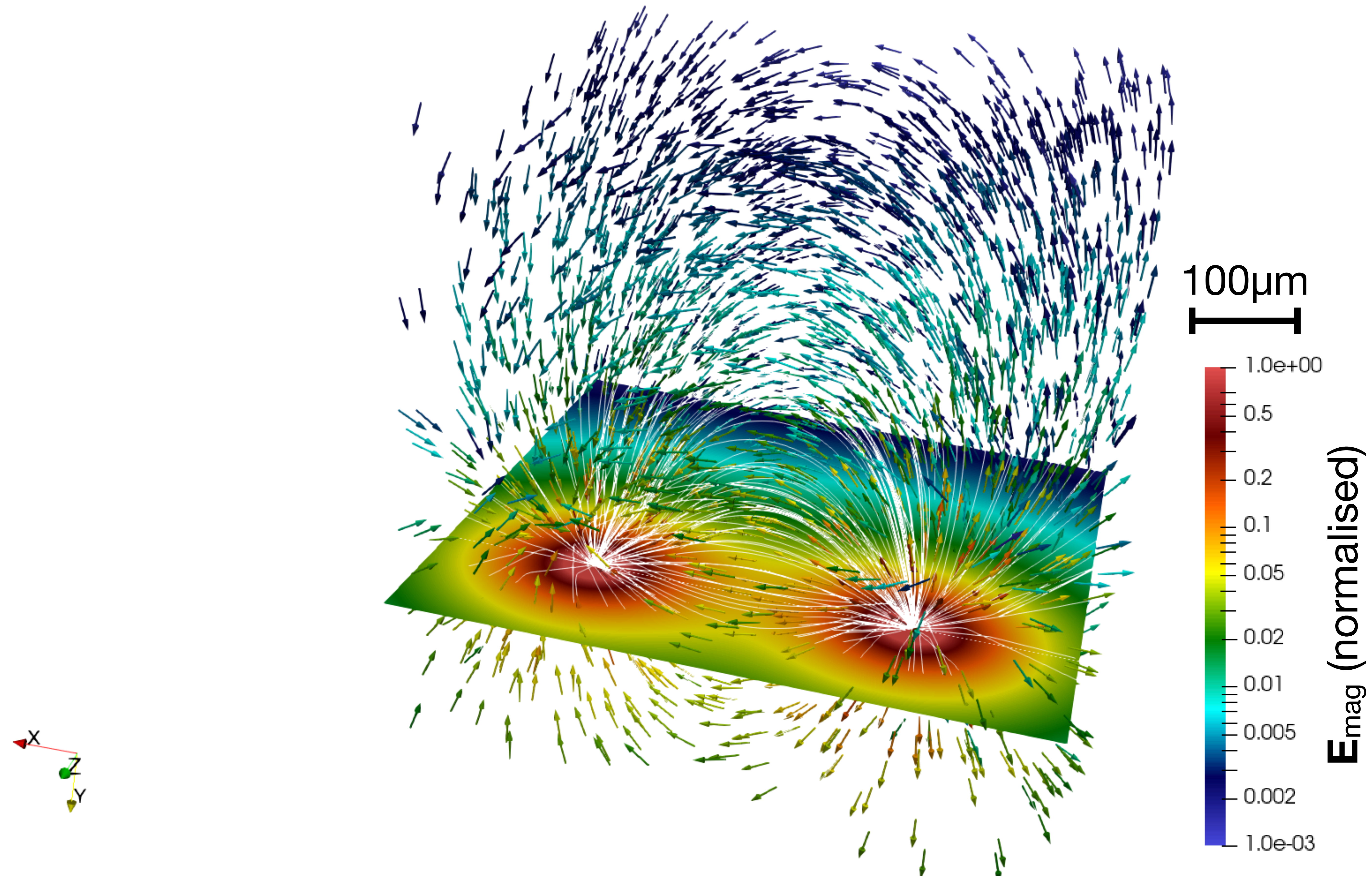
- Approximation algorithm designed for n-body simulations.
  - Divisions are constructed depending on particle/surface segment density.
  - Long-range interactions, use multipole expansion.





Barnes-Hut tree algorithm.

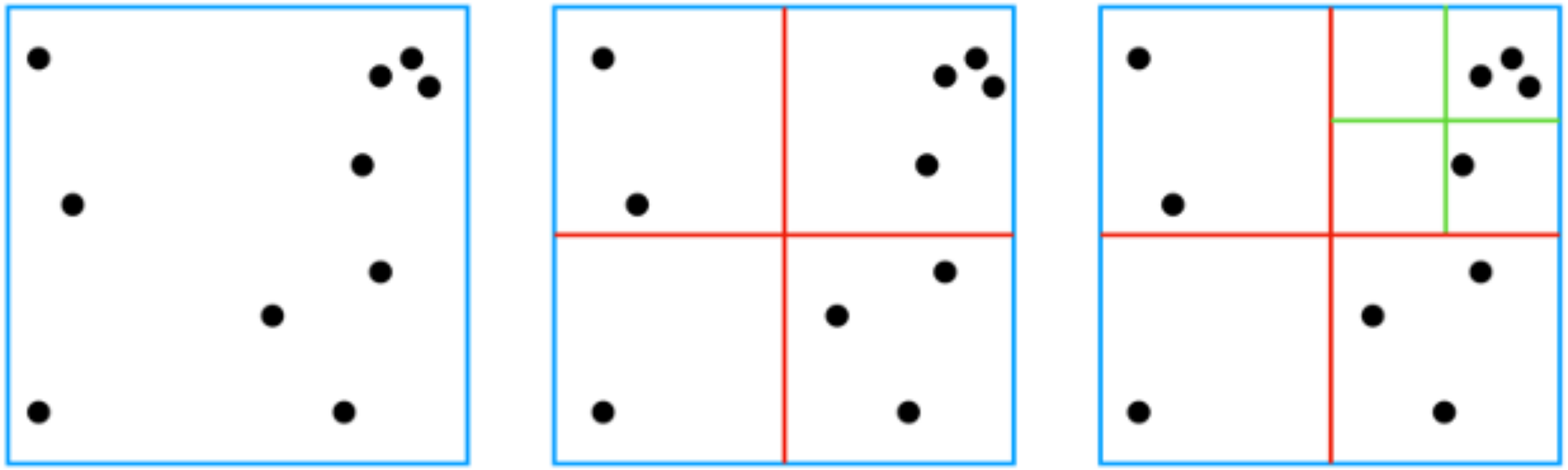
- **Key Points:**
  - Correct electric field values computed.
  - Smooth transition between the 'brute force' and multipole part of the solver.



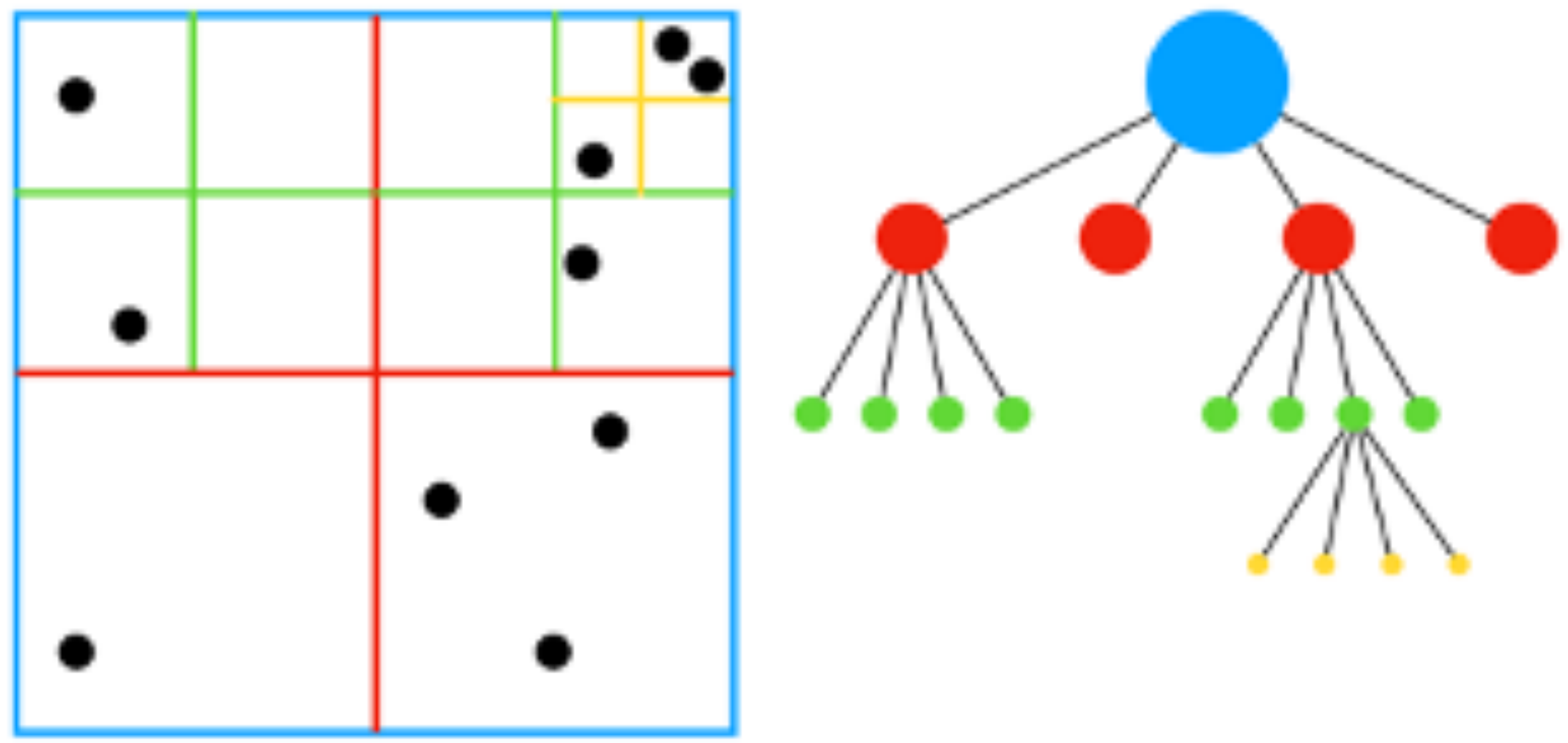
Parallelisation.

- **Paradigm:**
  - Every MPI thread/CPU is responsible for a specific part of the computational domain, i.e., domain decomposition (temporary solution).
  - Every MPI thread/CPU corresponds to at least one leaf of the Barnes-Hut tree.

- **Key Point:**
  - Plasma particles are distributed, grain information is 'global.'



Parallelisation.



<u>2D example, assume 16 CPUs.</u>

1 leaf, all CPUs perform the same work.

4 leaves, 2 CPUs perform the same work.

16 leaves, no CPUs perform the same work.

64 leaves, CPUs handle more than 1 leaf.

- **<u>In practice:</u>**
  - After a few computational cycles, you always end up in the scenario.
  - This approach allows for the MPI and particle reduction operation to run in unison.

Particle Shapes

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- **Design decisions:**
  - Keep grain information 'global' to reduce complexity.
  - Standalone input file for irregular volumes.
  - Mesh refinement to obtain preferred resolution.

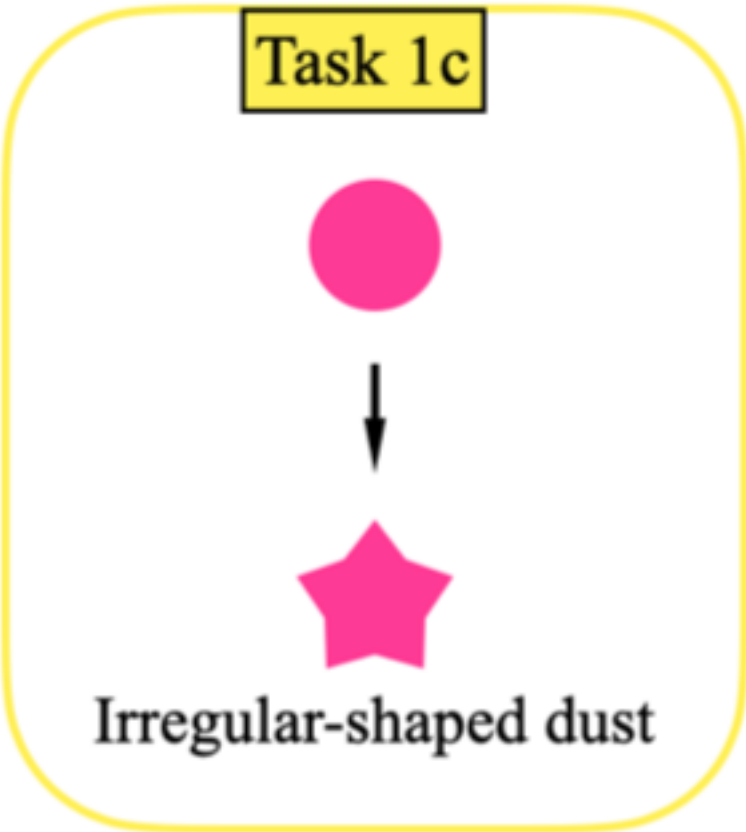
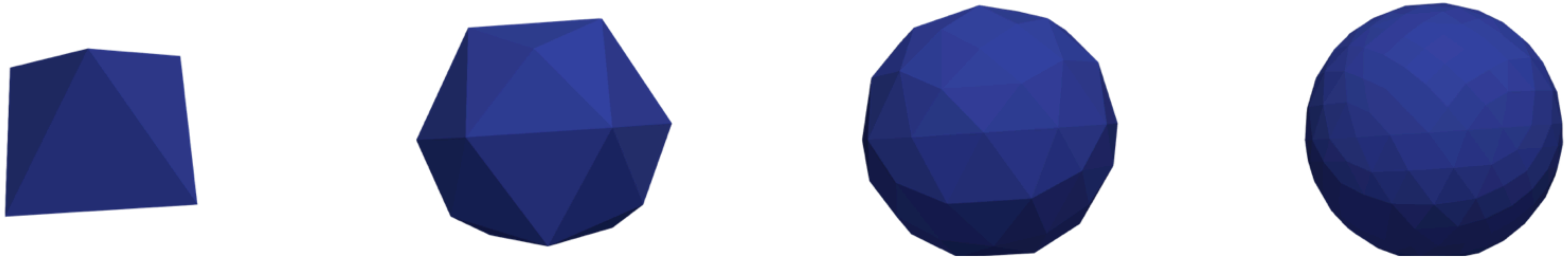
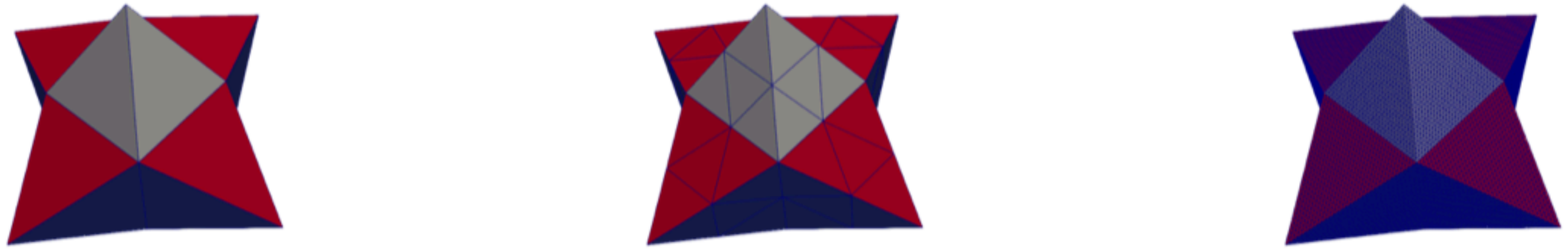


Illustration of the mesh refinement for spherical and irregularly shaped dust grains.



Refine = 0 Refine = 1 Refine = 2 Refine = 3



Refine = 0 Refine = 1 Refine = 5

Particle Shapes

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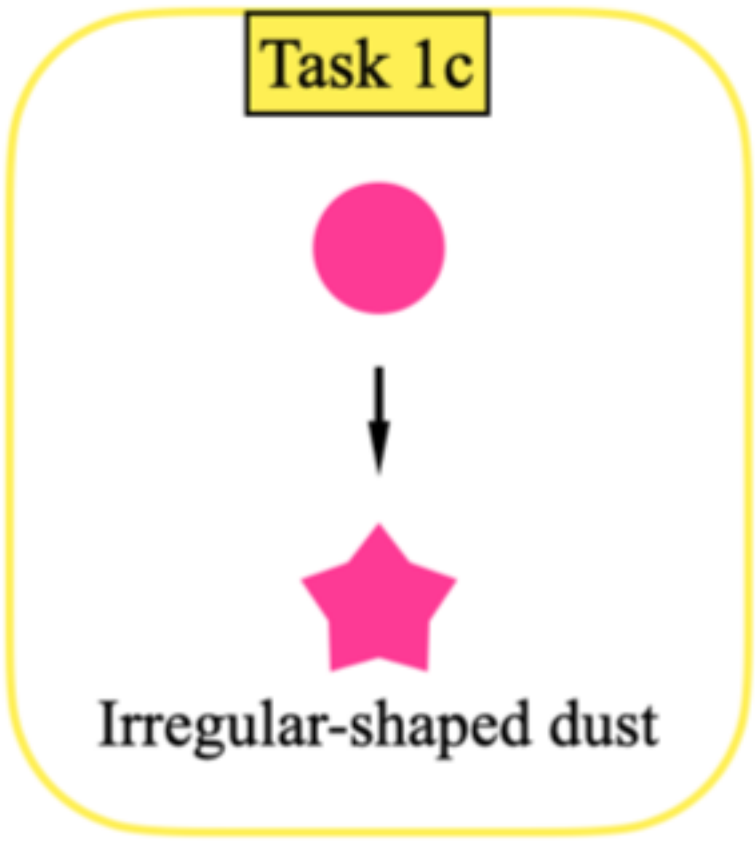
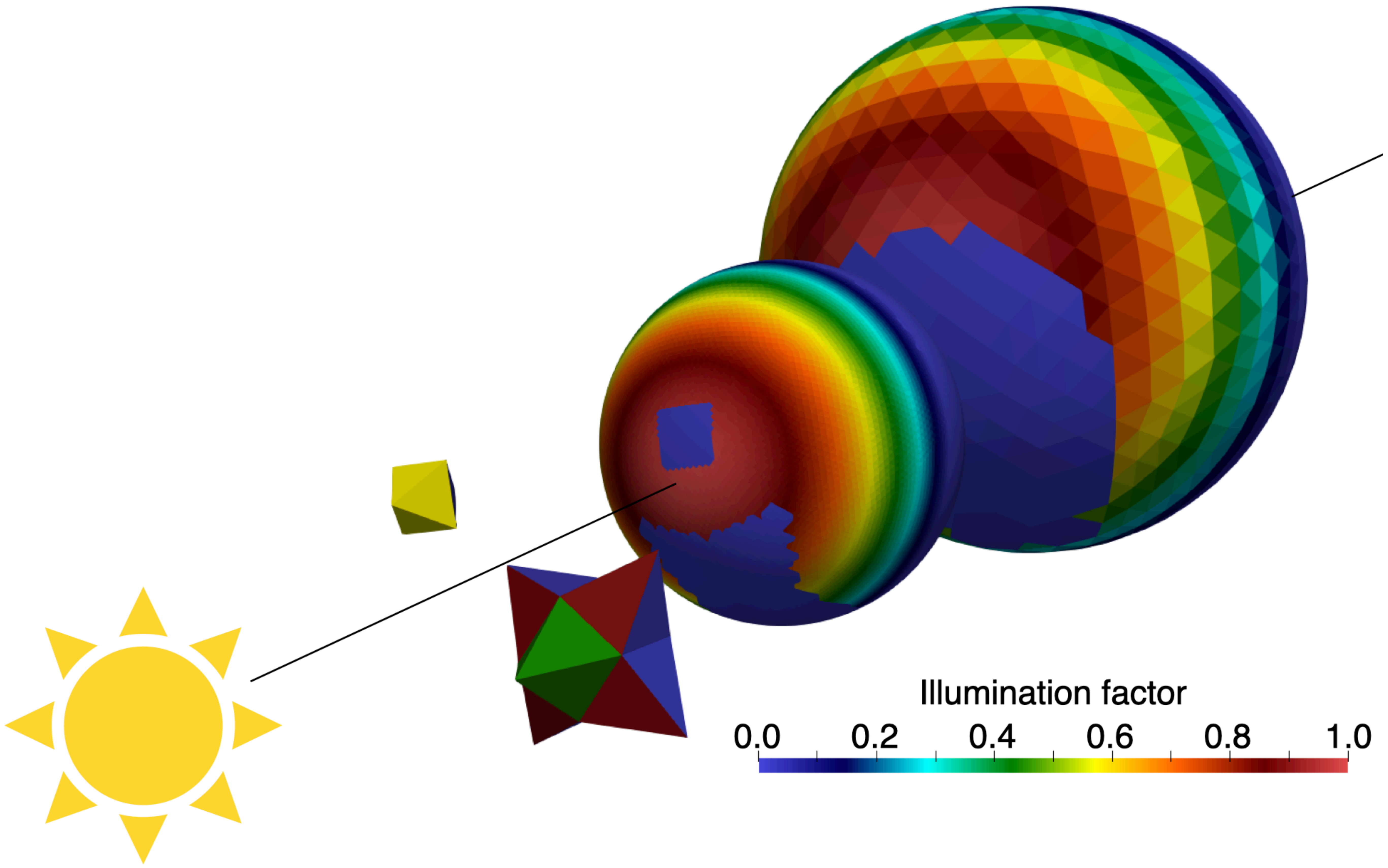
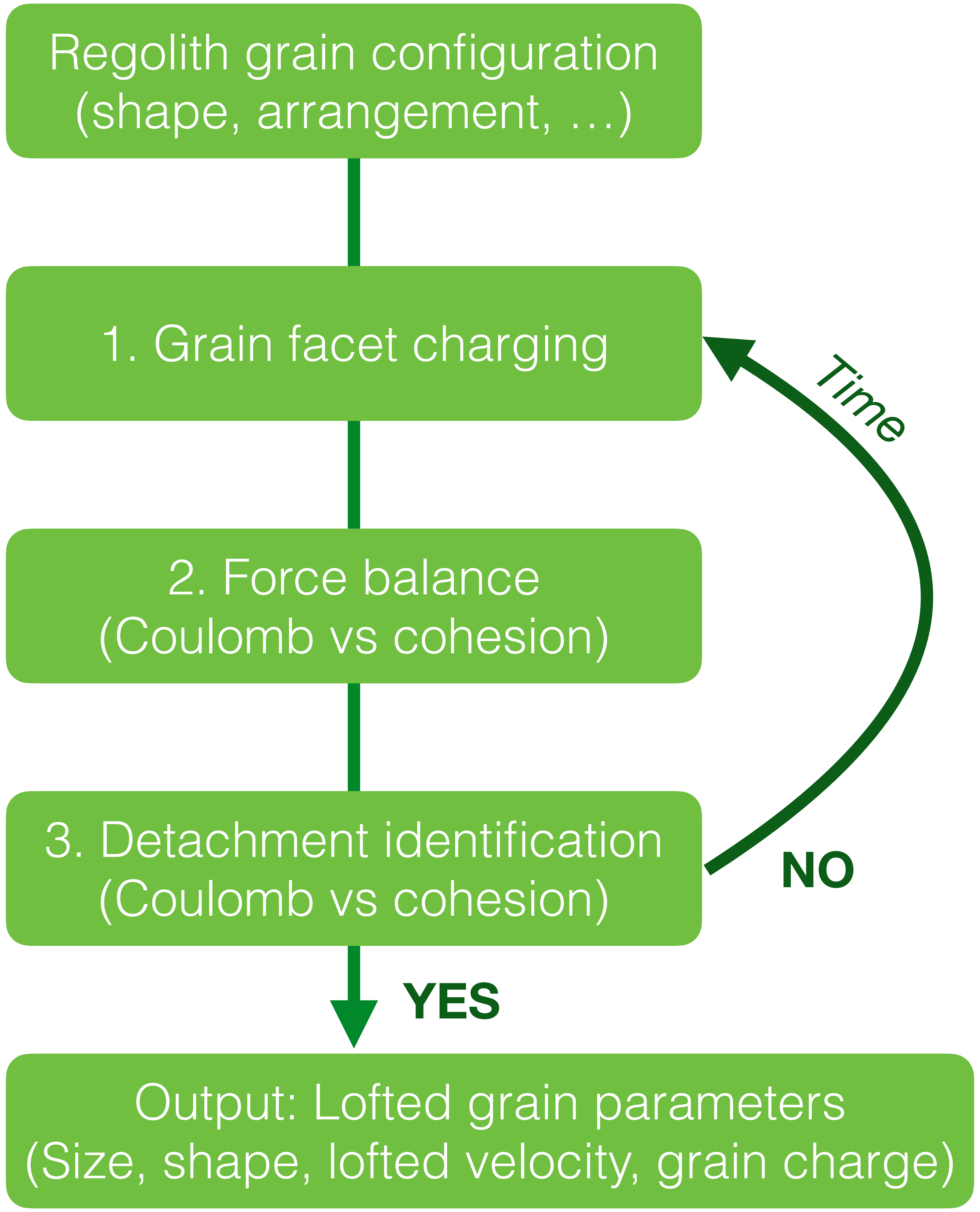
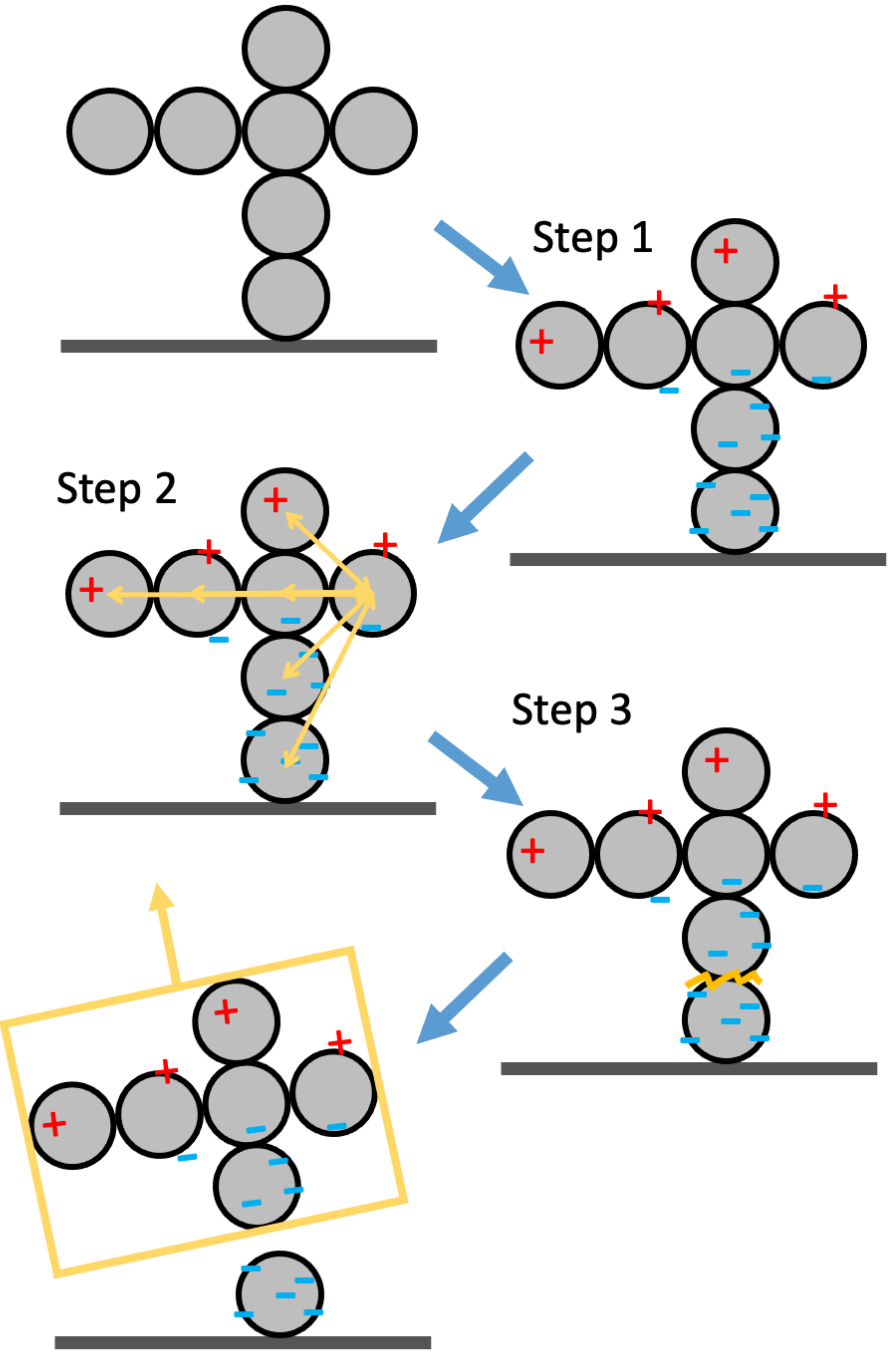
- **<u>Design decisions:</u>**
  - Mesh refinement to obtain preferred resolution.
  - Raytracing to obtain grain illumination/shadowing.

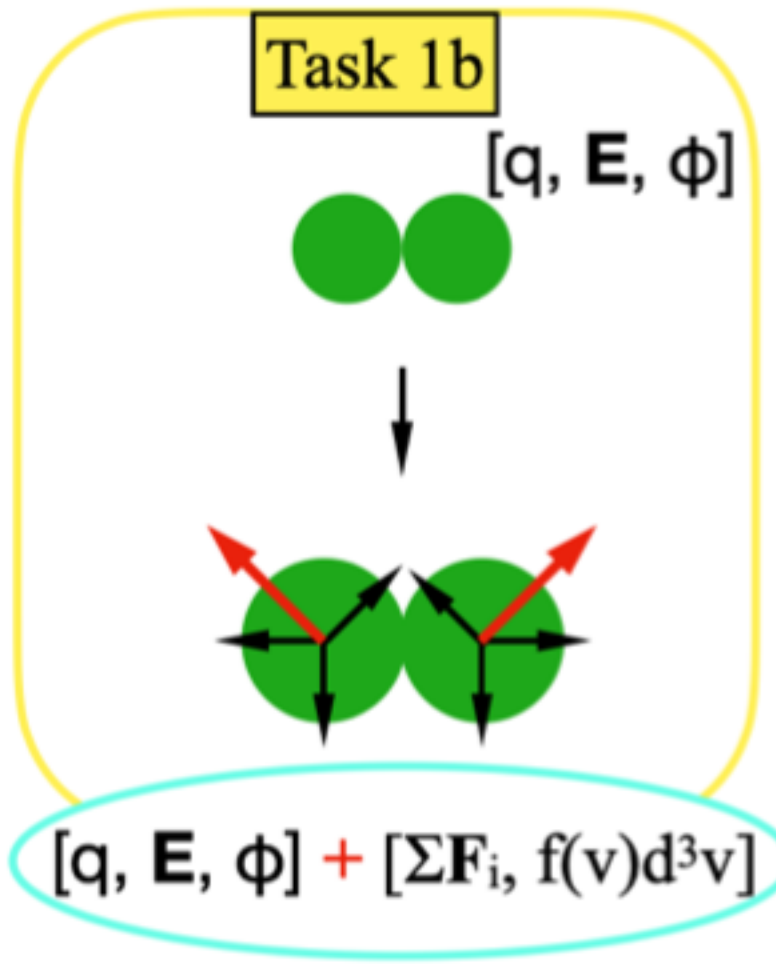




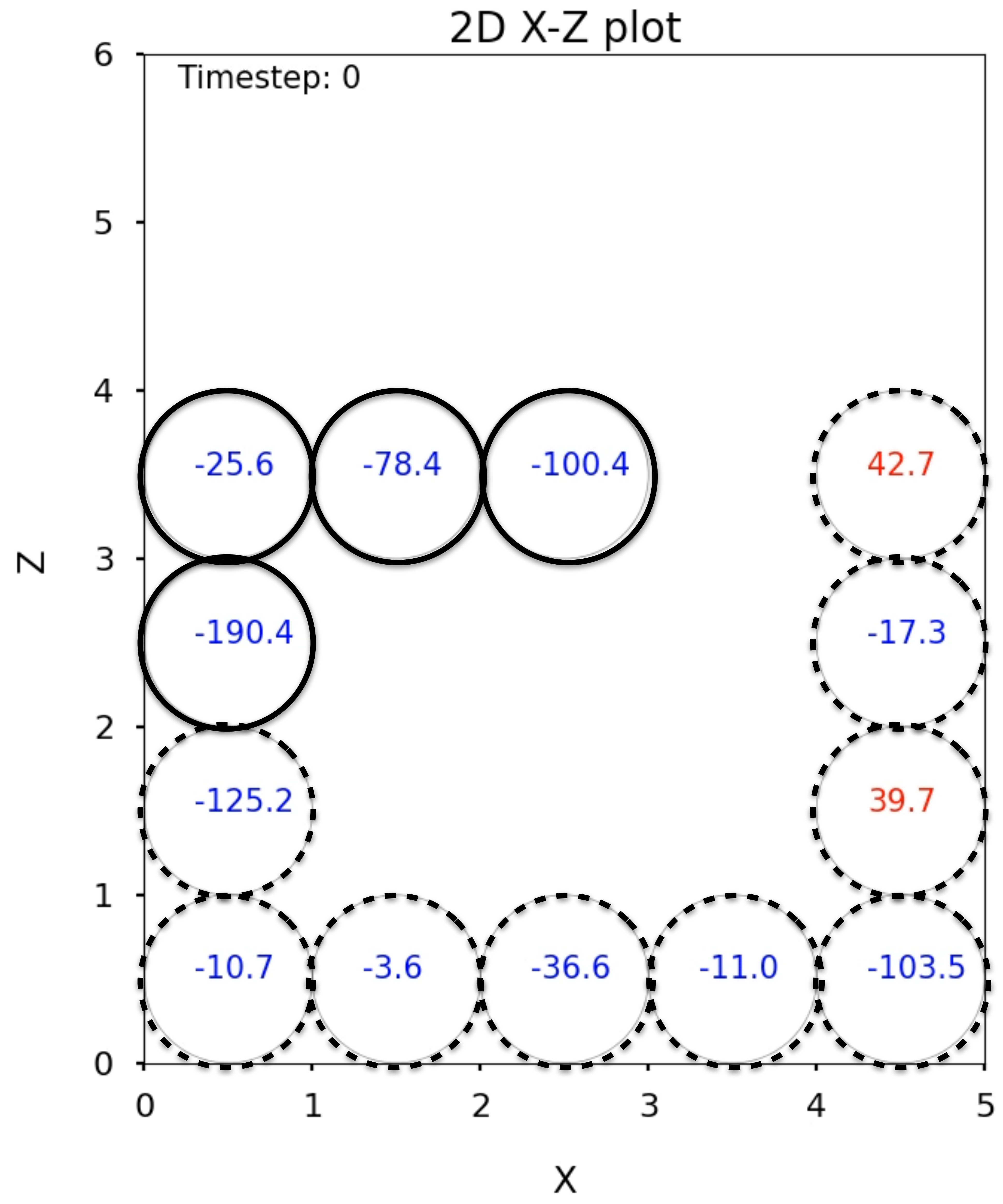
Particle mobilisation.







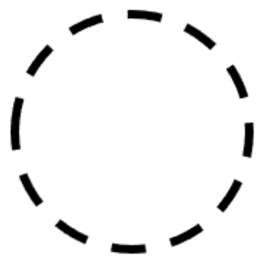
Particle mobilisation.



- Detachment criterion (artificial):

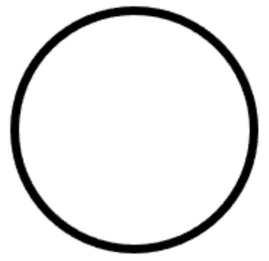
  Adjacent grains each carrying 10^3 elementary charges of the same polarity.

- Grain charging setup:



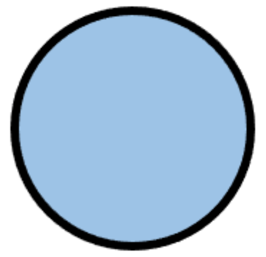
dQ/dt follows a Gaussian:

mean = 0e-, sigma 50e-

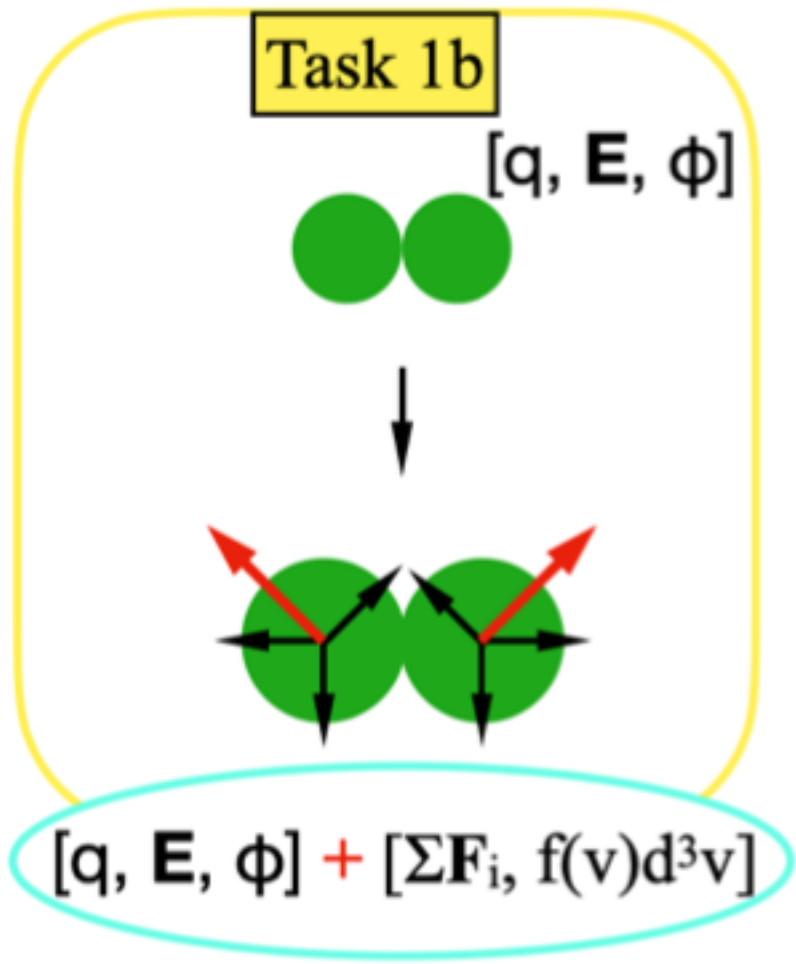


dQ/dt follows a Gaussian:

mean = 100e-, sigma = 50e-



Detached from surface.



Patched Charge Model Benchmark.

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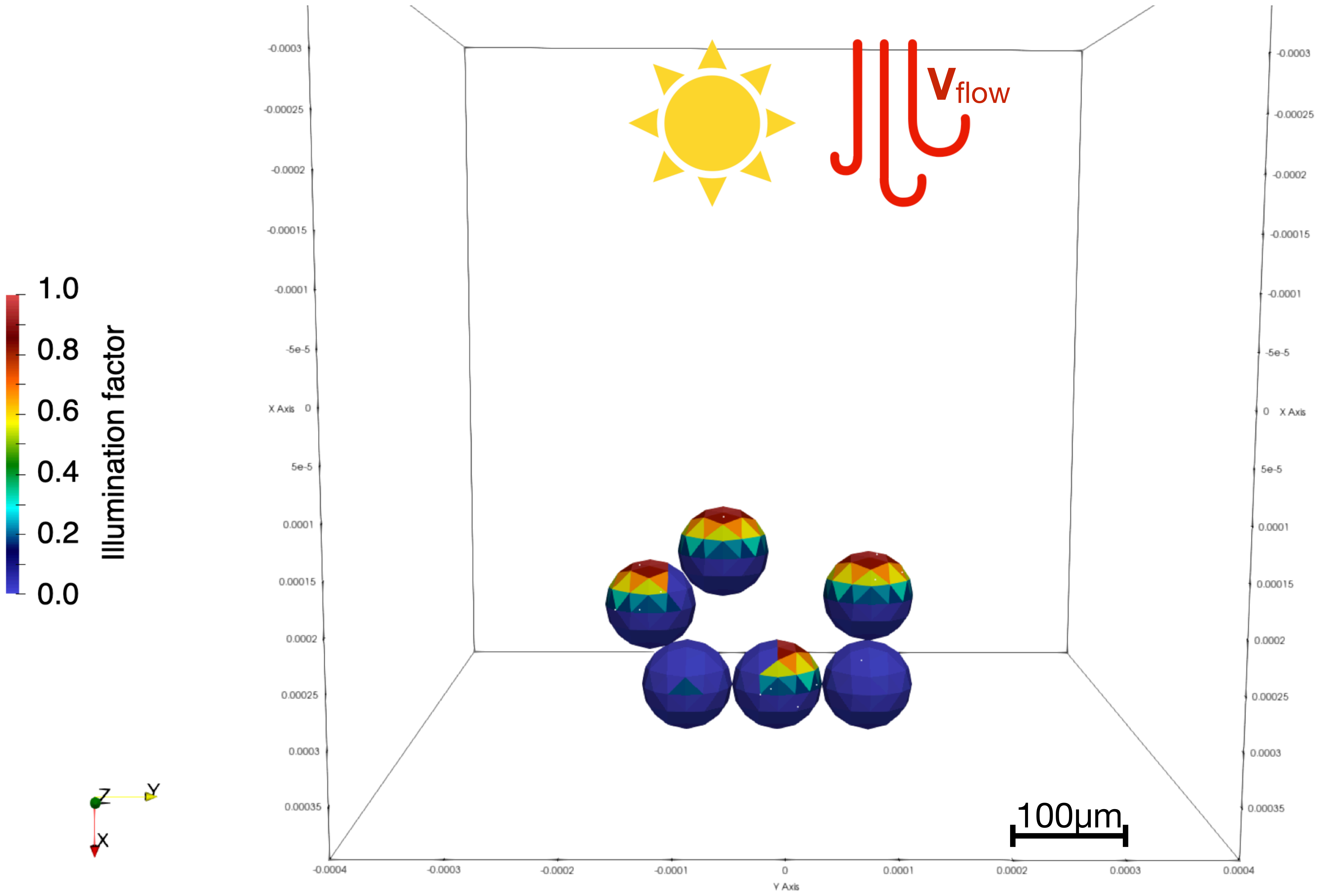

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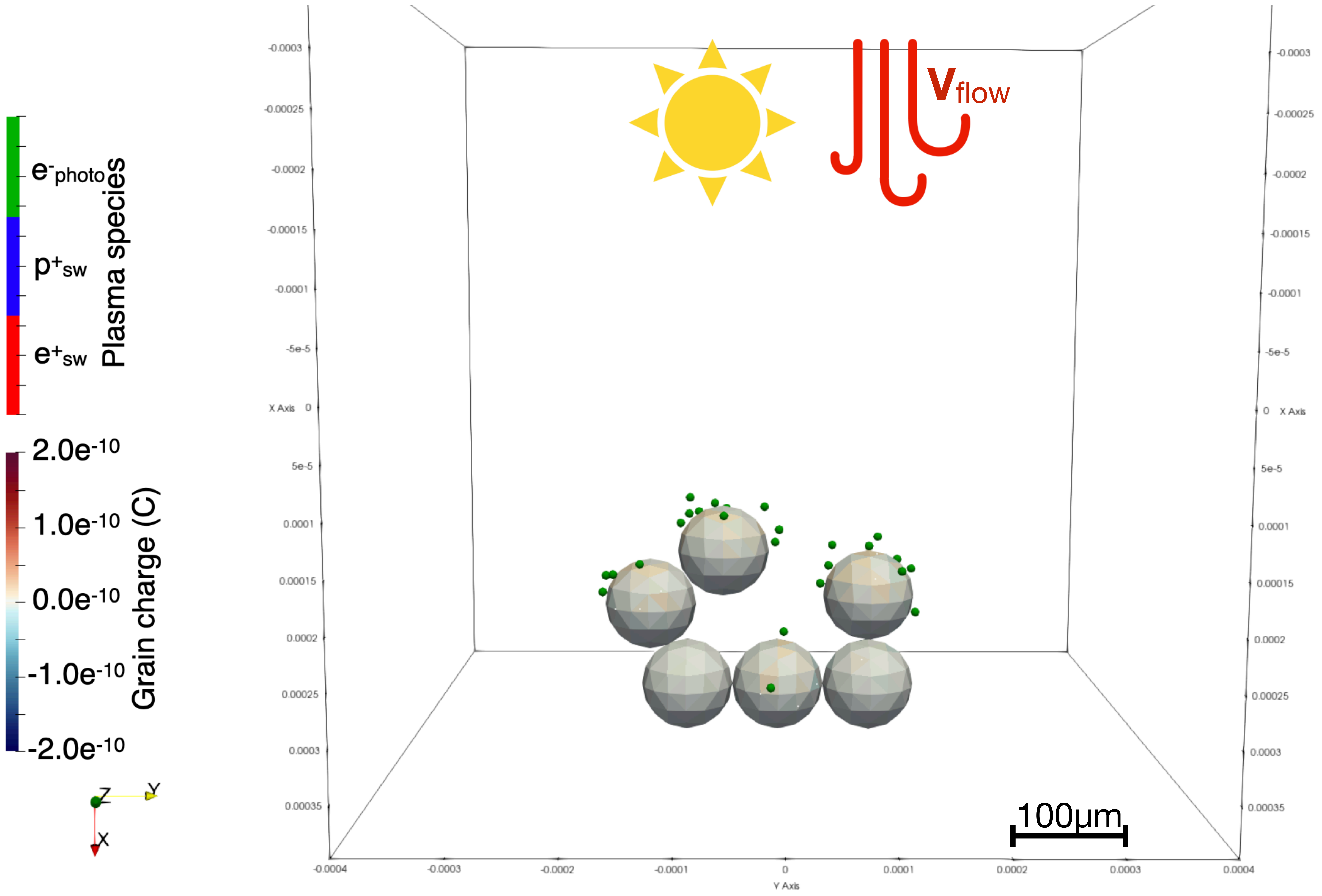

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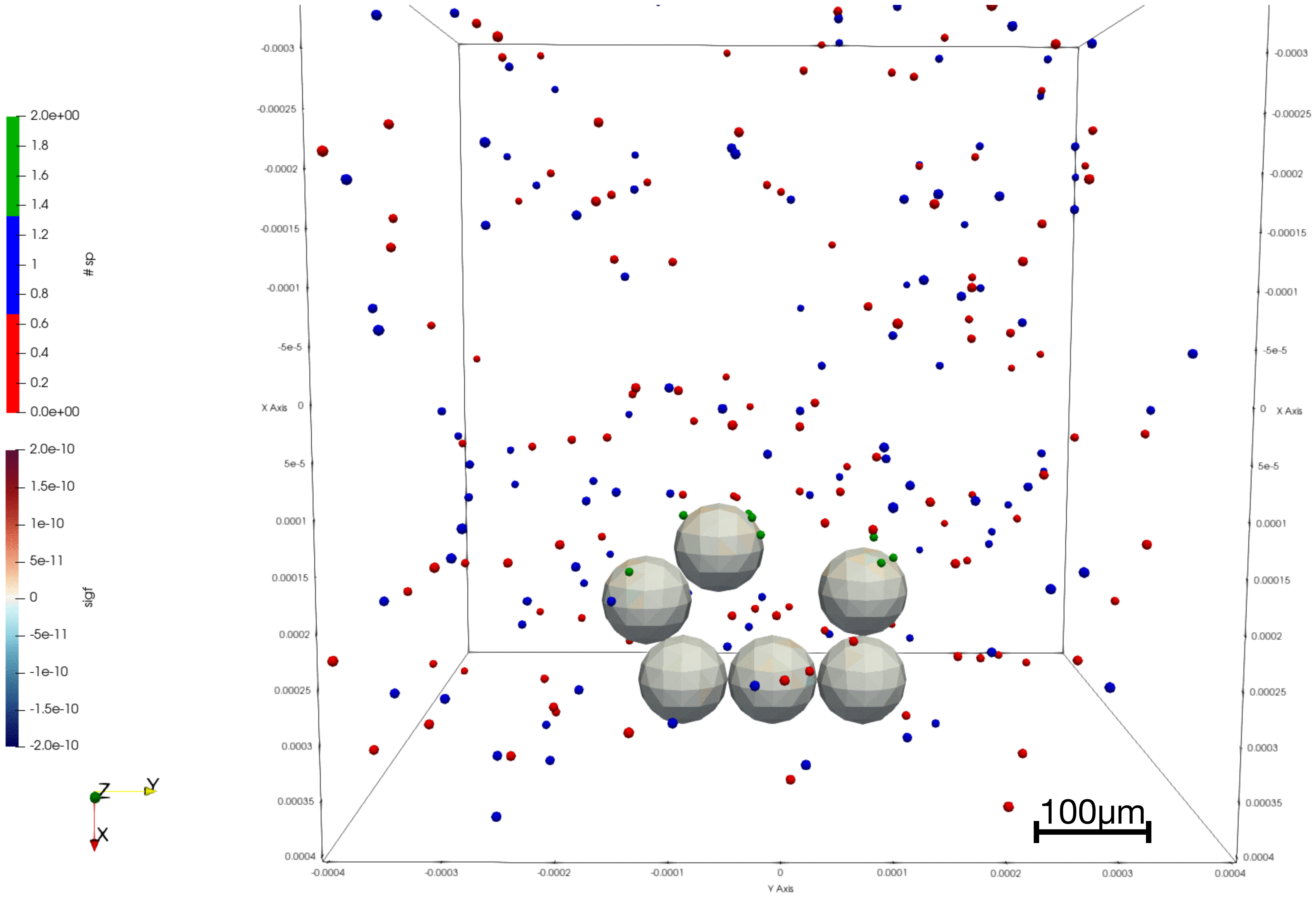

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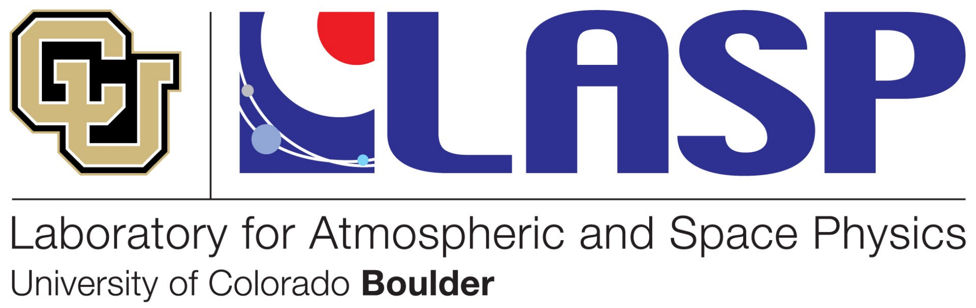

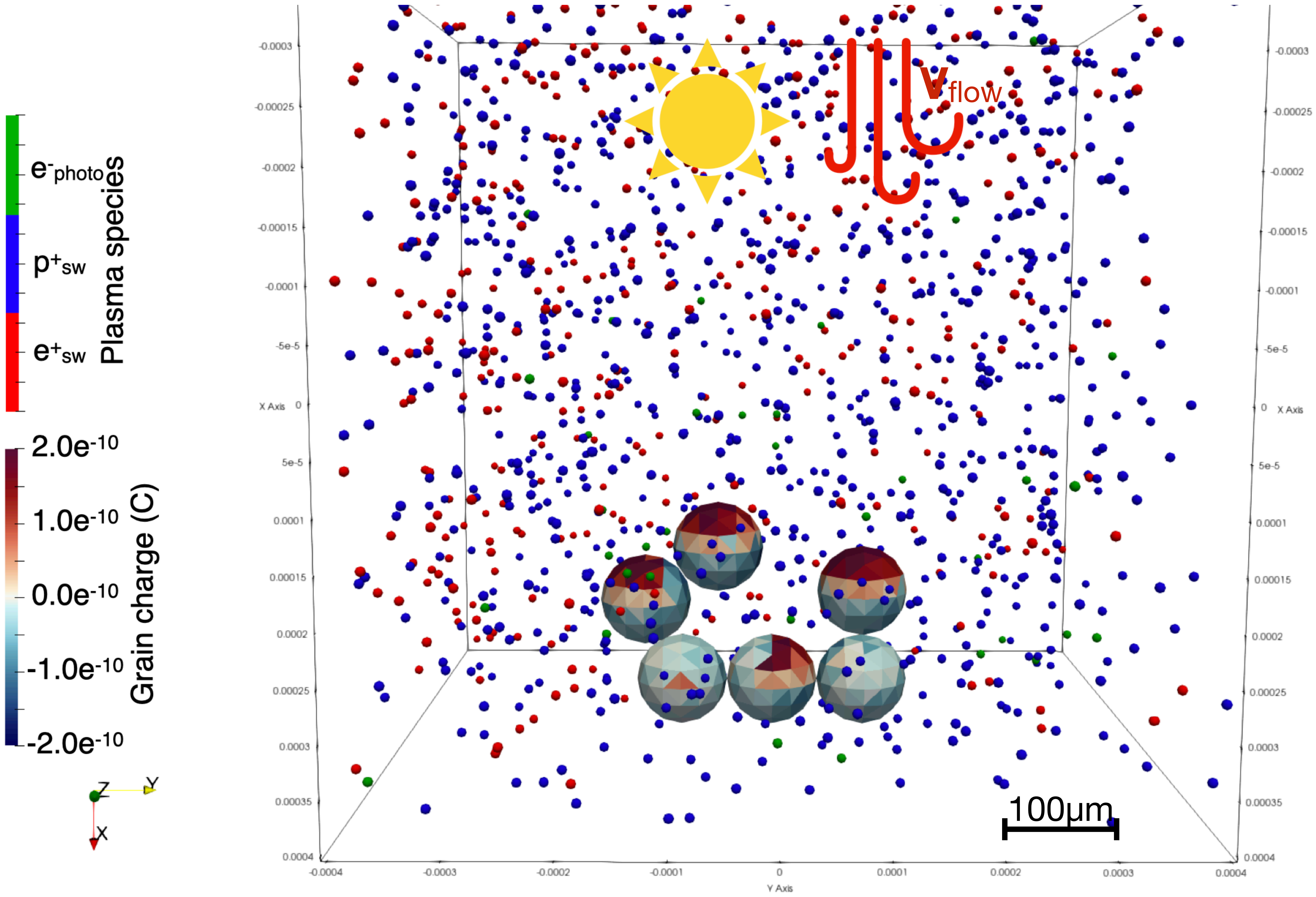

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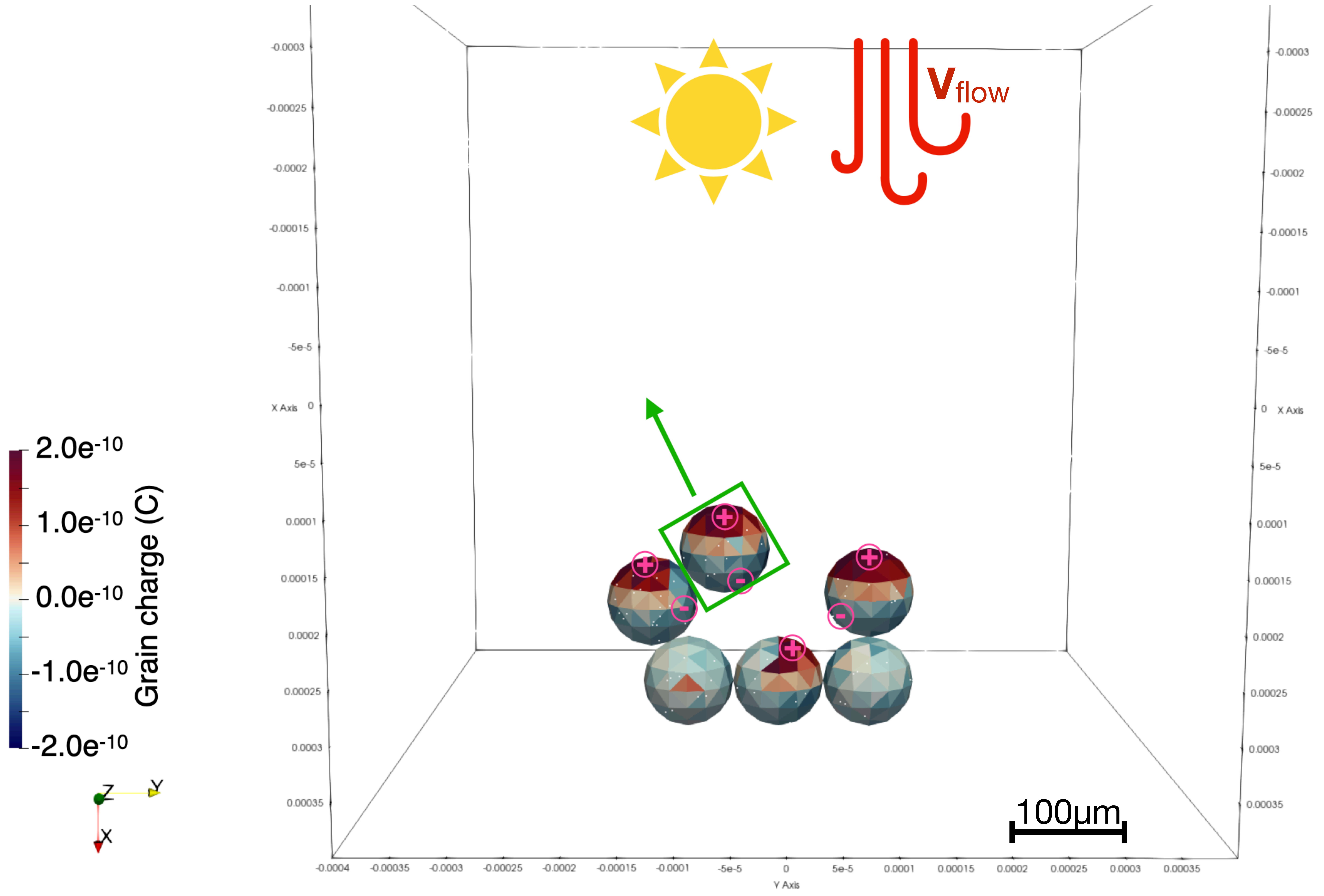

Particle-in-Cell approach.

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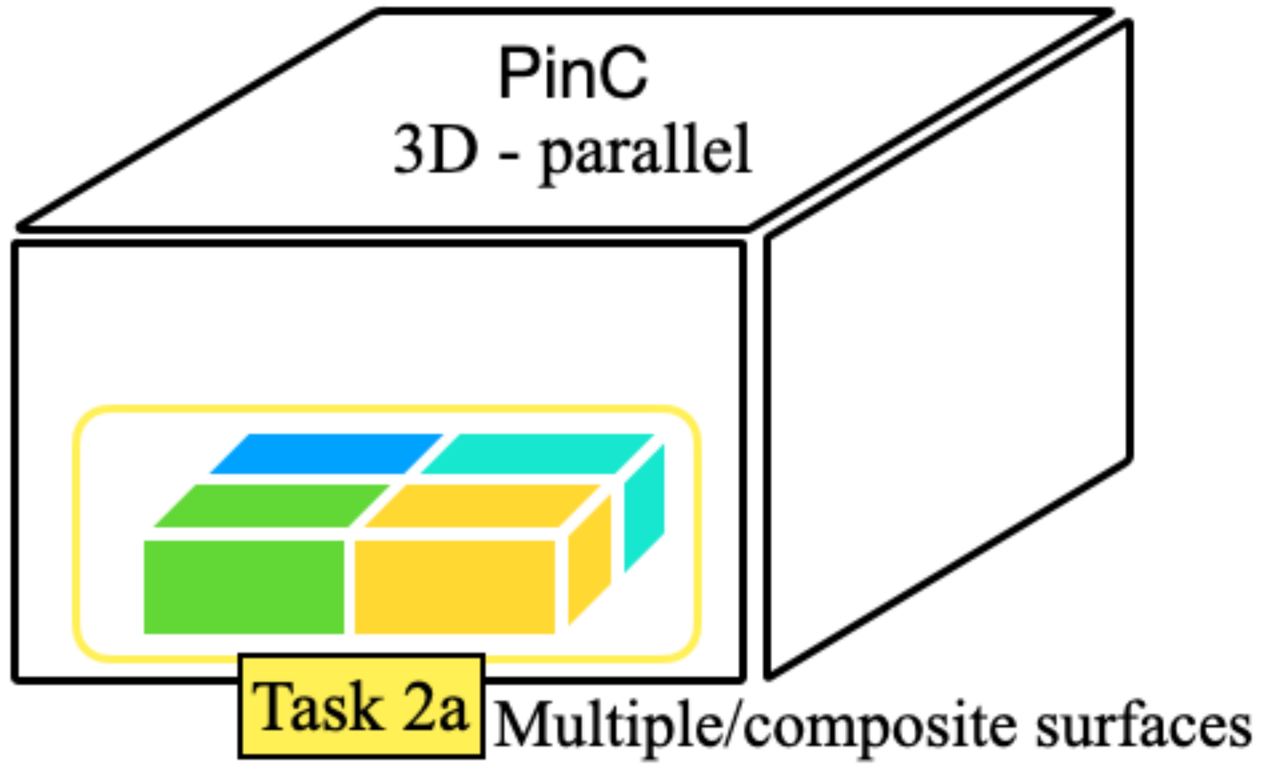
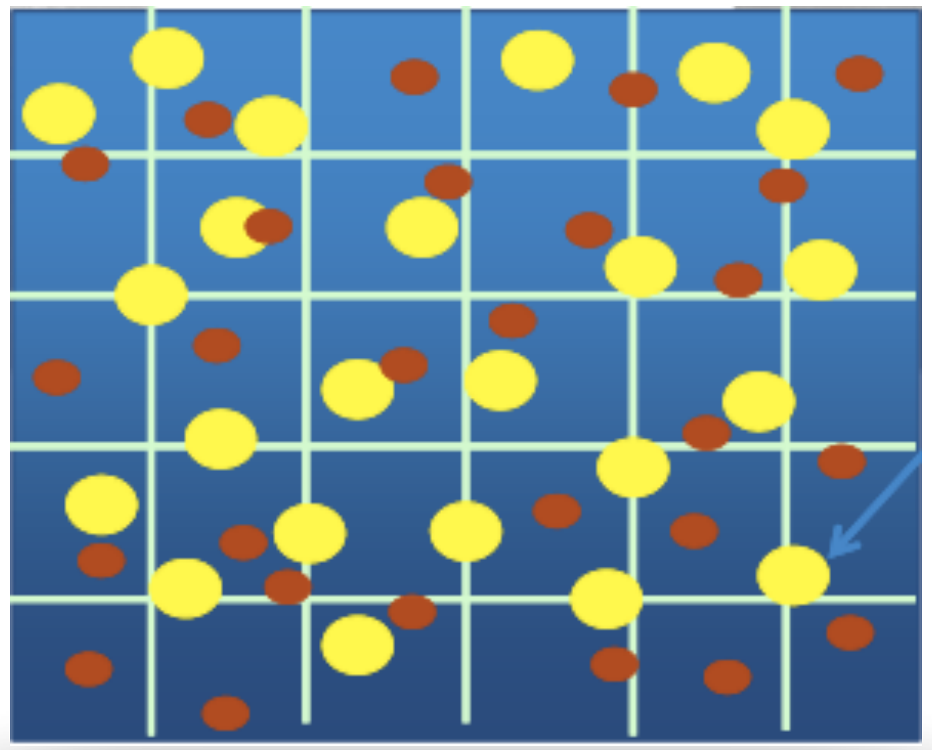
- PinC: C++/MPI-parallelised particle-in-cell code.
  - Before: Can handle 1 object/surface.
  - Today: Can handle multiple/composite objects/surfaces by leveraging the Capacitance Matrix method.



- Basic Particle-in-Cell algorithm:



$$\nabla \cdot \boldsymbol{E} = 4\pi\rho,$$

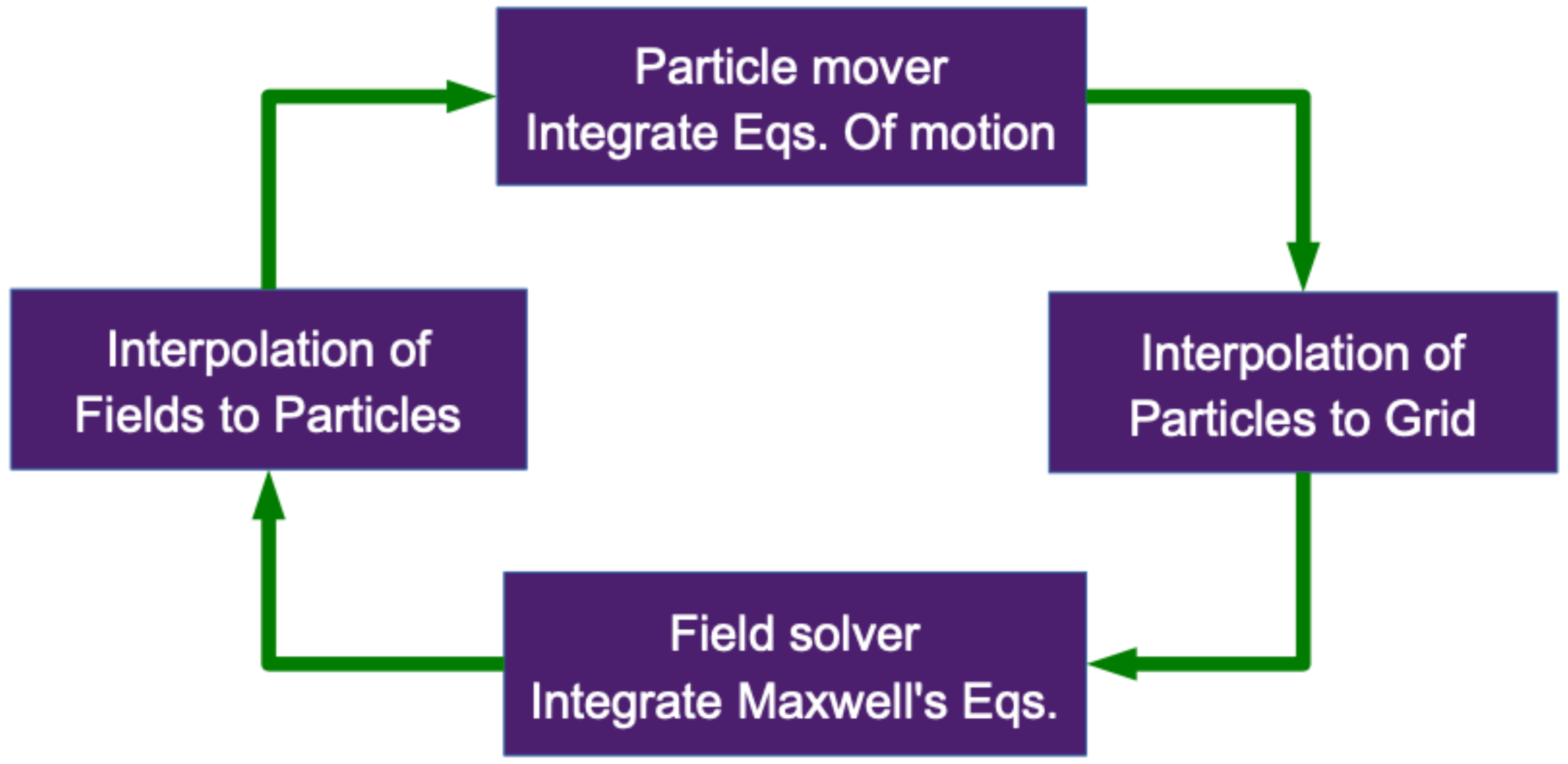
$$\nabla \cdot \boldsymbol{B} = 0,$$

$$\nabla \times \boldsymbol{E} = -\frac{1}{c}\frac{\partial \boldsymbol{B}}{\partial t},$$

$$\nabla \times \boldsymbol{B} = \frac{4\pi}{c}\boldsymbol{J} + \frac{1}{c}\frac{\partial \boldsymbol{E}}{\partial t}$$

$$\frac{d\boldsymbol{x}_p}{dt} = \boldsymbol{v}_p,$$

$$\frac{d\boldsymbol{v}_p}{dt} = \frac{q_s}{m_s}\left(\boldsymbol{E}_p + \frac{\boldsymbol{v}_p \times \boldsymbol{B}_p}{c}\right)$$



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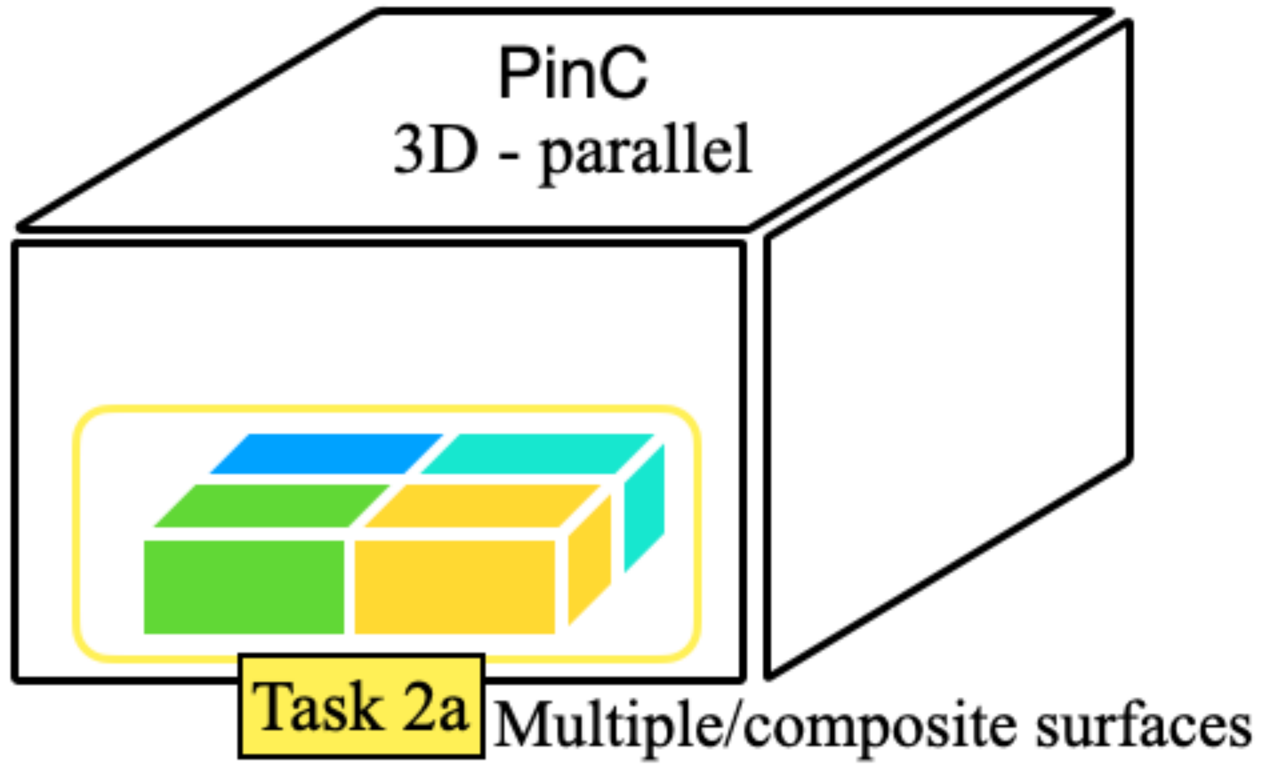
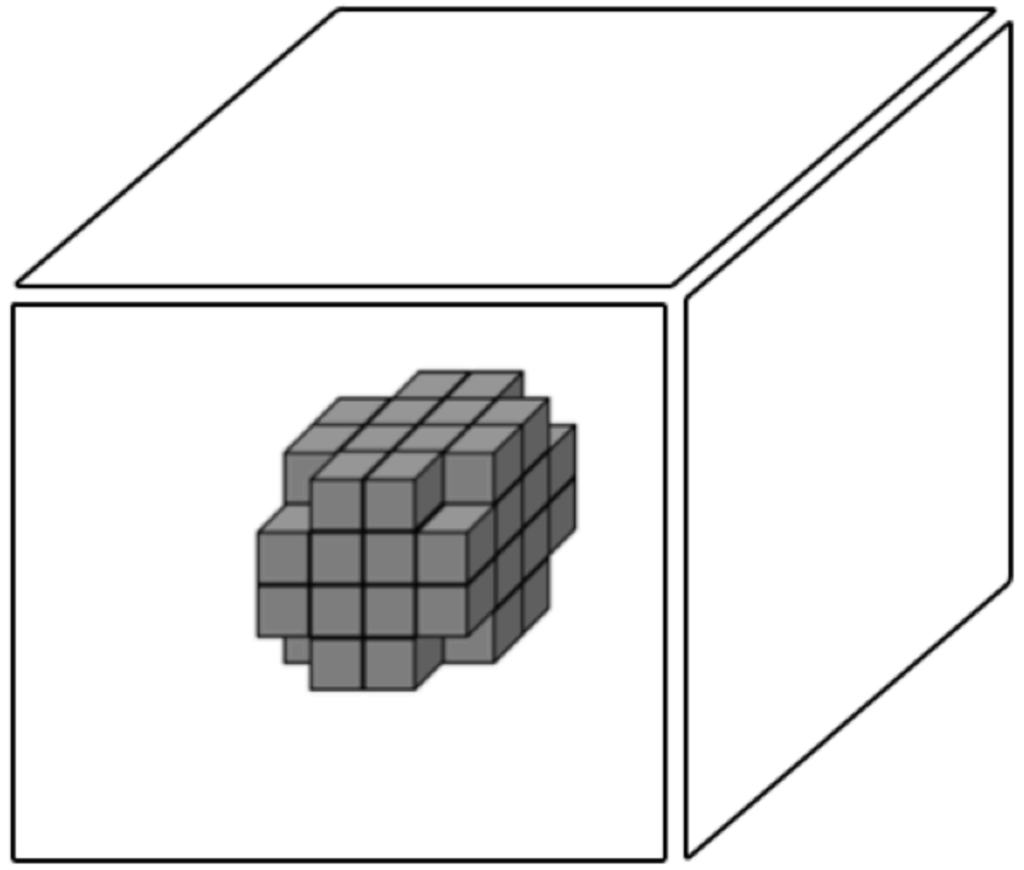


  - **Capacitance Matrix method** (Miyake et al. [2009,2011]).

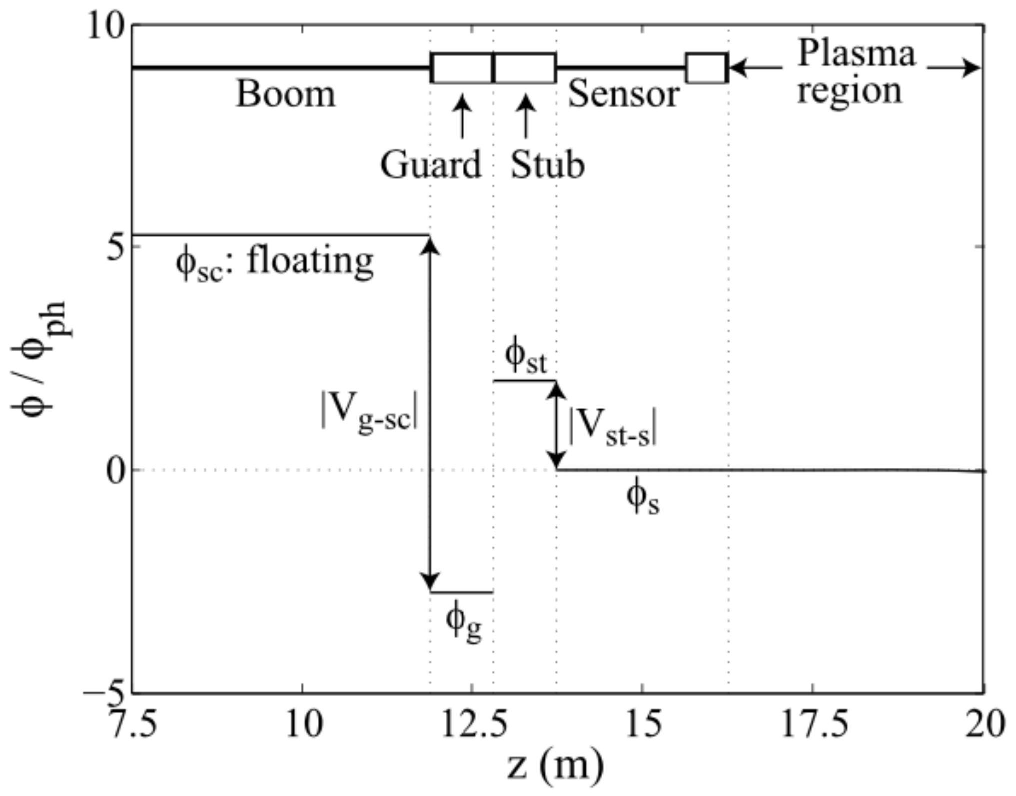


Relation between density and potential
(N_G: # grid nodes; N_B: # body nodes)

$$\rho_i = \sum_{j=1}^{N_G} A_{ij}\phi_j, \quad (i = 1, \cdots, N_G),$$

$$\delta\rho_{s,i} = \sum_{j=1}^{N_B} C_{ij}\delta\phi_{s,j}, \quad (i = 1, \cdots, N_B).$$

$$\phi_c = \frac{\Sigma_i \Sigma_j C_{ij}\phi_{s,j}}{\Sigma_i \Sigma_j C_{ij}}$$



$$\begin{aligned}
\Delta Q_{s1} &= \sum_{i\in G_{s1}}\sum_{j} c_{ij}(\phi_j - \phi'_j) \\
&= \phi_{s1}\sum_{i\in G_{s1}}\sum_{j\in G_{s1}} c_{ij} + \phi_{st1}\sum_{i\in G_{s1}}\sum_{j\in G_{st1}} c_{ij} \\
&\quad + \phi_{g1}\sum_{i\in G_{s1}}\sum_{j\in G_{g1}} c_{ij} + \phi_{sc}\sum_{i\in G_{s1}}\sum_{j\in G_{sc}} c_{ij} \\
&\quad + \phi_{g2}\sum_{i\in G_{s1}}\sum_{j\in G_{g2}} c_{ij} + \phi_{st2}\sum_{i\in G_{s1}}\sum_{j\in G_{st2}} c_{ij} \\
&\quad + \phi_{s2}\sum_{i\in G_{s1}}\sum_{j\in G_{s2}} c_{ij} - \sum_{i\in G_{s1}}\sum_{j} c_{ij}\phi'_j \\
&= \phi_{s1}\sum_{i\in G_{s1}}\sum_{j\in G_{s1+st1}} c_{ij} + V_{st1-s1}\sum_{i\in G_{s1}}\sum_{j\in G_{st1}} c_{ij} \\
&\quad + V_{g1-sc}\sum_{i\in G_{s1}}\sum_{j\in G_{g1}} c_{ij} + \phi_{sc}\sum_{i\in G_{s1}}\sum_{j\in G_{g1+sc+g2}} c_{ij} \\
&\quad + V_{g2-sc}\sum_{i\in G_{s1}}\sum_{j\in G_{g2}} c_{ij} + V_{st2-s2}\sum_{i\in G_{s1}}\sum_{j\in G_{st2}} c_{ij} \\
&\quad + \phi_{s2}\sum_{i\in G_{s1}}\sum_{j\in G_{st2+s2}} c_{ij} - \sum_{i\in G_{s1}}\sum_{j} c_{ij}\phi'_j,
\end{aligned}$$

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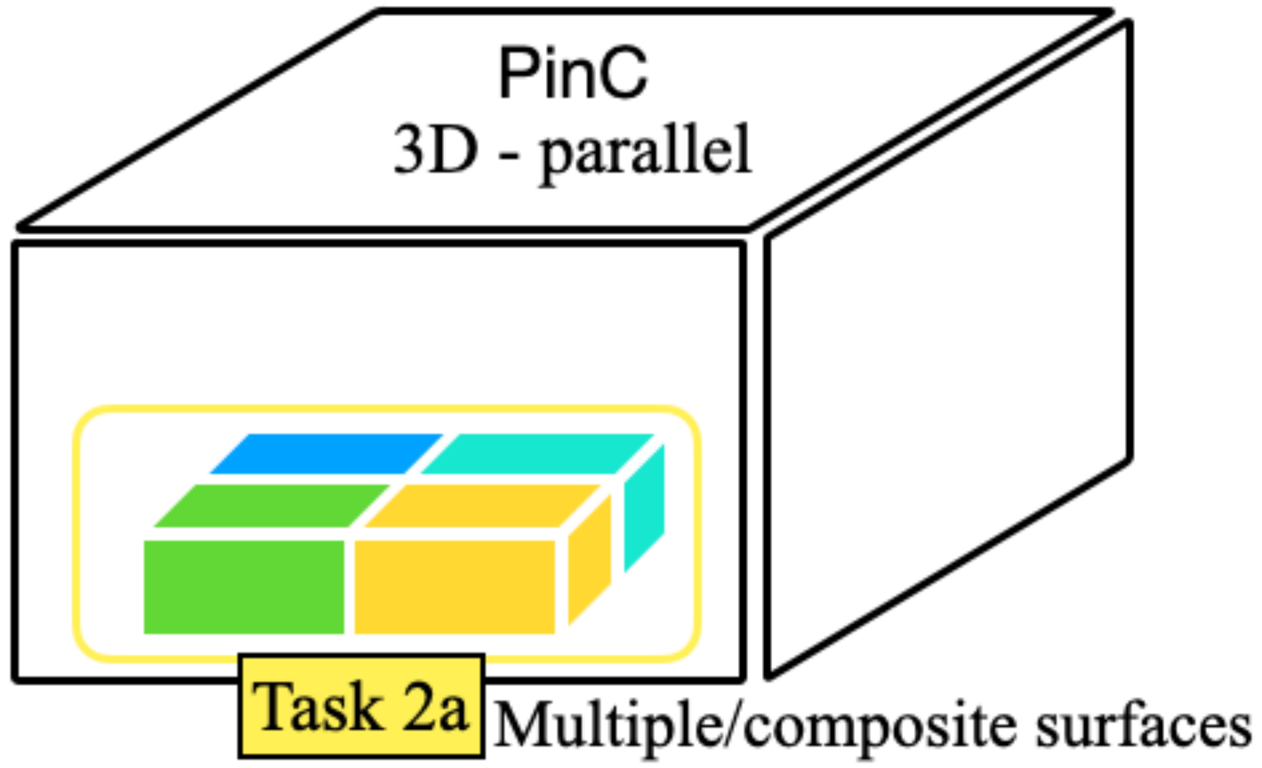
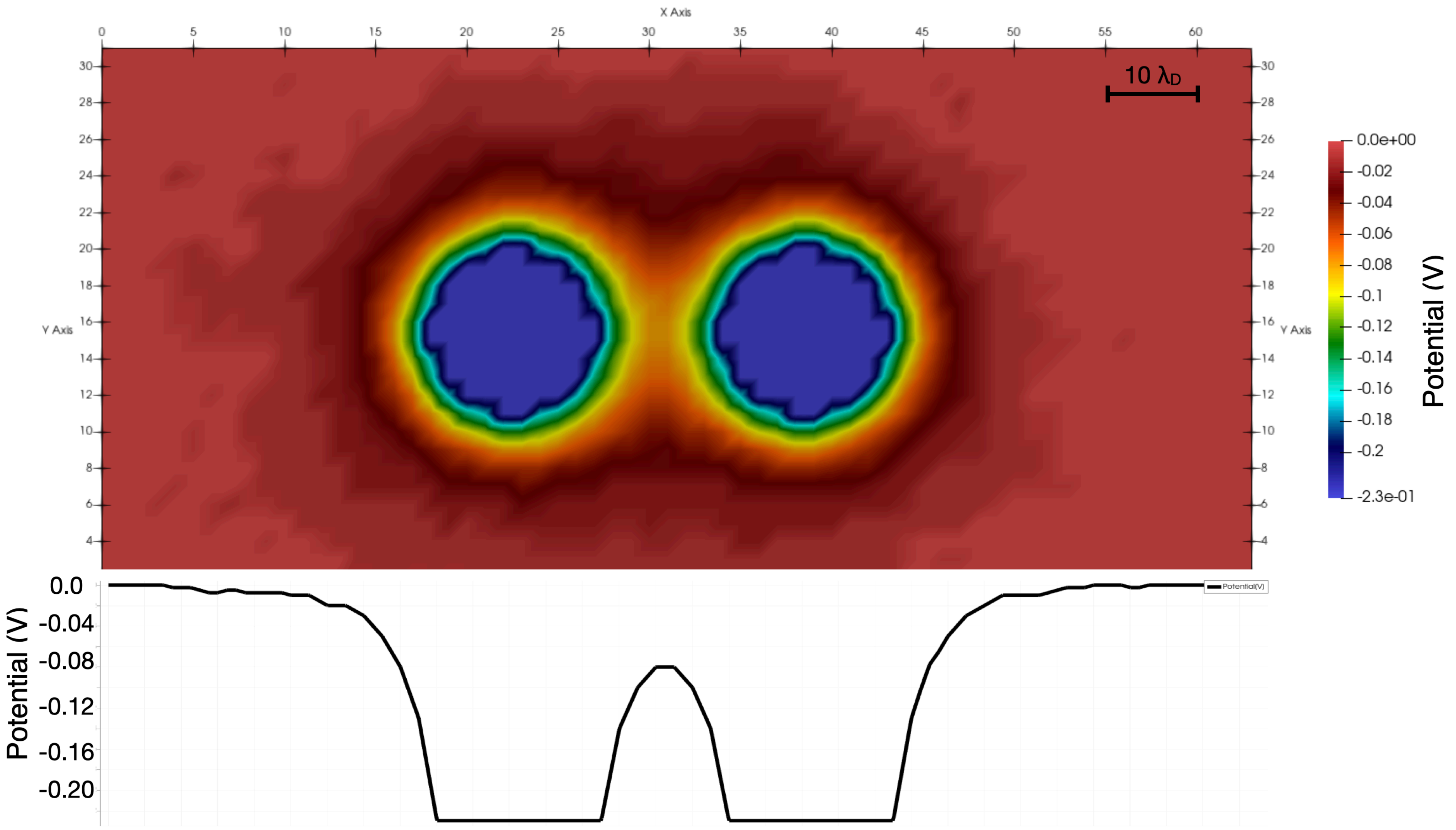
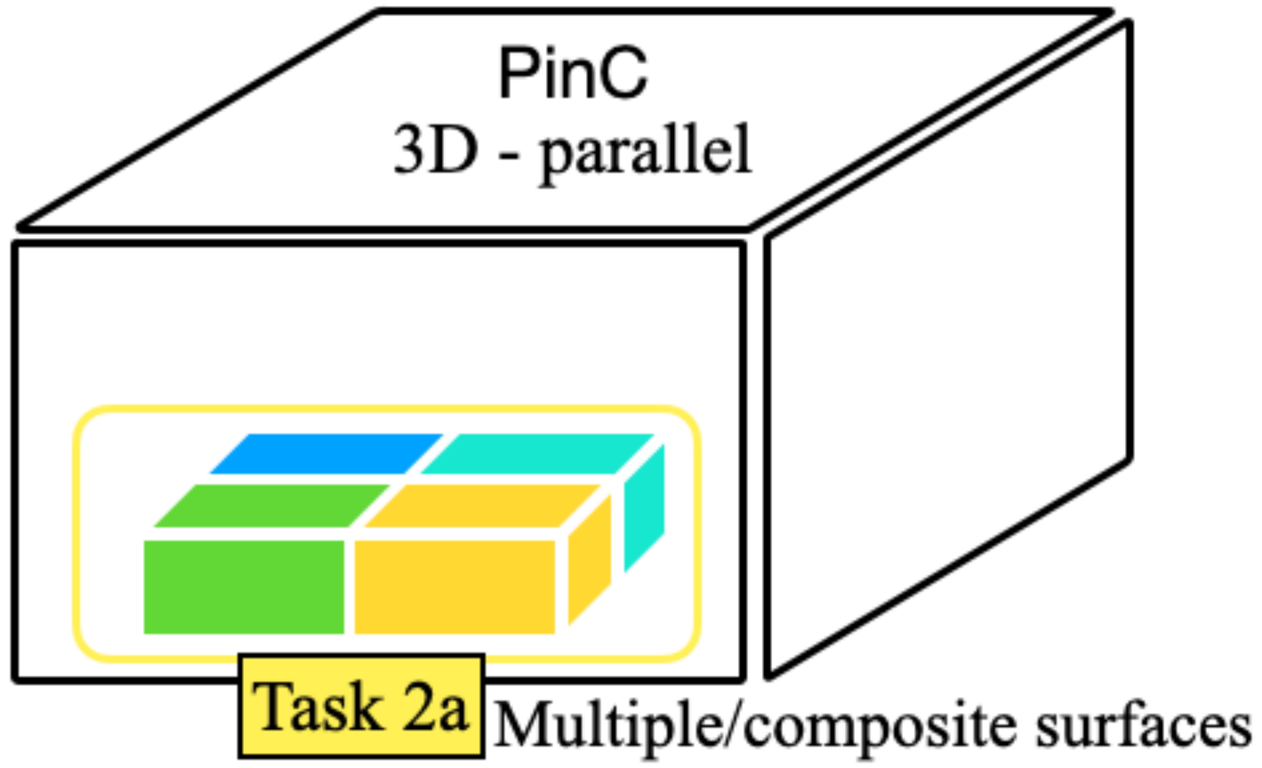
  - Before: Can handle 1 object/surface.
  - Today: Can handle multiple/composite objects/surfaces by leveraging the Capacitance Matrix method.
  - Example: two spheres in a stationary plasma.

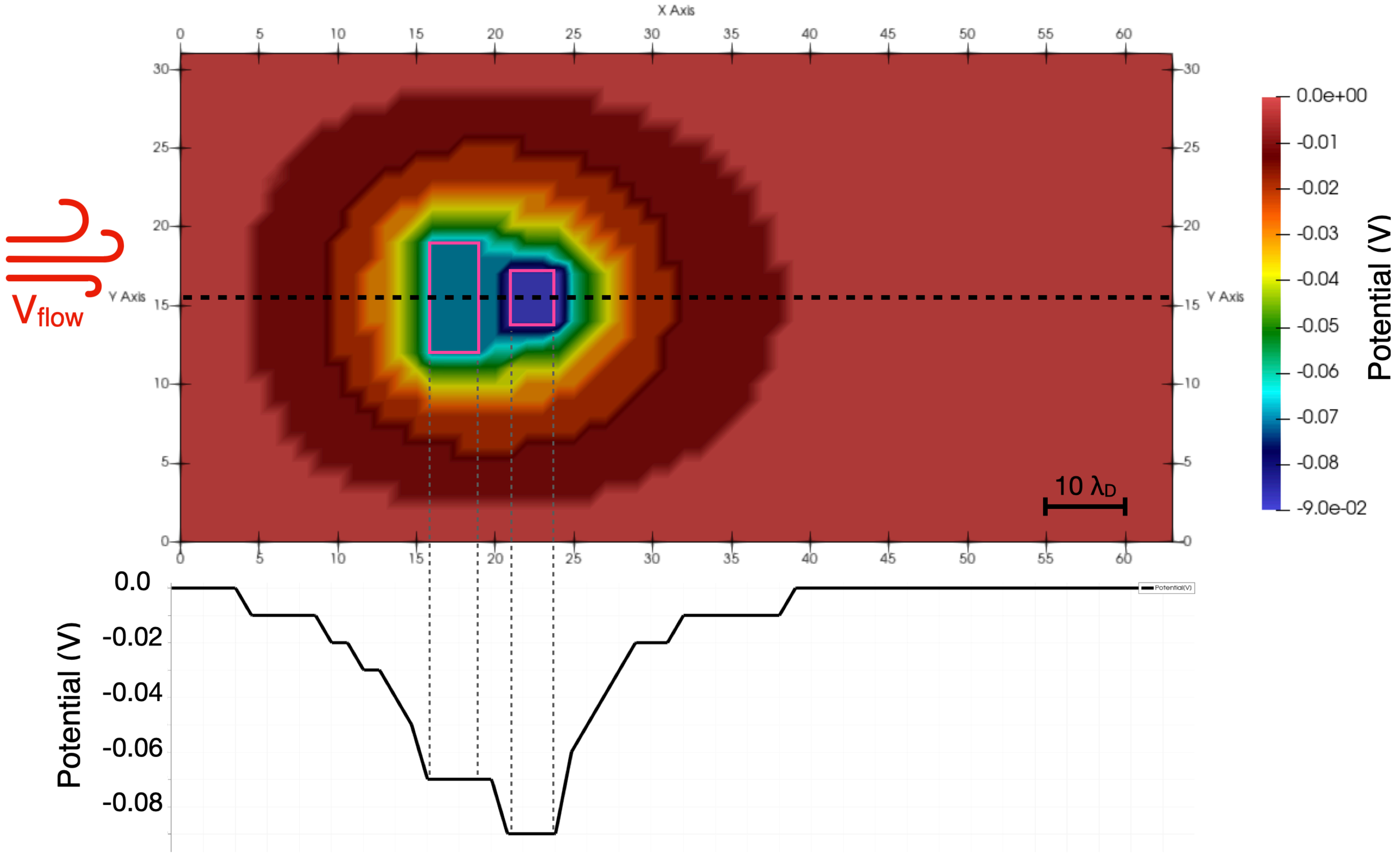




Particle-in-Cell approach.

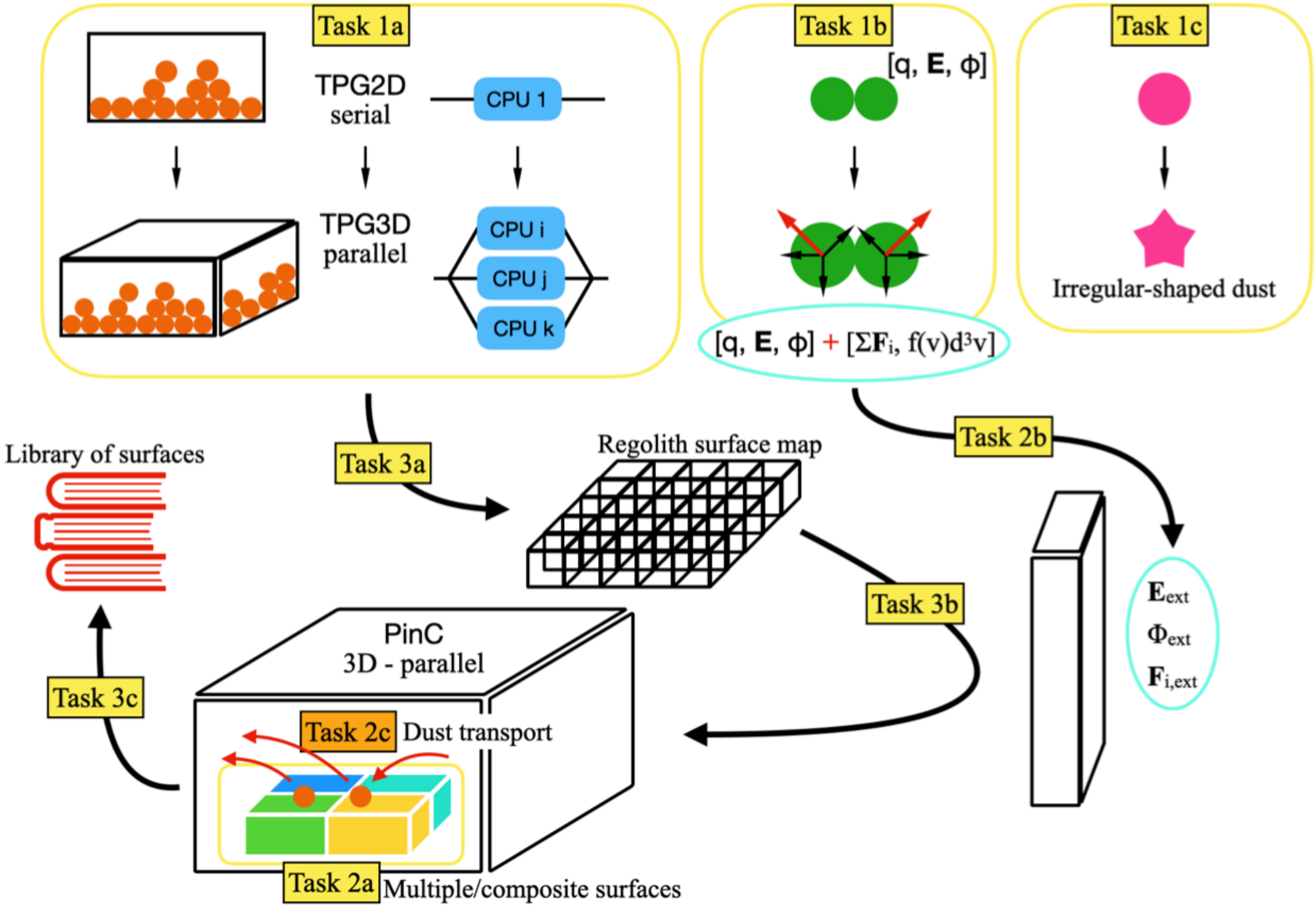
- PinC: C++/MPI-parallelised particle-in-cell code.
  - Multiple objects by leveraging the Capacitance Matrix method.
  - Example: two differently-sized prisms in flowing plasma.





To-dos

- Code-coupling (Tasks 3a-b).
- Dust transport model (Task 2c).
- Validate the framework against lab and flight results.



Thank you for your attention!

Questions?

Draw here.

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