3.3.2 Numerical method

In this subsection, we propose a procedure to simulate the dynamics of the whole fluids-membrane system. The procedure mainly contains two FEM based numerical schemes for weak formulations (3.56a)-(3.56f) and (3.57a)-(3.57f), respectively, and the modification of the numerical mesh.

We uniformly partition the time domain [0,T] as $[0,T] = \bigcup_{m=1}^{M} [t_{m-1},t_m]$ with $t_m = m\tau$ and $\tau = T/M$, and the reference domain $D_{\mathbf{r}} = [0,1]$ for the fluid-fluid interface as $D_{\mathbf{r}} = \bigcup_{j=1}^{\mathcal{R}} D_{\mathbf{r},j}$ where $D_{\mathbf{r},j} = [\zeta_{j-1},\zeta_j]$ with $\zeta_j = jh_{\mathbf{r}}$ and $h_{\mathbf{r}} = 1/\mathcal{R}$. The reference domain of the membrane at time $t = t_m$ is discretized as $D_{\mathbf{q}}^m = [-1,x_l^m] \cup [x_l^m,x_r^m] \cup [x_r^m,1]$ with $D_{\mathbf{q}}^m = \bigcup_{j=1}^{\mathcal{Q}} D_{\mathbf{q},j}^m$, where x_l^m,x_r^m denote the left and right contact lines' x value and $D_{\mathbf{q},j}^m = [x_{j-1}^m,x_j^m]$ with $-1 = x_0^m < x_1^m < x_2^m < \cdots < x_{j_l}^m = x_l^m < \cdots < x_{j_r}^m = x_r^m < \cdots < x_{\mathcal{Q}}^m = 1$. We use the following finite-dimensional spaces to approximate $H^1(D_{\mathbf{q}}^m)$, $H^1_0(D_{\mathbf{q}}^m)$, $H^1_0(D_{\mathbf{r}})$, respectively,

$$V^{m} := \left\{ f \in C(D_{\mathbf{q}}^{m}) : f|_{D_{\mathbf{q},j}^{m}} \in \mathcal{P}_{2}(D_{\mathbf{q},j}^{m}), \ \forall j = 1, 2, \cdots, \mathcal{Q} \right\},$$
(3.58a)

$$V_0^m := \{ f \in V^m : f(-1) = f(1) = 0 \},$$
(3.58b)

$$V_1^m := \left\{ g \in C([x_l^m, x_r^m]) : g|_{D_{\mathbf{q}, j}^m} \in \mathcal{P}_2(D_{\mathbf{q}, j}^m), \ \forall j = j_l + 1, \cdots, j_r \right\},$$
(3.58c)

$$V_2^m := \left\{ g \in C([-1, x_l^m] \cup [x_r^m, 1]) : g|_{D_{\mathbf{q}, j}^m} \in \mathcal{P}_2(D_{\mathbf{q}, j}^m), \right.$$

$$\forall j = 1, 2, \dots, j_l, j_r + 1, \dots, Q, \ g(-1) = g(1) = 0$$
, (3.58d)

$$W^h := \{ \psi \in C(D_{\mathbf{r}}) : \psi|_{D_{\mathbf{r},i}} \in \mathcal{P}_2(D_{\mathbf{r},i}), \ \forall j = 1, 2, \cdots, \mathcal{R} \},$$
 (3.58e)

$$W_0^h := \left\{ \psi \in W^h : \psi(0) = \psi(1) = 0 \right\}, \tag{3.58f}$$

where $\mathcal{P}_2(D)$ denotes the space of polynomials with degrees at most 2 on D.

Let $\Xi^m := \mathbf{q}^m = (x^m, y^m) \in D^m_{\mathbf{q}} \times V^m$ be the numerical approximation to the whole membrane Ξ at the time step t_m . Then it is straightforward to define Σ^m_1 and Σ^m_2 with $\Xi^m = \Sigma^m_1 \cup \Sigma^m_2$ as separated by x^m_l and x^m_r . For piecewise continuous functions u and v defined on $D^m_{\mathbf{q}}$, the inner products on Σ^m_1 , Σ^m_2 and Ξ^m can be

approximated as

$$(u, v)_{\Sigma_1^m} := \sum_{j=j_l+1}^{j_r} |\partial_x \mathbf{q}^m|_j \int_{x_{j-1}^m}^{x_j^m} u(x)v(x) dx,$$
 (3.59a)

$$(u, v)_{\Sigma_2^m} := \left(\sum_{j=1}^{j_l} + \sum_{j=j_r+1}^{\mathcal{Q}}\right) |\partial_x \mathbf{q}^m|_j \int_{x_{j-1}^m}^{x_j^m} u(x)v(x) dx,$$
(3.59b)

$$(u, v)_{\Xi^m} := (u, v)_{\Sigma_1^m} + (u, v)_{\Sigma_2^m},$$
 (3.59c)

where $|\partial_x \mathbf{q}^m|_j = \sqrt{1 + \left(\frac{y^m(x_j^m) - y^m(x_{j-1}^m)}{x_j^m - x_{j-1}^m}\right)^2}$, $j = 1, 2, \dots, \mathcal{Q}$. We could further compute them using the Boole's rule as

$$\int_{x_{j-1}^m}^{x_j^m} u(x)v(x)dx = \frac{x_j^m - x_{j-1}^m}{90} \left[7(u \cdot v)(x_{j-1}^{m,+}) + 32(u \cdot v)(x_{j-3/4}^m) + 12(u \cdot v)(x_{j-\frac{1}{2}}^m) + 32(u \cdot v)(x_{j-1/4}^m) + 7(u \cdot v)(x_j^{m,-}) \right],$$
(3.60)

where $u(x_j^{m,\pm})$ are the one-sided limits of u approaching x_j^m from the right and left sides, $x_{j-3/4}^m = \frac{1}{4}(3x_{j-1}^m + x_j^m)$, $x_{j-\frac{1}{2}}^m = \frac{1}{2}(x_{j-1}^m + x_j^m)$ and $x_{j-1/4}^m = \frac{1}{4}(x_{j-1}^m + 3x_j^m)$. Let $\boldsymbol{\tau}^m$, \mathbf{n}^m , κ^m , ν^m be the numerical approximations to the membrane's unit tangential and normal vectors, the membrane curvature, and the membrane inner tension, respectively, at the time step t_m .

Let $\Sigma_3^m := \mathbf{r}^m = (x_{\mathbf{r}}^m(\zeta), y_{\mathbf{r}}^m(\zeta)) \in W^h \times W^h$ be the numerical approximation to the fluid-fluid interface Σ_3 at the time step t_m . For piecewise continuous functions u and v defined on $D_{\mathbf{r}}$, the inner products on Σ_3^m can be approximated as

$$(u, v)_{\Sigma_3^m} := \sum_{j=1}^{\mathcal{R}} |\mathbf{r}^m(\zeta_j) - \mathbf{r}^m(\zeta_{j-1})| \int_{\zeta_{j-1}}^{\zeta_j} u(\zeta)v(\zeta)d\zeta,$$
(3.61)

where $|\mathbf{r}^m(\zeta_j) - \mathbf{r}^m(\zeta_{j-1})| = \sqrt{(x_{\mathbf{r}}^m(\zeta_j) - x_{\mathbf{r}}^m(\zeta_{j-1}))^2 + (y_{\mathbf{r}}^m(\zeta_j) - y_{\mathbf{r}}^m(\zeta_{j-1}))^2}, \ j = 1, 2, \dots, \mathcal{R}$. Similarly, we could further compute it using the Boole's rule.

Based on the discretization of $D_{\mathbf{r}}$ and $D_{\mathbf{q}}^m$, we denote $\mathbf{r}_j^m = \mathbf{r}^m(\zeta_j), \ j = 0, 1, \cdots, \mathcal{R}$

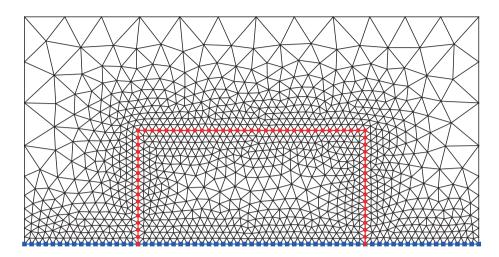


Figure 3.3: The initial mesh used for wetting and nonwetting examples with $\mathcal{R} = 64$, $\mathcal{Q} = 64$, $J^0 = 1120$, $N^0 = 2142$. The red line with circle markers represents the fluid-fluid interface. The blue line with square markers represents the membrane.

and $\mathbf{q}_j^m = (x_j^m, y^m(x_j^m)), \ j = 0, 1, \dots, \mathcal{Q}$ as markers to represent the fluid-fluid interface Σ_3^m and the membrane Ξ^m , respectively. Especially, we have $\mathbf{r}_0^m = \mathbf{q}_{j_l}^m = (x_l^m, y^m(x_l^m))$ marking the left contact line Λ_l^m and $\mathbf{r}_{\mathcal{R}}^m = \mathbf{q}_{j_r}^m = (x_r^m, y^m(x_r^m))$ marking the right contact line Λ_r^m .

Let $\mathcal{T}^m := \bigcup_{j=1}^{N^m} \bar{o}_j^m$ be a triangulation of Ω^m at the time step $t = t_m$. The mesh contains J^m vertices denoted by $\{\mathbf{p}_k^m\}_{k=1}^{J^m}$. We use a fitted mesh (see Fig. 3.3) such that line segments of Ξ^m and Σ_3^m are edges from \mathcal{T}^m , i.e., $\Xi^m \cup \Sigma_3^m \subset \bigcup_{j=1}^{N^m} \partial o_j^m$. Besides, markers \mathbf{r}_j^m , $j = 0, 1, \dots, \mathcal{R}$ and markers \mathbf{q}_j^m , $j = 0, 1, \dots, \mathcal{Q}$ are vertices of the mesh. We define the following finite element spaces over \mathcal{T}^m ,

$$S_k^m := \{ \varphi_h \in C(\bar{\Omega}^m) : \varphi_h|_{o_i^m} \in \mathcal{P}_k(o_j^m), \ j = 1, \dots, N^m \},$$
 (3.62a)

$$S_0^m := \{ \varphi_h \in L^2(\Omega^m) : \varphi_h|_{o_i^m} \in \mathcal{P}_0(o_j^m), \ j = 1, \dots, N^m \},$$
 (3.62b)

where $\mathcal{P}_k(D)$ denotes the space of polynomials with degrees at most k on D.

The fluid-fluid interface Σ_3^m divides the domain Ω^m into Ω_1^m and Ω_2^m . Correspondingly, the mesh \mathcal{T}^m is divided into \mathcal{T}_1^m and \mathcal{T}_2^m . Based on the spatial discretization,

we define the viscosity η^m and the surface tension γ^m as

$$\eta^{m} = \eta_{1} \chi_{\Omega_{1}^{m}} + \eta_{2} \chi_{\Omega_{2}^{m}}, \quad \gamma^{m} = \gamma_{1} \chi_{\Sigma_{1}^{m}} + \gamma_{2} \chi_{\Sigma_{2}^{m}}. \tag{3.63}$$

We denote the corresponding finite element spaces for \mathbb{U}_i (i = 1, 2, 3) and \mathbb{P} as \mathbb{U}_i^m (i = 1, 2, 3) and \mathbb{P}^m , respectively. These finite element spaces are chosen to use the standard P2-(P1+P0) elements as

$$\mathbb{U}_{1}^{m} = [S_{2}^{m}]^{2} \cap \mathbb{U}_{1}, \quad \mathbb{U}_{2}^{m} = [S_{2}^{m}]^{2} \cap \mathbb{U}_{2}, \quad \mathbb{P}^{m} = (S_{1}^{m} + S_{0}^{m}) \cap \mathbb{P},$$
 (3.64a)

$$\mathbb{U}_{3}^{m} = \left\{ \boldsymbol{\omega} \in \mathbb{U}_{1}^{m} : \boldsymbol{\omega} \cdot \mathbf{n}^{m} = -\frac{1}{|\partial_{x} \mathbf{q}^{m}|} \frac{y^{m} - y^{m-1}}{\tau} \text{ on } \Xi^{m} \right\},$$
(3.64b)

where $|\partial_x \mathbf{q}^m| = \sqrt{1 + (\frac{\partial y^m}{\partial x})^2}$. These choices satisfy the inf-sup stability condition,

$$\inf_{\varphi \in \mathbb{P}^m} \sup_{0 \neq \boldsymbol{\omega} \in \mathbb{U}_i^m} \frac{(\varphi, \nabla \cdot \boldsymbol{\omega})_{\Omega^m}}{\|\varphi\|_0 \|\boldsymbol{\omega}\|_1} \ge C_0 > 0, \quad i = 1, 2,$$
(3.65)

where C_0 is a constant, and $\|\cdot\|_0$ and $\|\cdot\|_1$ denote the L^2 and H^1 -norm on Ω^m , respectively.

The overall procedure of the numerical method is summarized as follows. Given the initial configuration of the system including $D_{\mathbf{q}}^0$, y^0 and κ^0 for the membrane Ξ^0 , \mathbf{r}^0 for the fluid-fluid interface Σ_3^0 , and \mathcal{T}^0 for the triangulation of Ω^0 . Set m=0 and then go through the following steps.

(1) Fix the current configuration of fluid-fluid interface \mathbf{r}^m and the positions of the contact lines x_l^m and x_r^m , based on the mesh \mathcal{T}^m , find the fluid velocity $\mathbf{u}^{m+\frac{1}{2}} \in \mathbb{U}_1^m$, the fluid pressure $p^{m+\frac{1}{2}} \in \mathbb{P}^m$, the membrane configuration $y^{m+\frac{1}{2}} \in V^m$, the curvature of the membrane $\kappa^{m+\frac{1}{2}} \in V_0^m$, and the inner tension of the membrane $\nu^{m+\frac{1}{2}} \in V_1^m \cup V_2^m$ such that

$$+ \frac{c_b}{Ca} \left(\partial_s^m (\frac{\kappa^{m+\frac{1}{2}}}{|\partial_x \mathbf{q}^m|}), \ \partial_s^m (|\partial_x \mathbf{q}^m| \boldsymbol{\omega}^h \cdot \mathbf{n}^m) \right)_{\Xi^m}$$
(3.66a)
$$+ \frac{3c_b}{2Ca} \left((\kappa^m)^2 \partial_s^m y^m, \ \partial_s^m (|\partial_x \mathbf{q}^m| \boldsymbol{\omega}^h \cdot \mathbf{n}^m) \right)_{\Xi^m} + \frac{1}{Ca} \left(\partial_s \mathbf{r}^m, \ \partial_s \boldsymbol{\omega}^h \right)_{\Sigma_3^m}$$
$$+ \frac{\gamma_1 - \gamma_2}{Ca} \left(\left(|\partial_x \mathbf{q}^m| \boldsymbol{\omega}_1^h \right) \Big|_{\Lambda_r^m} - \left(|\partial_x \mathbf{q}^m| \boldsymbol{\omega}_1^h \right) \Big|_{\Lambda_l^m} \right) = 0, \quad \forall \boldsymbol{\omega}^h = (\omega_1^h, \omega_2^h) \in \mathbb{U}_1^m,$$
$$\left(\nabla \cdot \mathbf{u}^{m+\frac{1}{2}}, \varphi^h \right)_{\Omega^m} = 0, \quad \forall \varphi^h \in \mathbb{P}^m,$$
(3.66b)
$$\underbrace{\mathbf{M41}}_{\mathbf{V}} \left(\frac{y^{m+\frac{1}{2}} - y^m}{\tau}, f^h \right)_{\Xi^m} + \left(|\partial_x \mathbf{q}^m| \mathbf{u}^{m+\frac{1}{2}} \cdot \mathbf{n}^m, f^h \right)_{\Xi^m} = 0, \quad \forall f^h \in V^m,$$
(3.66c)
$$\underbrace{\left(\frac{\kappa^{m+\frac{1}{2}}}{|\partial_x \mathbf{q}^m|}, \beta^h \right)_{\Xi^m}}_{\mathbf{E}^m} + \left(\partial_s^m y^{m+\frac{1}{2}}, \partial_s^m \beta^h \right)_{\Xi^m} = 0, \quad \forall \beta^h \in V_0^m,$$
(3.66d)
$$\underbrace{\frac{l_s}{|\partial_x \mathbf{q}^m|}}_{\mathbf{E}^m}, \beta^h \underbrace{\frac{l_s}{|\partial_x \mathbf{q}^m|}}_{\mathbf{E}^m} + Ca \left(\nabla_s^m \cdot \mathbf{u}^{m+\frac{1}{2}}, g_1^h \right)_{\Sigma_1^m} \\ + \underbrace{\frac{1}{\mu_1}}_{\mathbf{L}} \left([\nu^{m+\frac{1}{2}}]_2^1 g_1^h \right) \Big|_{\Lambda^m} = 0, \quad \forall g_1^h \in V_1^m,$$
(3.66e)
$$\underbrace{\frac{l_s}{\mu_2}}_{\mathbf{L}^m} \left(\partial_s^m \nu^{m+\frac{1}{2}}, \partial_s^m g_2^h \right)_{\Sigma_2^m} + Ca \left(\nabla_s^m \cdot \mathbf{u}^{m+\frac{1}{2}}, g_2^h \right)_{\Sigma_2^m} \\ - \underbrace{\frac{1}{\mu_1}}_{\mathbf{L}^m} \left([\nu^{m+\frac{1}{2}}]_2^1 g_2^h \right) \Big|_{\Lambda^m} = 0, \quad \forall g_2^h \in V_2^m,$$
(3.66f)

where $\partial_s^m = \frac{1}{|\partial_x \mathbf{q}^m|} \frac{\partial}{\partial x}$, $\nabla_s^m = \boldsymbol{\tau}^m \partial_s^m$, and the superscript $m + \frac{1}{2}$ is used to denote the temporary state from the time step t_m to t_{m+1} .

(2) Due to the condition that the fluid-fluid interface always attaches the membrane, update the y value of $\mathbf{r}^m(0)$ and $\mathbf{r}^m(1)$ as

$$\mathbf{r}^{m+\frac{1}{2}}(\zeta) = \begin{cases} (x_l^m, y^{m+\frac{1}{2}}(x_l^m)), & \zeta = 0, \\ (x_r^m, y^{m+\frac{1}{2}}(x_r^m)), & \zeta = 1, \\ \mathbf{r}^m(\zeta), & 0 < \zeta < 1. \end{cases}$$
(3.67)

Use the computed membrane configuration $y^{m+\frac{1}{2}}$ to update the numerical mesh from \mathcal{T}^m to $\mathcal{T}^{m+\frac{1}{2}}$. Since $x_j^m, j=0,1,\cdots,\mathcal{Q}$ are not modified, set $D_{\mathbf{q}}^{m+\frac{1}{2}}$ as $D_{\mathbf{q},j}^{m+\frac{1}{2}}=D_{\mathbf{q},j}^m$ for $j=1,2,\cdots,\mathcal{Q}$.

(3) Using the computed $y^{m+\frac{1}{2}}$, based on the mesh $\mathcal{T}^{m+\frac{1}{2}}$, find the fluid velocity

 $\mathbf{u}^{m+1} \in \mathbb{U}_3^{m+\frac{1}{2}}$, the fluid pressure $p^{m+1} \in \mathbb{P}^{m+\frac{1}{2}}$, the inner tension of the membrane $\nu^{m+1} \in V_1^{m+\frac{1}{2}} \cup V_2^{m+\frac{1}{2}}$, and the fluid-fluid interface $\mathbf{r}^{m+1} \in W^h \times W^h$ such that

$$\frac{y_{\mathbf{r}}^{m+1}(0) - y_{\mathbf{r}}^{m+\frac{1}{2}}(0)}{\tau} = \frac{\partial y^{m+\frac{1}{2}}}{\partial x} \Big|_{x=x_l^m} \frac{x_{\mathbf{r}}^{m+1}(0) - x_{\mathbf{r}}^{m+\frac{1}{2}}(0)}{\tau},$$
(3.68f)

$$\frac{y_{\mathbf{r}}^{m+1}(1) - y_{\mathbf{r}}^{m+\frac{1}{2}}(1)}{\tau} = \frac{\partial y^{m+\frac{1}{2}}}{\partial x} \Big|_{x=x^m} \frac{x_{\mathbf{r}}^{m+1}(1) - x_{\mathbf{r}}^{m+\frac{1}{2}}(1)}{\tau}, \tag{3.68g}$$

where Eq. (3.68f) and Eq. (3.68g)) are numerical approximations to the time derivatives of $y_{\mathbf{r}}(0,t) = y^{m+\frac{1}{2}}(x_{\mathbf{r}}(0,t))$ and $y_{\mathbf{r}}(1,t) = y^{m+\frac{1}{2}}(x_{\mathbf{r}}(1,t))$, respectively. These two equations are approximating the motion of contact lines along the membrane.

(4) Update x_l^{m+1} , x_r^{m+1} with

$$x_l^{m+1} = x_{\mathbf{r}}^{m+1}(0), \quad x_r^{m+1} = x_{\mathbf{r}}^{m+1}(1),$$
 (3.69)

Then we could update markers for the membrane \mathbf{q}_{j}^{m+1} , $j=0,1,\cdots,\mathcal{Q}$ as

$$\mathbf{q}_{j}^{m+1} = \begin{cases} (x_{l}^{m+1}, y_{\mathbf{r}}^{m+1}(0)), & j = j_{l}, \\ (x_{r}^{m+1}, y_{\mathbf{r}}^{m+1}(1)), & j = j_{r}, \\ (x_{j}^{m}, y^{m+\frac{1}{2}}(x_{j}^{m})), & j = 0, 1, \dots, \mathcal{Q} \text{ but } j \neq j_{l}, j_{r}. \end{cases}$$
(3.70)

- (5) Fix the markers $\mathbf{r}_0^{m+1} = \mathbf{q}_{j_l}^{m+1}$, $\mathbf{r}_{\mathcal{R}}^{m+1} = \mathbf{q}_{j_r}^{m+1}$ for the contact lines. According to the equal arclength, redistribute markers \mathbf{r}_j^{m+1} , $j=1,2,\cdots,\mathcal{R}-1$ for the fluid-fluid interface Σ_3^{m+1} , markers \mathbf{q}_j^{m+1} , $j=j_l+1,\cdots,j_r-1$ for the membrane Σ_1^{m+1} under the droplet, and markers \mathbf{q}_j^{m+1} , $j=0,1,\cdots,j_l-1,j_r+1,\cdots,\mathcal{Q}$ for the membrane Σ_2^{m+1} outside the droplet. A ratio ρ between the average arclengths of Σ_1^{m+1} and Σ_2^{m+1} is computed. If the ratio $\rho \in [1/1.3,1.3]$, no further redistribution is conducted. If the ratio $\rho > 1.3$ or $\rho < 1/1.3$, to guarantee a good approximation accuracy of markers, our operation is to redetermine the numbers of markers for Σ_1^{m+1} and Σ_2^{m+1} to make the ratio ρ as closed to one as possible, while the total number of markers for the membrane remains unchanged. Then, new markers can be determined by interpolation. After these redistribution, we obtain $D_{\mathbf{q}}^{m+1}$ and $y^{m+1} \in V^{m+1}$, and then we could compute the membrane curvature $\kappa^{m+1} \in V_0^{m+1}$.
- (6) If no redetermination is conducted in the previous step, use the moving mesh method to generate the new fitted mesh \mathcal{T}^{m+1} from \mathcal{T}^m , which is introduced in Appendix B.3. Otherwise, use the same method for the initial mesh to generate the new mesh \mathcal{T}^{m+1} . Then, go to step (1) with m = m + 1.

3.3.3 Well-posedness of the FEM schemes

We show that the FEM schemes (3.66a)-(3.66f) and (3.68a)-(3.68g) both yield a unique solution.

Theorem 1. (Well-posedness). Let $(\mathbb{U}_1^m, \mathbb{P}^m)$ satisfy the inf-sup condition (3.65). Then the FEM scheme (3.66a)-(3.66f) admits a unique solution.