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1 Definitions and math convention

$$\begin{aligned}\eta^2 &\equiv [-H, H] \times [-H, H] \subset \mathbb{R}^2 \\ \Delta &\equiv \frac{2H}{K} \\ \Pi\left(\frac{x}{b}\right) &\equiv \Theta\left(\frac{b}{2} - x\right) \cdot \Theta\left(x + \frac{b}{2}\right) \\ \epsilon_x &\equiv \frac{x_i - x_k}{\Delta} + \frac{1}{2} \\ \epsilon_y &\equiv \frac{y_i - y_l}{\Delta} + \frac{1}{2}\end{aligned}\tag{1}$$

2 Exercise 1.1.: Weight coefficients and shape functions

2.1 Criteria for the cell indices

$$\begin{aligned}k' &= \left\lfloor \frac{(x_i + H) \cdot K}{2H} \right\rfloor \\ l' &= \left\lfloor \frac{(y_i + H) \cdot K}{2H} \right\rfloor\end{aligned}\tag{2}$$

The indices k' and l' from equation (2) indicate the allocation of the particle to the cell with the ID (k', l') .

2.2 Density matrix with zeroth order method

In the zeroth order method the particles are assumed to be point-like. As a consequence, the particle is represented as a Dirac-delta function in the convolution integral with the mesh function. The particle density matrix ρ_{kl} will result as the quotient of the convolution divided by the discretized area element Δ^2 (1) as indicated in equation (3). The integral can be solved by using Kronecker deltas.

$$\begin{aligned}\rho_{kl} &= \frac{1}{\Delta^2} \cdot \sum_{i=1}^N \int_{\eta^2} \Pi\left(\frac{\vec{x} - \vec{x}_{kl}}{\Delta}\right) \cdot \delta(\vec{x} - \vec{x}_i) d\vec{x} \\ \rho_{kl} &= \frac{1}{\Delta^2} \cdot \sum_{i=1}^N \delta_{kk'}^{(i)} \cdot \delta_{ll'}^{(i)} \\ \rho_{kl} &= \frac{K^2}{4H^2} \cdot \sum_{i=1}^N \delta_{kk'}^{(i)} \cdot \delta_{ll'}^{(i)}\end{aligned}\tag{3}$$

To receive the mass density it is necessary to include the particle mass m_i into the sum of equation (3).

3 Exercise 1.2.: Weight matrix for the 1st and 2nd-order method

3.1 Weight matrix W for the first order method

In contrast to the zeroth order method the first order method assigns a top-hat function to the particle. The entries of the weight matrix are obtained by the convolution of the single particle function with the mesh function.

$$\begin{aligned}W_{kl}^{(i)} &= \frac{1}{\Delta^2} \cdot \int_{\eta^2} \Pi\left(\frac{\vec{x} - \vec{x}_{kl}}{\Delta}\right) \cdot \Pi\left(\frac{\vec{x}_i - \vec{x}}{\Delta}\right) d\vec{x} \\ W_{kl}^{(i)} &= \frac{1}{\Delta^2} \cdot \int_{\eta} \Pi\left(\frac{x - x_k}{\Delta}\right) \cdot \Pi\left(\frac{x_i - x}{\Delta}\right) dx \cdot \int_{\eta} \Pi\left(\frac{y - y_l}{\Delta}\right) \cdot \Pi\left(\frac{y_i - y}{\Delta}\right) dy \\ W_{kl}^{(i)} &= \frac{1}{\Delta^2} \cdot \int_{\max\left\{x_k - \frac{\Delta}{2}, x_i - \frac{\Delta}{2}\right\}}^{\min\left\{x_k + \frac{\Delta}{2}, x_i + \frac{\Delta}{2}\right\}} dx \cdot \int_{\max\left\{y_l - \frac{\Delta}{2}, y_i - \frac{\Delta}{2}\right\}}^{\min\left\{y_l + \frac{\Delta}{2}, y_i + \frac{\Delta}{2}\right\}} dy \\ W_{kl}^{(i)} &= \left(\min\left\{\frac{x_k}{\Delta} + \frac{1}{2}, \frac{x_i}{\Delta} + \frac{1}{2}\right\} - \max\left\{\frac{x_k}{\Delta} - \frac{1}{2}, \frac{x_i}{\Delta} - \frac{1}{2}\right\} \right) \\ &\quad \times \left(\min\left\{\frac{y_l}{\Delta} + \frac{1}{2}, \frac{y_i}{\Delta} + \frac{1}{2}\right\} - \max\left\{\frac{y_l}{\Delta} - \frac{1}{2}, \frac{y_i}{\Delta} - \frac{1}{2}\right\} \right)\end{aligned}\tag{4}$$

To further resolve the expression (4) for the weight matrix $W_{kl}^{(i)}$ it is required to split the calculation in four different cases.

- Case 1.: Constraints: $x_k \stackrel{!}{<} x_i$ and $y_l \stackrel{!}{<} y_i$

$$\begin{aligned}
W_{kl}^{(i)}[C1] &= \left(1 - \frac{x_i - x_k}{\Delta}\right) \cdot \left(1 - \frac{y_i - y_l}{\Delta}\right) \\
W_{kl}^{(i)}[C1] &= \left(1 - \frac{x_i - \left(x_{k-0.5} + \frac{\Delta}{2}\right)}{\Delta}\right) \cdot \left(1 - \frac{y_i - \left(y_{l-0.5} + \frac{\Delta}{2}\right)}{\Delta}\right) \\
W_{kl}^{(i)}[C1] &\stackrel{(1)}{=} \left(\frac{3}{2} - \epsilon_x\right) \cdot \left(\frac{3}{2} - \epsilon_y\right)
\end{aligned} \tag{5}$$

- Case 2.: Constraints: $x_k \stackrel{!}{>} x_i$ and $y_l \stackrel{!}{<} y_i$

$$\begin{aligned}
W_{kl}^{(i)}[C2] &= \left(1 + \frac{x_i - x_k}{\Delta}\right) \cdot \left(1 - \frac{y_i - y_l}{\Delta}\right) \\
W_{kl}^{(i)}[C2] &= \left(1 + \frac{x_i - \left(x_{k-0.5} + \frac{\Delta}{2}\right)}{\Delta}\right) \cdot \left(1 - \frac{y_i - \left(y_{l-0.5} + \frac{\Delta}{2}\right)}{\Delta}\right) \\
W_{kl}^{(i)}[C2] &\stackrel{(1)}{=} \left(\frac{1}{2} + \epsilon_x\right) \cdot \left(\frac{3}{2} - \epsilon_y\right)
\end{aligned} \tag{6}$$

- Case 3.: Constraints: $x_k \stackrel{!}{>} x_i$ and $y_l \stackrel{!}{>} y_i$

$$\begin{aligned}
W_{kl}^{(i)}[C3] &= \left(1 + \frac{x_i - x_k}{\Delta}\right) \cdot \left(1 + \frac{y_i - y_l}{\Delta}\right) \\
W_{kl}^{(i)}[C3] &= \left(1 + \frac{x_i - \left(x_{k-0.5} + \frac{\Delta}{2}\right)}{\Delta}\right) \cdot \left(1 + \frac{y_i - \left(y_{l-0.5} + \frac{\Delta}{2}\right)}{\Delta}\right) \\
W_{kl}^{(i)}[C3] &\stackrel{(1)}{=} \left(\frac{1}{2} + \epsilon_x\right) \cdot \left(\frac{1}{2} + \epsilon_y\right)
\end{aligned} \tag{7}$$

- Case 4.: Constraints: $x_k \overset{!}{<} x_i$ and $y_l \overset{!}{>} y_i$

$$\begin{aligned}
W_{kl}^{(i)} [C4] &= \left(1 - \frac{x_i - x_k}{\Delta}\right) \cdot \left(1 + \frac{y_i - y_l}{\Delta}\right) \\
W_{kl}^{(i)} [C4] &= \left(1 - \frac{x_i - \left(x_{k-0.5} + \frac{\Delta}{2}\right)}{\Delta}\right) \cdot \left(1 + \frac{y_i - \left(y_{l-0.5} + \frac{\Delta}{2}\right)}{\Delta}\right) \\
W_{kl}^{(i)} [C4] &\stackrel{(1)}{=} \left(\frac{3}{2} - \epsilon_x\right) \cdot \left(\frac{1}{2} + \epsilon_y\right)
\end{aligned} \tag{8}$$

The results from equations (5) to (8) for the restricted weight matrix $W_{kl}^{(i)}$ under the respective constraints can be used to determine the explicit matrix representation of $W_{kl}^{(i)}$ as shown in the equations (9) to (12).

- Case 1.: Constraints: $x_k \overset{!}{<} x_i$ and $y_l \overset{!}{<} y_i$

$$W_{kl}^{(i)} [C1] = \begin{bmatrix} 0 & \left(\frac{3}{2} - \epsilon_x\right) \cdot \left(\epsilon_y - \frac{1}{2}\right) & \left(\epsilon_x - \frac{1}{2}\right) \cdot \left(\epsilon_y - \frac{1}{2}\right) \\ 0 & \left(\frac{3}{2} - \epsilon_x\right) \cdot \left(\frac{3}{2} - \epsilon_y\right) & \left(\epsilon_x - \frac{1}{2}\right) \cdot \left(\frac{3}{2} - \epsilon_y\right) \\ 0 & 0 & 0 \end{bmatrix} \tag{9}$$

- Case 2.: Constraints: $x_k \overset{!}{>} x_i$ and $y_l \overset{!}{<} y_i$

$$W_{kl}^{(i)} [C2] = \begin{bmatrix} \left(\frac{1}{2} - \epsilon_x\right) \cdot \left(\epsilon_y - \frac{1}{2}\right) & \left(\frac{1}{2} + \epsilon_x\right) \cdot \left(\epsilon_y - \frac{1}{2}\right) & 0 \\ \left(\frac{1}{2} - \epsilon_x\right) \cdot \left(\frac{3}{2} - \epsilon_y\right) & \left(\frac{1}{2} + \epsilon_x\right) \cdot \left(\frac{3}{2} - \epsilon_y\right) & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{10}$$

- Case 3.: Constraints: $x_k \overset{!}{>} x_i$ and $y_l \overset{!}{>} y_i$

$$W_{kl}^{(i)} [C3] = \begin{bmatrix} 0 & 0 & 0 \\ \left(\frac{1}{2} - \epsilon_x\right) \cdot \left(\frac{1}{2} + \epsilon_y\right) & \left(\frac{1}{2} + \epsilon_x\right) \cdot \left(\frac{1}{2} + \epsilon_y\right) & 0 \\ \left(\frac{1}{2} - \epsilon_x\right) \cdot \left(\frac{1}{2} - \epsilon_y\right) & \left(\frac{1}{2} + \epsilon_x\right) \cdot \left(\frac{1}{2} - \epsilon_y\right) & 0 \end{bmatrix} \tag{11}$$

- Case 4.: Constraints: $x_k \overset{!}{<} x_i$ and $y_l \overset{!}{>} y_i$

$$W_{kl}^{(i)} [C4] = \begin{bmatrix} 0 & 0 & 0 \\ 0 & \left(\frac{3}{2} - \epsilon_x\right) \cdot \left(\frac{1}{2} + \epsilon_y\right) & \left(\epsilon_x - \frac{1}{2}\right) \cdot \left(\frac{1}{2} + \epsilon_y\right) \\ 0 & \left(\frac{3}{2} - \epsilon_x\right) \cdot \left(\frac{1}{2} - \epsilon_y\right) & \left(\epsilon_x - \frac{1}{2}\right) \cdot \left(\frac{1}{2} - \epsilon_y\right) \end{bmatrix} \tag{12}$$

Consider that the weight matrix $W_{kl}^{(i)}$ of the cell (kl) is related to a particle that is within the reference cell in the context of center of mass position.

3.2 Weight matrix W for the second order method

In contrast to the first order method the second order method assigns a triangular function to the particle. The entries of the weight matrix are obtained by the convolution of the single particle function with the mesh function. Since the full calculation requires to have a look to 16 different cases we will only show for one entry of the weight matrix that the given solution on the exercise sheet is valid.

$$\begin{aligned}
W_{kl}^{(i)} &= \frac{1}{\Delta^4} \cdot \int_{\eta^2} \int_{\eta^2} \Pi\left(\frac{\vec{x} - \vec{x}_{kl}}{\Delta}\right) \cdot \Pi\left(\frac{\vec{x}_i - \vec{\alpha} - \vec{x}}{\Delta}\right) \cdot \Pi\left(\frac{\vec{\alpha}}{\Delta}\right) d\vec{x} d\vec{\alpha} \\
W_{kl}^{(i)} &= \frac{1}{\Delta^2} \cdot \int_{\eta} \Pi\left(\frac{x - x_k}{\Delta}\right) \cdot \Pi\left(\frac{x_i - \alpha_x - x}{\Delta}\right) \cdot \Pi\left(\frac{\alpha_x}{\Delta}\right) dx d\alpha_x \\
&\quad \times \frac{1}{\Delta^2} \cdot \int_{\eta} \Pi\left(\frac{y - y_l}{\Delta}\right) \cdot \Pi\left(\frac{y_i - \alpha_y - y}{\Delta}\right) \cdot \Pi\left(\frac{\alpha_y}{\Delta}\right) dy d\alpha_y \\
W_{kl}^{(i)} &= \frac{1}{\Delta} \cdot \int_{\eta} \left(\min\left\{\frac{x_k}{\Delta} + \frac{1}{2}, \frac{x_i - \alpha_x}{\Delta} + \frac{1}{2}\right\} - \max\left\{\frac{x_k}{\Delta} - \frac{1}{2}, \frac{x_i - \alpha_x}{\Delta} - \frac{1}{2}\right\} \right) \cdot \Pi\left(\frac{\alpha_x}{\Delta}\right) d\alpha_x \\
&\quad \times \frac{1}{\Delta} \cdot \int_{\eta} \left(\min\left\{\frac{y_l}{\Delta} + \frac{1}{2}, \frac{y_i - \alpha_y}{\Delta} + \frac{1}{2}\right\} - \max\left\{\frac{y_l}{\Delta} - \frac{1}{2}, \frac{y_i - \alpha_y}{\Delta} - \frac{1}{2}\right\} \right) \cdot \Pi\left(\frac{\alpha_y}{\Delta}\right) d\alpha_y
\end{aligned} \tag{13}$$

Here, α denotes the lag vector between the two convolutions. To further resolve the expression (13) for the weight matrix $W_{kl}^{(i)}$ it is required to split the calculation in 4×4 different cases. From now on, we will restrict the calculation to one single case and calculate the corresponding entry of the weight matrix. It is up to the reader to further deploy the introduced procedure to convince himself from the truthiness of the full solution given on the exercise sheet.

- Case 1. | First level restriction: $x_k \stackrel{!}{<} x_i$ and $y_l \stackrel{!}{<} y_i$
- Case 1. | Second level restriction (L1): $x_k \stackrel{!}{<} x_i - \alpha_x$ and $y_k \stackrel{!}{<} y_i - \alpha_y$

$$\begin{aligned}
W_{kl}^{(i)} [C1 | L1] &= \frac{1}{\Delta^2} \cdot \int_{-0.5 \cdot \Delta}^{\Delta \cdot (\epsilon_x - 0.5)} \left[\frac{3}{2} - \epsilon_x + \frac{\alpha_x}{\Delta} \right] d\alpha_x \cdot \int_{-0.5 \cdot \Delta}^{\Delta \cdot (\epsilon_y - 0.5)} \left[\frac{3}{2} - \epsilon_y + \frac{\alpha_y}{\Delta} \right] d\alpha_y \\
W_{kl}^{(i)} [C1 | L1] &= \frac{1}{\Delta^2} \cdot \left[\left(\frac{3}{2} - \epsilon_x \right) \cdot \alpha_x + \frac{\alpha_x^2}{2\Delta} \right] \Big|_{-0.5 \cdot \Delta}^{\Delta \cdot (\epsilon_x - 0.5)} \cdot \left[\left(\frac{3}{2} - \epsilon_y \right) \cdot \alpha_y + \frac{\alpha_y^2}{2\Delta} \right] d\alpha_y \Big|_{-0.5 \cdot \Delta}^{\Delta \cdot (\epsilon_y - 0.5)} \\
W_{kl}^{(i)} [C1 | L1] &= \left(\epsilon_x - \frac{\epsilon_x^2}{2} \right) \cdot \left(\epsilon_y - \frac{\epsilon_y^2}{2} \right)
\end{aligned} \tag{14}$$

- Case 1. | Second level restriction (L2): $x_k \stackrel{!}{>} x_i - \alpha_x$ and $y_k \stackrel{!}{<} y_i - \alpha_y$

$$\begin{aligned}
W_{kl}^{(i)} [C1 | L2] &= \frac{1}{\Delta^2} \cdot \int_{\Delta \cdot (\epsilon_x - 0.5)}^{0.5 \cdot \Delta} \left[\frac{1}{2} + \epsilon_x - \frac{\alpha_x}{\Delta} \right] d\alpha_x \cdot \int_{-0.5 \cdot \Delta}^{\Delta \cdot (\epsilon_y - 0.5)} \left[\frac{3}{2} - \epsilon_y + \frac{\alpha_y}{\Delta} \right] d\alpha_y \\
W_{kl}^{(i)} [C1 | L2] &= \frac{1}{\Delta^2} \cdot \left[\left(\frac{1}{2} + \epsilon_x \right) \cdot \alpha_x - \frac{\alpha_x^2}{2\Delta} \right] \Big|_{\Delta \cdot (\epsilon_x - 0.5)}^{0.5 \cdot \Delta} \cdot \left[\left(\frac{3}{2} - \epsilon_y \right) \cdot \alpha_y + \frac{\alpha_y^2}{2\Delta} \right] d\alpha_y \Big|_{-0.5 \cdot \Delta}^{\Delta \cdot (\epsilon_y - 0.5)} \\
W_{kl}^{(i)} [C1 | L2] &= \left(\frac{1}{2} - \frac{\epsilon_x^2}{2} \right) \cdot \left(\epsilon_y - \frac{\epsilon_y^2}{2} \right)
\end{aligned} \tag{15}$$

- Case 1. | Second level restriction (L3): $x_k \stackrel{!}{<} x_i - \alpha_x$ and $y_k \stackrel{!}{>} y_i - \alpha_y$

$$\begin{aligned}
W_{kl}^{(i)} [C1 | L3] &= \frac{1}{\Delta^2} \cdot \int_{-0.5 \cdot \Delta}^{\Delta \cdot (\epsilon_x - 0.5)} \left[\frac{3}{2} - \epsilon_x + \frac{\alpha_x}{\Delta} \right] d\alpha_x \cdot \int_{\Delta \cdot (\epsilon_y - 0.5)}^{0.5 \cdot \Delta} \left[\frac{1}{2} + \epsilon_y - \frac{\alpha_y}{\Delta} \right] d\alpha_y \\
W_{kl}^{(i)} [C1 | L3] &= \frac{1}{\Delta^2} \cdot \left[\left(\frac{3}{2} - \epsilon_x \right) \cdot \alpha_x + \frac{\alpha_x^2}{2\Delta} \right] \Big|_{-0.5 \cdot \Delta}^{\Delta \cdot (\epsilon_x - 0.5)} \cdot \left[\left(\frac{1}{2} + \epsilon_y \right) \cdot \alpha_y - \frac{\alpha_y^2}{2\Delta} \right] d\alpha_y \Big|_{\Delta \cdot (\epsilon_y - 0.5)}^{0.5 \cdot \Delta} \\
W_{kl}^{(i)} [C1 | L3] &= \left(\epsilon_x - \frac{\epsilon_x^2}{2} \right) \cdot \left(\frac{1}{2} - \frac{\epsilon_y^2}{2} \right)
\end{aligned} \tag{16}$$

- Case 1. | Second level restriction (L4): $x_k \stackrel{!}{>} x_i - \alpha_x$ and $y_k \stackrel{!}{>} y_i - \alpha_y$

$$\begin{aligned}
W_{kl}^{(i)} [C1 | L4] &= \frac{1}{\Delta^2} \cdot \int_{\Delta \cdot (\epsilon_x - 0.5)}^{0.5 \cdot \Delta} \left[\frac{1}{2} + \epsilon_x - \frac{\alpha_x}{\Delta} \right] d\alpha_x \cdot \int_{\Delta \cdot (\epsilon_y - 0.5)}^{0.5 \cdot \Delta} \left[\frac{1}{2} + \epsilon_y - \frac{\alpha_y}{\Delta} \right] d\alpha_y \\
W_{kl}^{(i)} [C1 | L4] &= \frac{1}{\Delta^2} \cdot \left[\left(\frac{1}{2} + \epsilon_x \right) \cdot \alpha_x - \frac{\alpha_x^2}{2\Delta} \right] \Big|_{\Delta \cdot (\epsilon_x - 0.5)}^{0.5 \cdot \Delta} \cdot \left[\left(\frac{1}{2} + \epsilon_y \right) \cdot \alpha_y - \frac{\alpha_y^2}{2\Delta} \right] d\alpha_y \Big|_{\Delta \cdot (\epsilon_y - 0.5)}^{0.5 \cdot \Delta} \\
W_{kl}^{(i)} [C1 | L4] &= \left(\frac{1}{2} - \frac{\epsilon_x^2}{2} \right) \cdot \left(\frac{1}{2} - \frac{\epsilon_y^2}{2} \right)
\end{aligned} \tag{17}$$

- Case 1. | First level restriction: $x_k \stackrel{!}{<} x_i$ and $y_l \stackrel{!}{<} y_i$

To obtain the full solution for the first case it is necessary to sum over all possibilities of second level conditions. The summation returns the first entry of the weight matrix $W_{kl}^{(i)}$.

$$\begin{aligned}
W_{kl}^{(i)} [C1] &= W_{kl}^{(i)} [C1 | L1] + W_{kl}^{(i)} [C1 | L2] + W_{kl}^{(i)} [C1 | L3] + W_{kl}^{(i)} [C1 | L4] \\
W_{kl}^{(i)} [C1] &= \left(\frac{1}{2} + \epsilon_x - \epsilon_x^2 \right) \cdot \left(\frac{1}{2} + \epsilon_y - \epsilon_y^2 \right)
\end{aligned} \tag{18}$$

Relation (18) is equivalent to the middle entry of the weight matrix $W_{kl}^{(i)}[1, 1]$ given on the exercise sheet. ■