Predicting micro-bubble system dynamics with PINN

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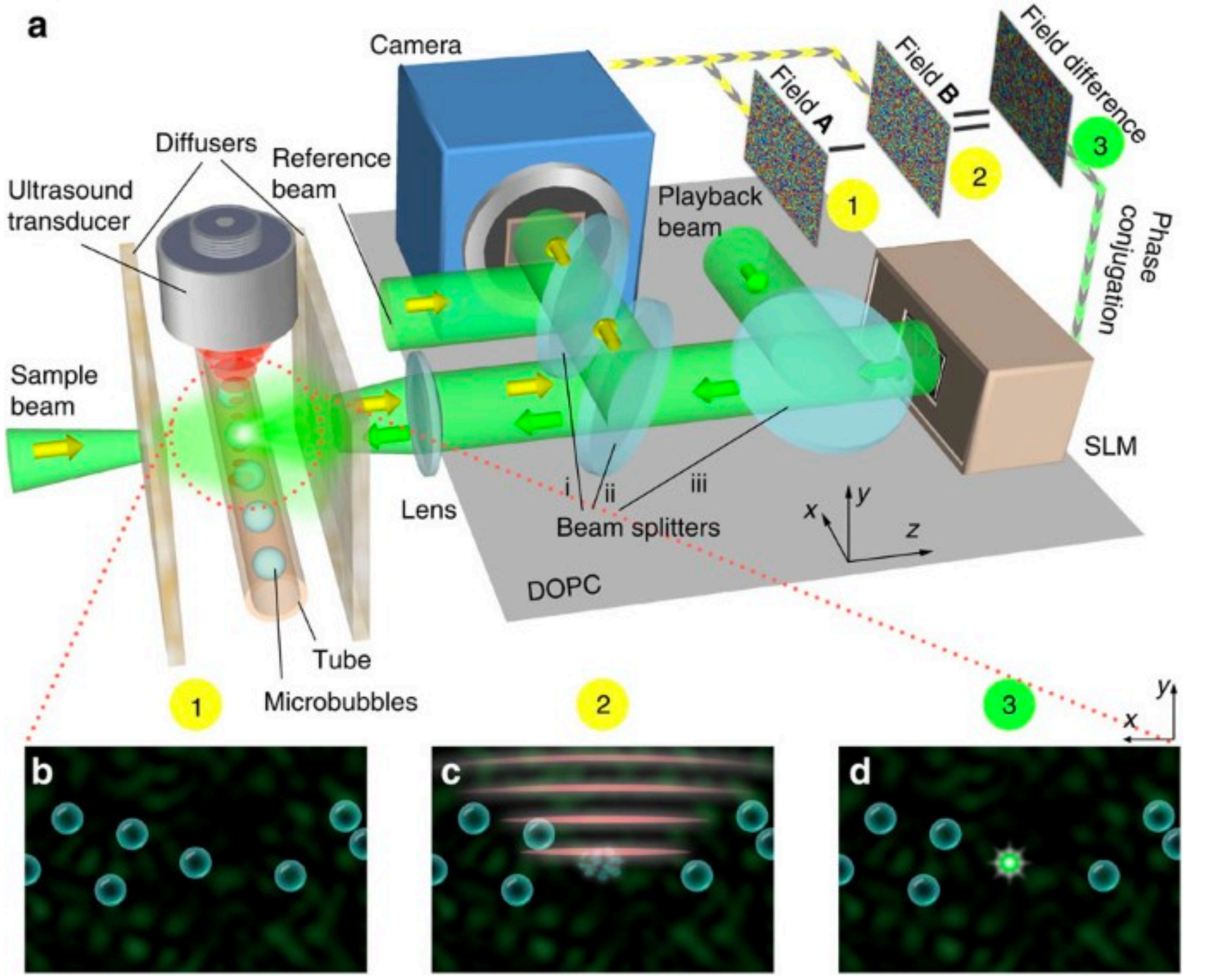
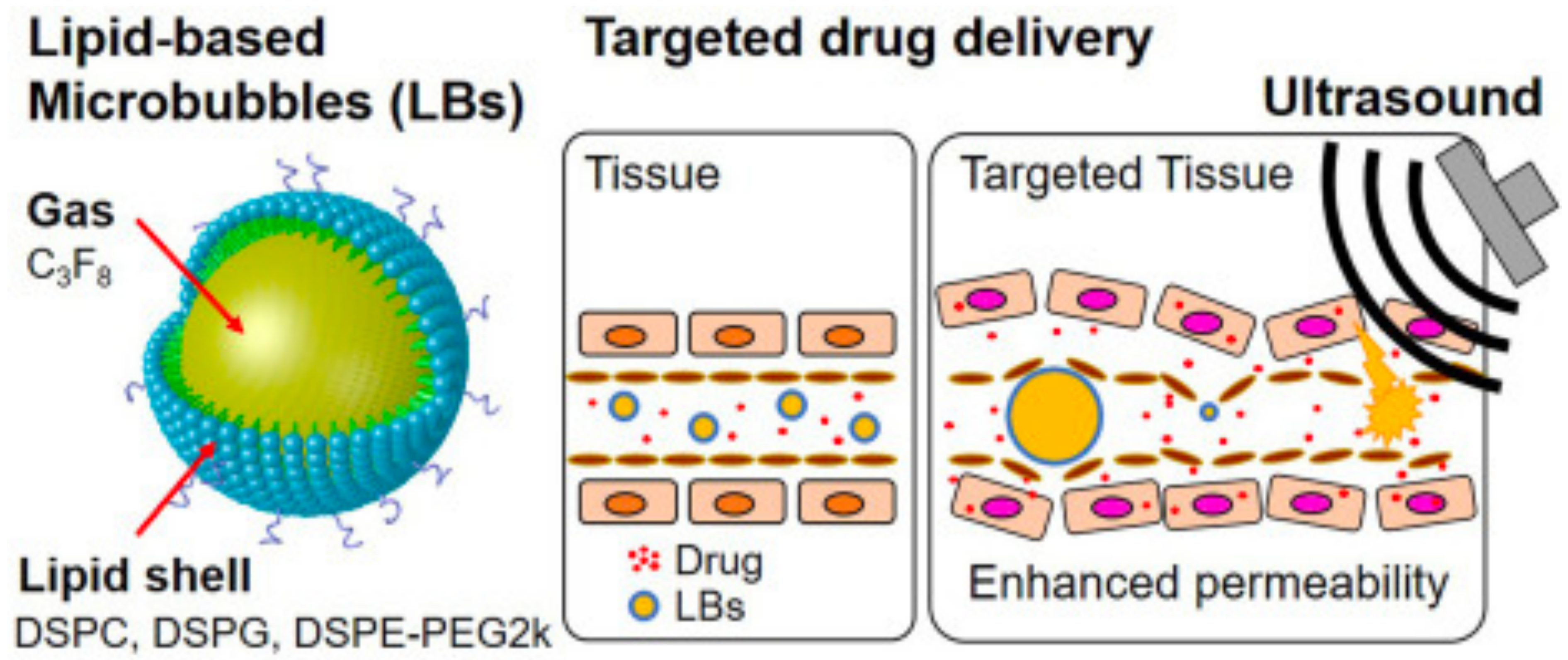
Mar 22, 2021

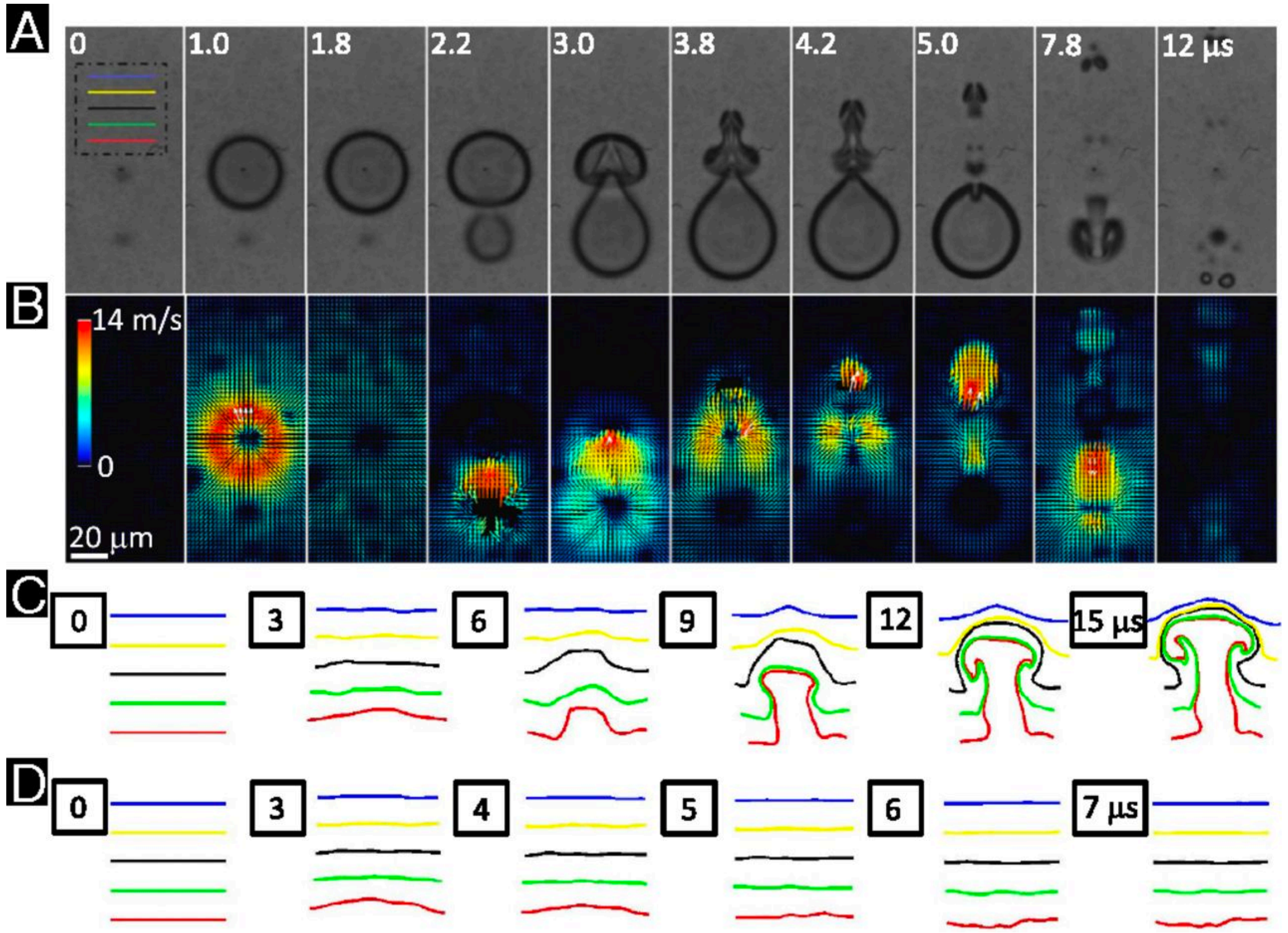
Background



Ruan *et al*., *Nat. Com.*, 2015



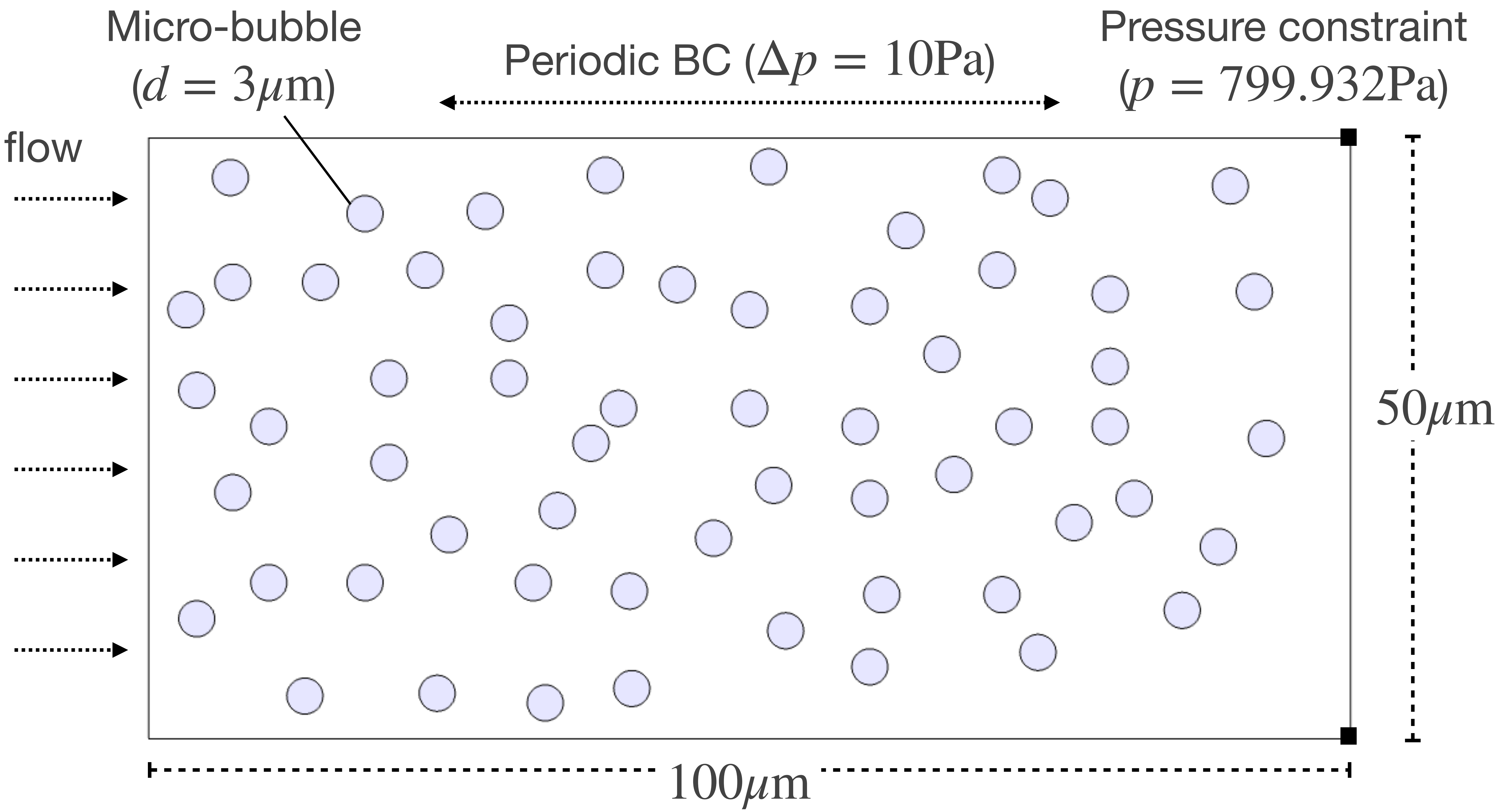
Omata *et al*., *Adv. Drug Deliv. Rev.*, 2020



Omata *et al*., *PNAS*, 2015

Modeling

Microfluids in pipe flow

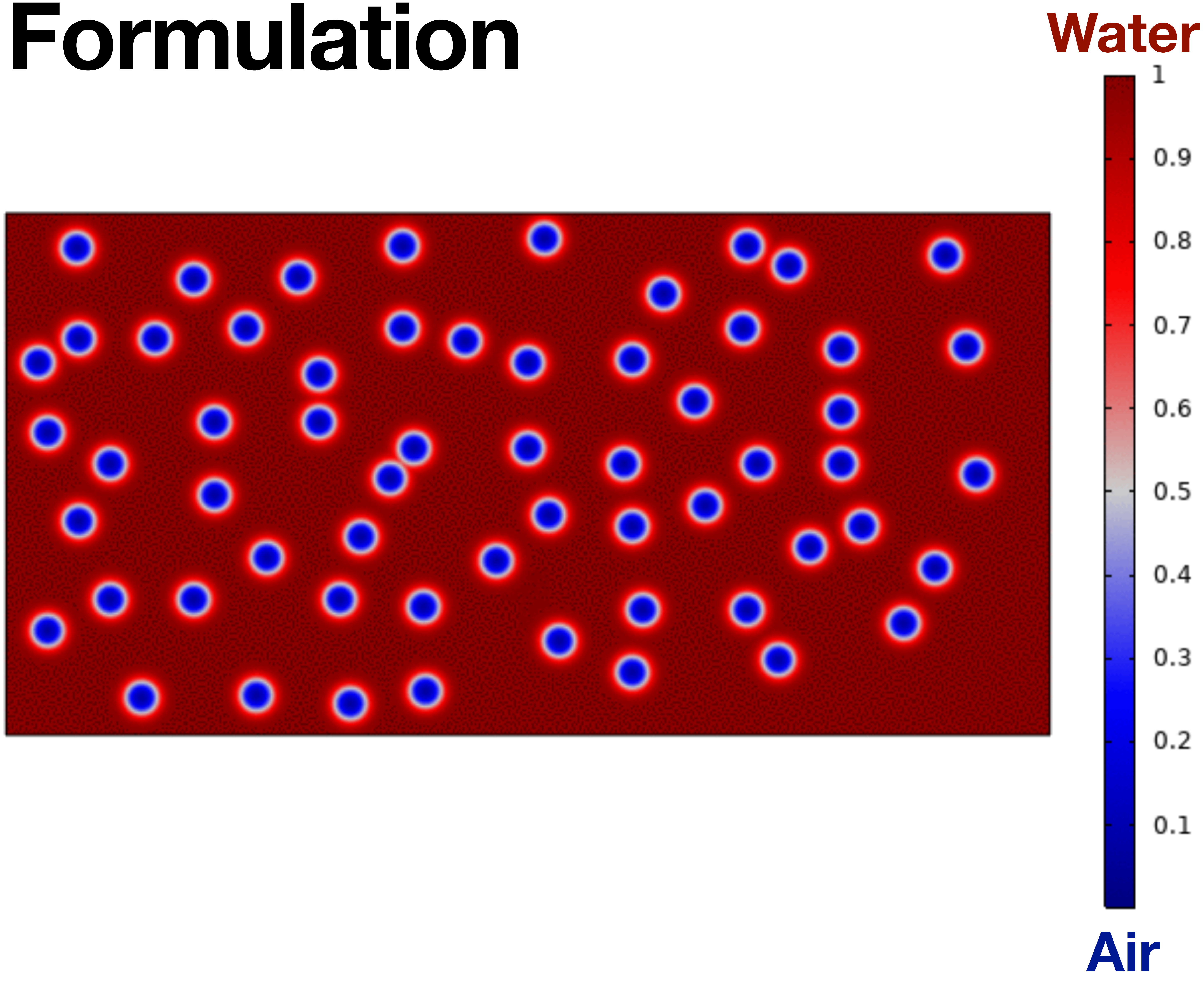


	Air	Water
ρ	1.204	998.23
μ	1.825×10^{-4}	1.0016×10^{-3}
%	0.0903	0.9097

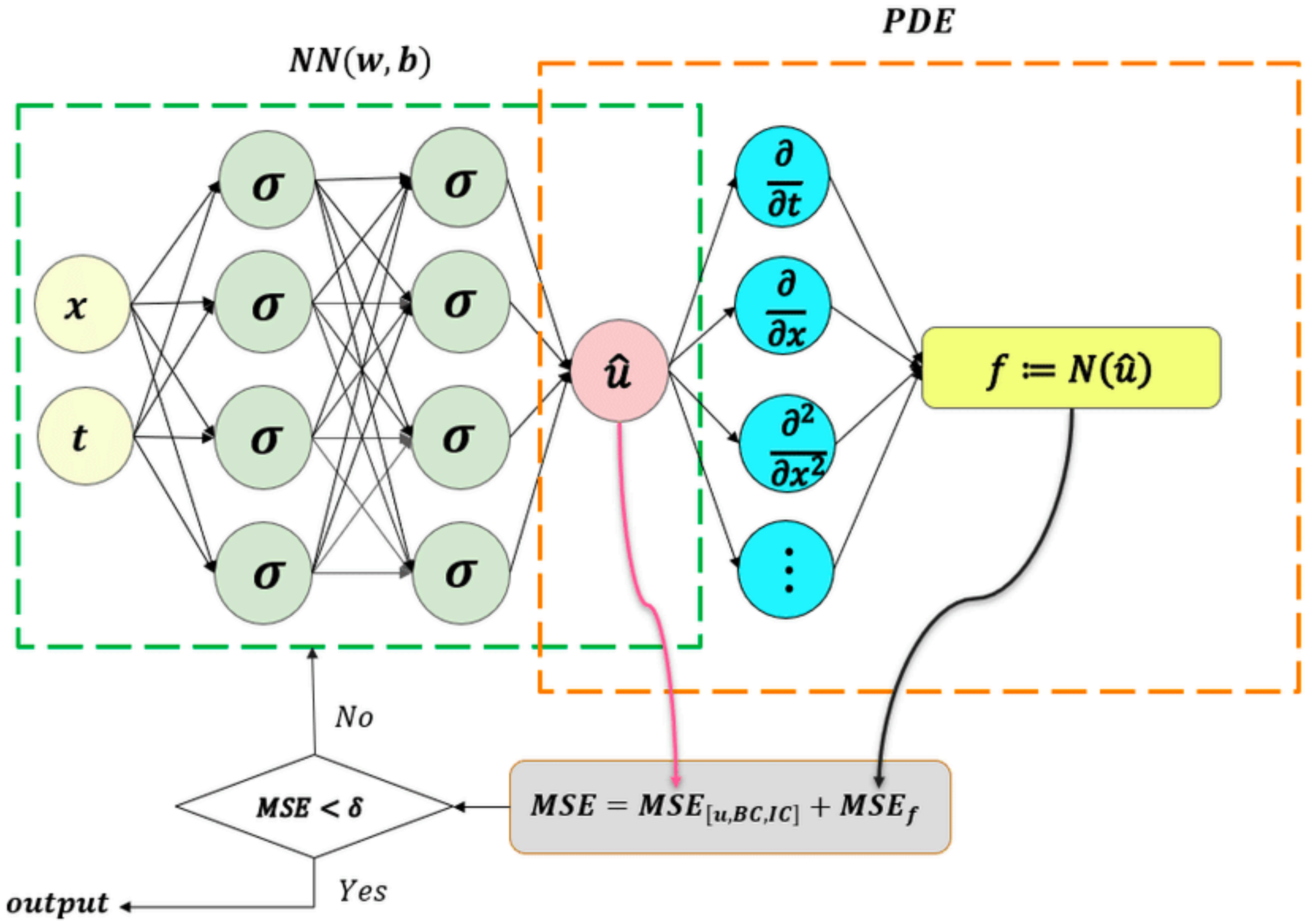
(All at 20℃, with SI system)

IC: $p_0 = 799.932\text{Pa}$ (6mmHg)

Problem Formulation



Physics-Informed Neural Network



Theory

The Navier-Stokes equation is given as

$$\rho(u_t + uu_x + vu_y) = -p_x + \mu(u_{xx} + u_{yy})$$
$$\rho(v_t + uv_x + vv_y) = -p_y + \mu(v_{xx} + v_{yy})$$

For two phase flows (bubble dynamics), we reconstruct density and viscosity into

$$(\alpha_1\rho_1 + \alpha_2\rho_2)(u_t + uu_x + vu_y) = -p_x + [\beta(\alpha_1\mu_1 + \alpha_2\mu_2)](u_{xx} + u_{yy})$$
$$(\alpha_1\rho_1 + \alpha_2\rho_2)(v_t + uv_x + vv_y) = -p_y + [\beta(\alpha_1\mu_1 + \alpha_2\mu_2)](v_{xx} + v_{yy}) \quad \text{(A)}$$

Where β is the *Bubble Coefficient* pertaining surface tension, velocity field, etc.

For PINNs, **PREDICTING** the solution & **IDENTIFYING** the equation (dynamics) can be applied simultaneously.

Review

When ρ takes 1, Raissi *et al*. reconstruct the N-S equation into

$$1(u_t + uu_x + vu_y) = -p_x + \mu(u_{xx} + u_{yy}) \qquad u_t + \lambda_1(uu_x + vu_y) = -p_x + \lambda_2(u_{xx} + u_{yy})$$

$$1(v_t + uv_x + vv_y) = -p_y + \mu(v_{xx} + v_{yy}) \dashrightarrow v_t + \lambda_1(uv_x + vv_y) = -p_y + \lambda_2(v_{xx} + v_{yy})$$

Where λ_1 and λ_2 is to be learnt from the neural network.

Here, we adopt λ_1 and λ_2 to reconstruct Eq. A into three forms

$$(\alpha_1\rho_1 + \alpha_2\rho_2)(u_t + uu_x + vu_y) = -p_x + [\beta(\alpha_1\lambda_1 + \alpha_2\lambda_2)](u_{xx} + u_{yy})$$

$$(\alpha_1\rho_1 + \alpha_2\rho_2)(v_t + uv_x + vv_y) = -p_y + [\beta(\alpha_1\lambda_1 + \alpha_2\lambda_2)](v_{xx} + v_{yy}) \tag{A.1}$$

… which doesn't work

Theory

$$(\lambda_1\rho_1+\lambda_2\rho_2)(u_t + uu_x + vu_y) = -p_x + [\beta(\lambda_1\mu_1+\lambda_2\mu_2)](u_{xx} + u_{yy})$$
$$(\lambda_1\rho_1+\lambda_2\rho_2)(v_t + uv_x + vv_y) = -p_y + [\beta(\lambda_1\mu_1+\lambda_2\mu_2)](v_{xx} + v_{yy})$$
(A.2)

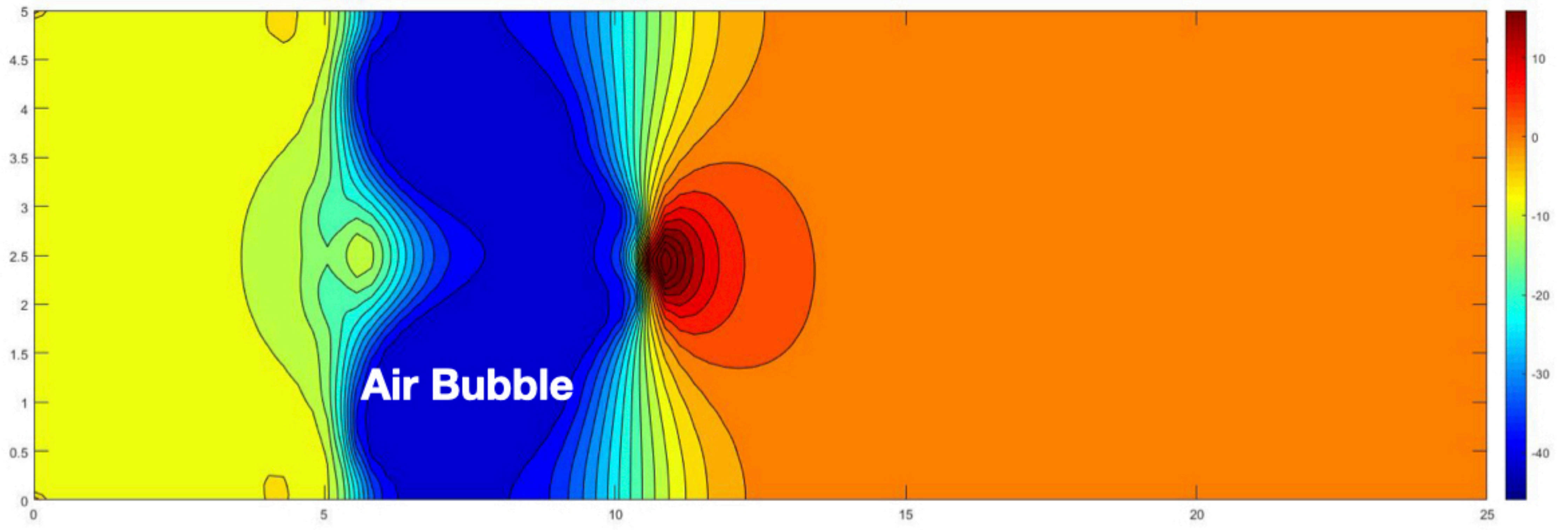
$$(\alpha_1\rho_1 + \alpha_2\rho_2)u_t+\lambda_1(uu_x + vu_y) = -p_x+\lambda_2(u_{xx} + u_{yy})$$
$$(\alpha_1\rho_1 + \alpha_2\rho_2)v_t+\lambda_1(uv_x + vv_y) = -p_y+\lambda_2(v_{xx} + v_{yy})$$
(A.3)

$$\lambda_1 u_t+\lambda_1(uu_x + vu_y) = -p_x+\lambda_2(u_{xx} + u_{yy})$$
$$\lambda_1 v_t+\lambda_1(uv_x + vv_y) = -p_x+\lambda_2(v_{xx} + v_{yy})$$
(A.3.1)

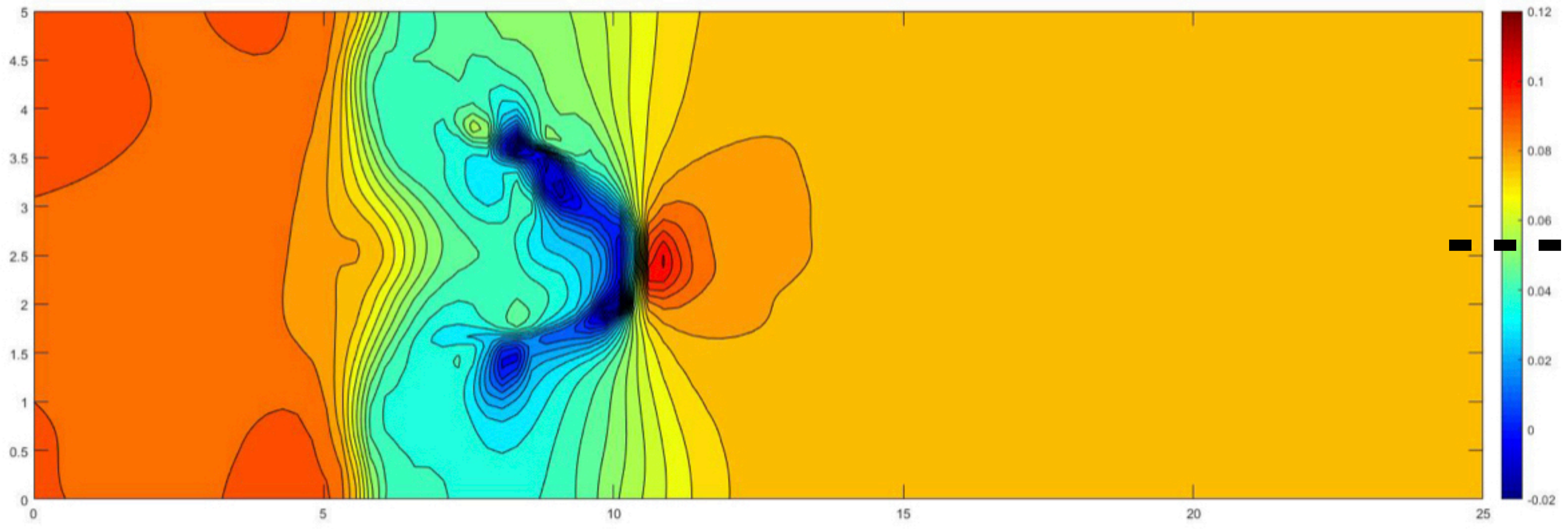
$$\lambda_1 = \beta_1(\alpha_1\rho_1 + \alpha_2\rho_2) \qquad \lambda_2 = \beta_2(\alpha_1\mu_1 + \alpha_2\mu_2)$$

Recall

CFD



PINN Prediction



Raissi *et al*., *JCP*, 2019:

Constitute a latent function ψ such that:

$$u = \psi_y, \quad v = -\psi_x$$

Therefore the continuum condition is automatically satisfied:

$$u_x + v_y = 0$$

For air bubble flows, the continuum condition is not satisfied.

Theory

The Raissi *et al*. work set the output as $[\psi(x, y, t) \quad p(x, y, t)]$, so that the NN can be trained by minimizing the MSE containing f_u & f_v while automatically satisfy the continuum condition.

Our approach break the original continuum condition and set the output as $[u \quad v \quad p \quad \phi]$

Where ϕ is the phase variant that satisfied:

$$\phi_t + \mathbf{u} \cdot \nabla \phi = \gamma \nabla \cdot \left(\epsilon_{ls} \nabla \phi - \phi(1 - \phi) \frac{\nabla \phi}{|\nabla \phi|} \right)$$

Recall the density and dynamics viscosity we assumed the bubble flow to satisfy:

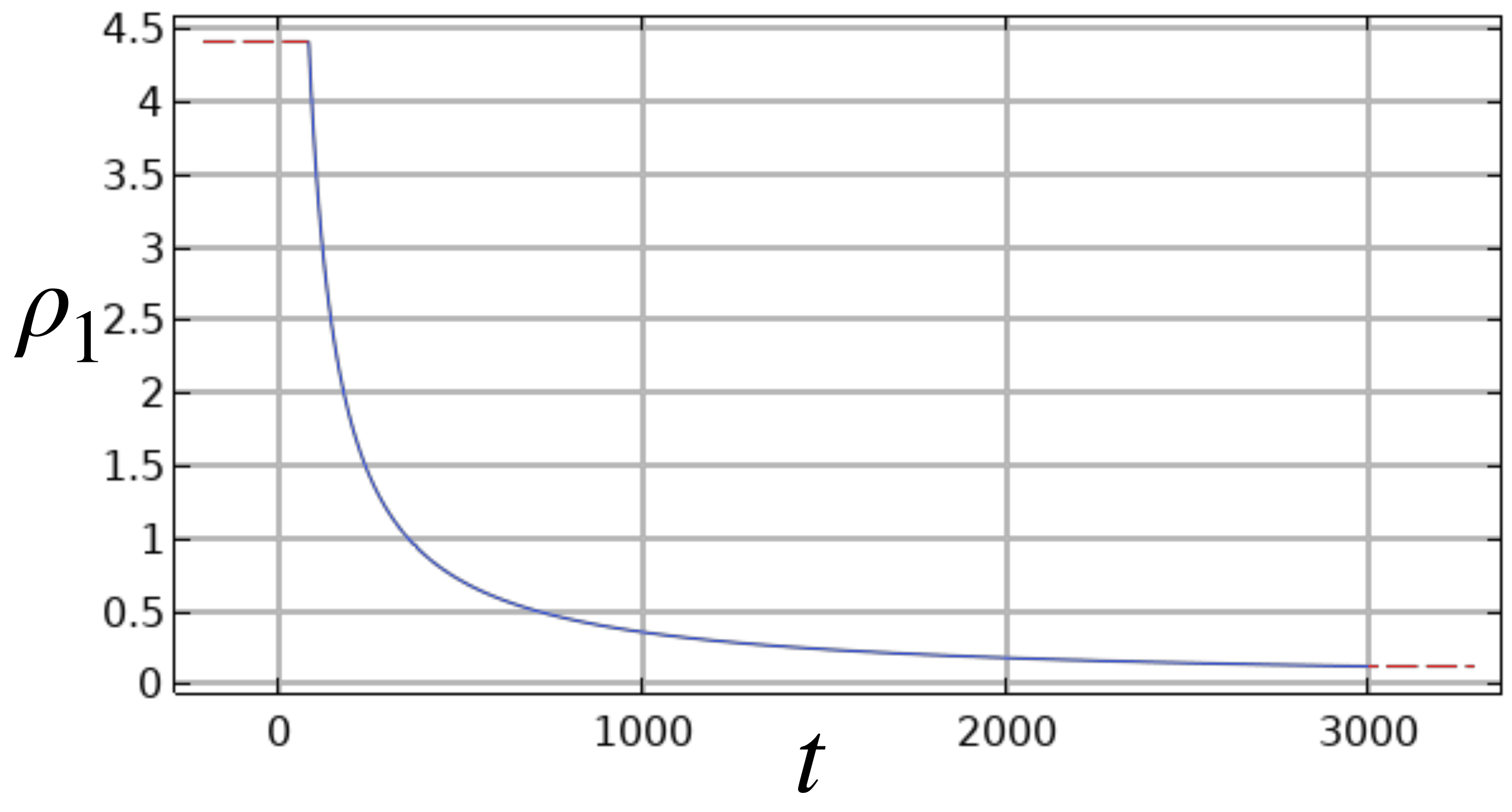
$$\lambda_1 = \beta_1(\alpha_1 \rho_1 + \alpha_2 \rho_2) \qquad \lambda_2 = \beta_2(\alpha_1 \mu_1 + \alpha_2 \mu_2)$$

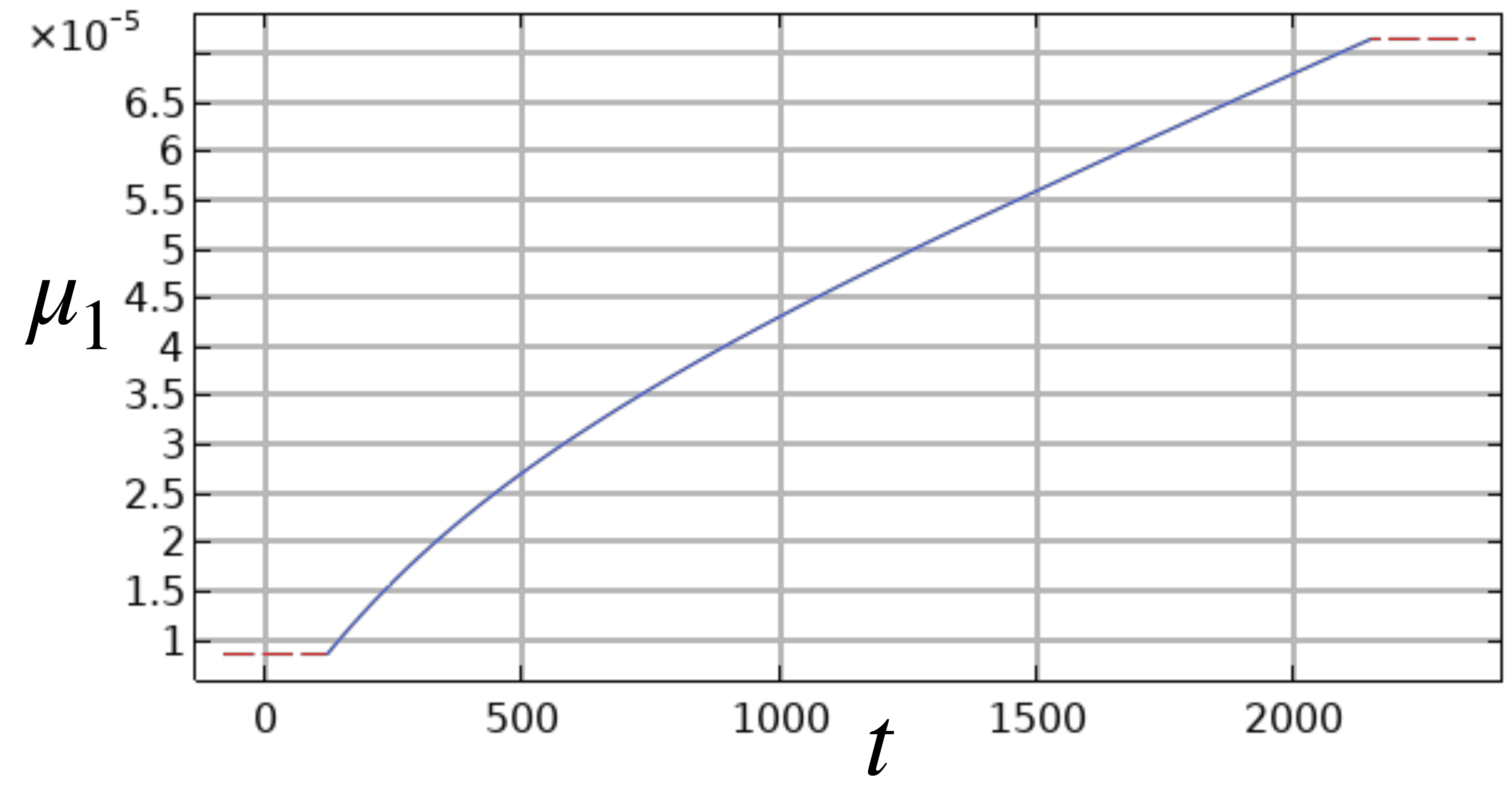
$$\rho_1 + \phi(\rho_2 - \rho_1) \qquad \mu_1 + \phi(\mu_2 - \mu_1)$$

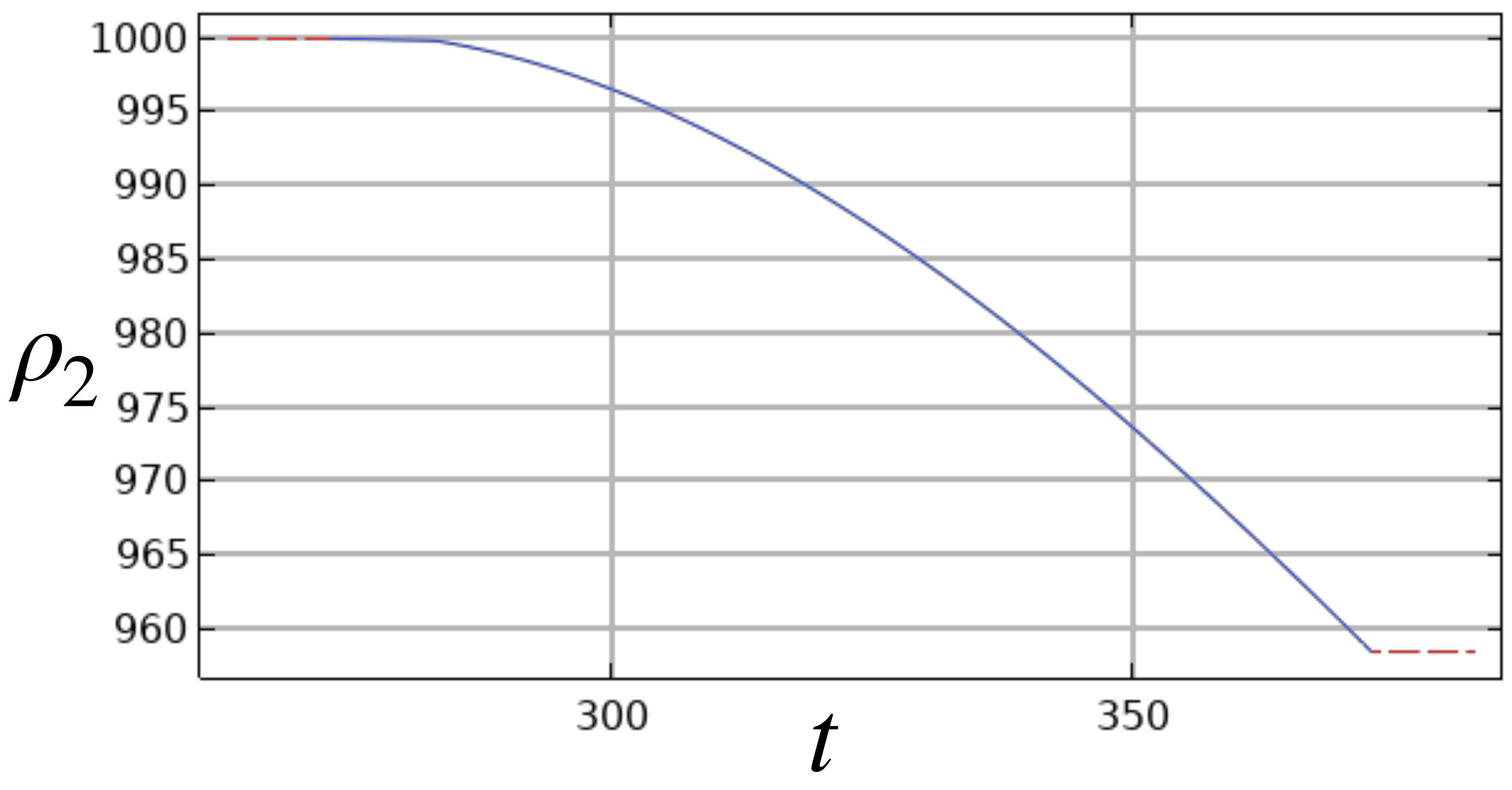
Theory

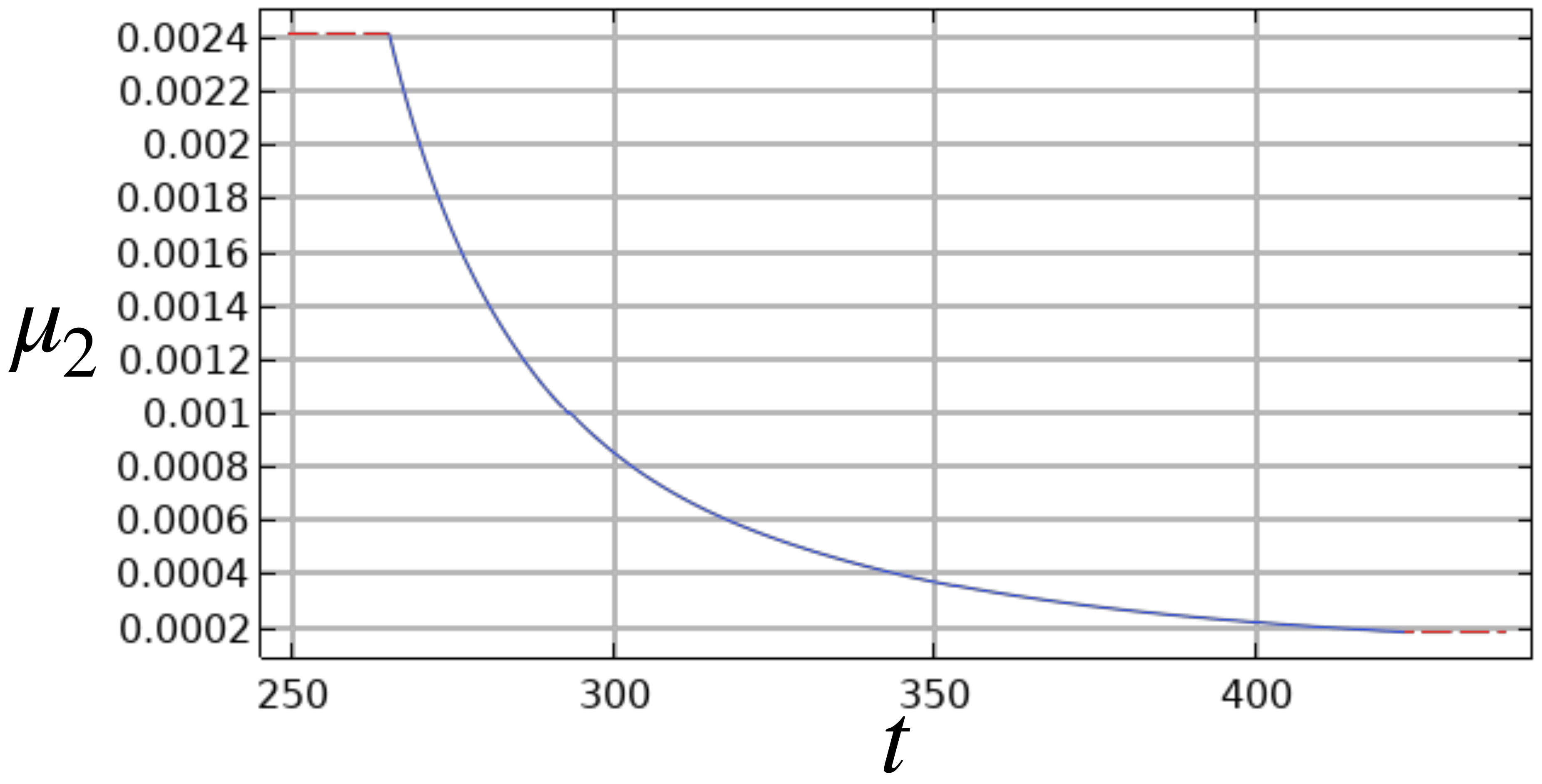
$$(1-\phi)\rho_1 + \phi\rho_2$$

$$(1-\phi)\mu_1 + \phi\mu_2$$









Physics-Informed Neural Network