Dispersion in porous media with evolving heterogeneities

Morgan Chabanon[1], J. Alberto Ochoa-Tapia[2], & Benoît Goyeau[1]

[1] EM2C, CNRS, CentraleSupelec, Paris-Saclay University, France
[2] Universidad Autonoma Metropolitana de Mexico, Mexico

Spatially evolving heterogeneities

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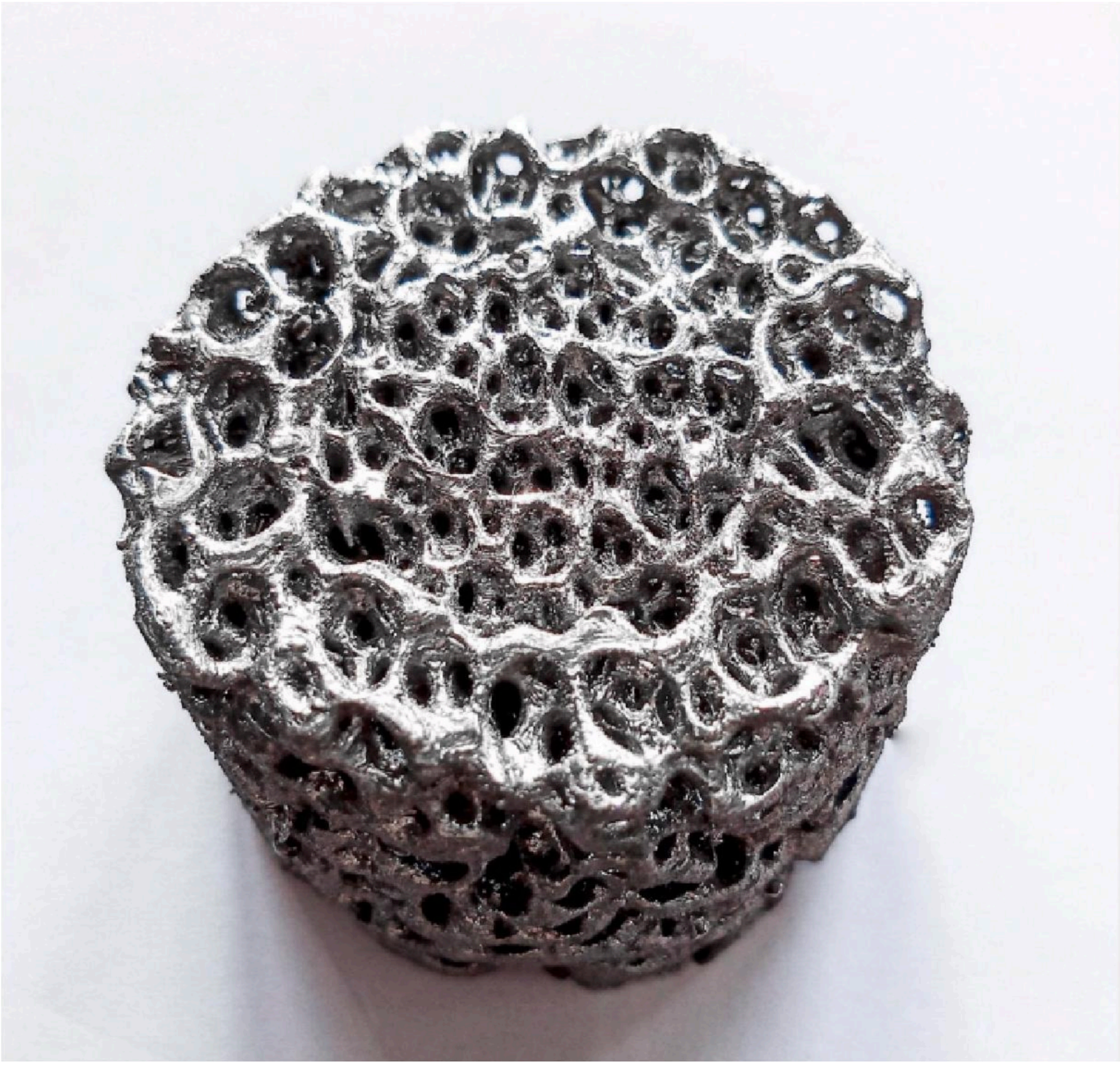
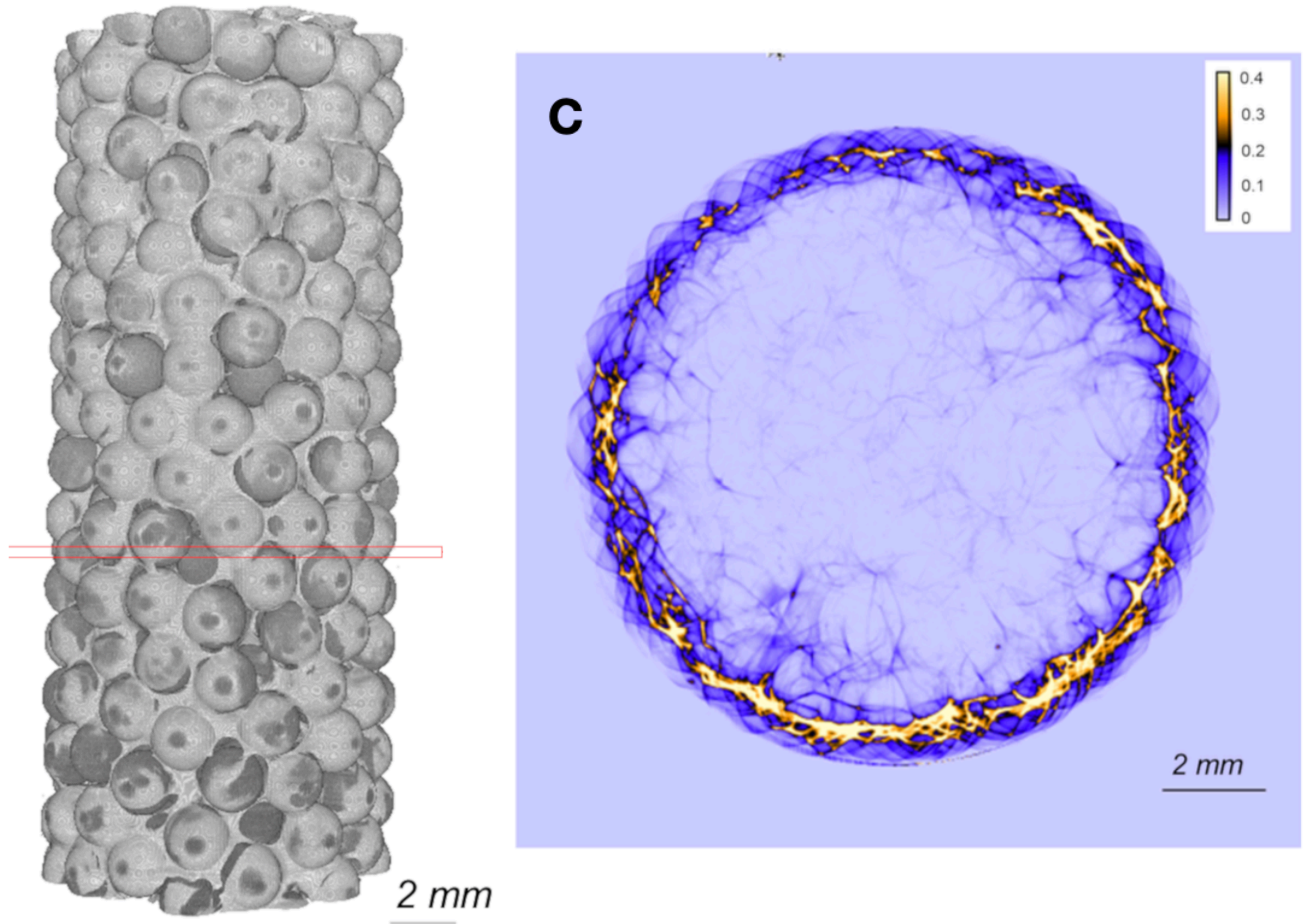
  - Definition of a representative volume ?
- Focus on PM with **continuous spatial variations of average properties**
  - Energy efficiency [Du et al. 2020]
  - Bioreactors [Chabanon et al. 2019, Beauchesne, Chabanon et al. 2020]
  - Filters in process engineering [Dalwadi et al. 2015]
  - Dendritic solidification [Goyeau et al. 1999]
  - Fluid-porous interfaces [Goyeau et al, 2003]





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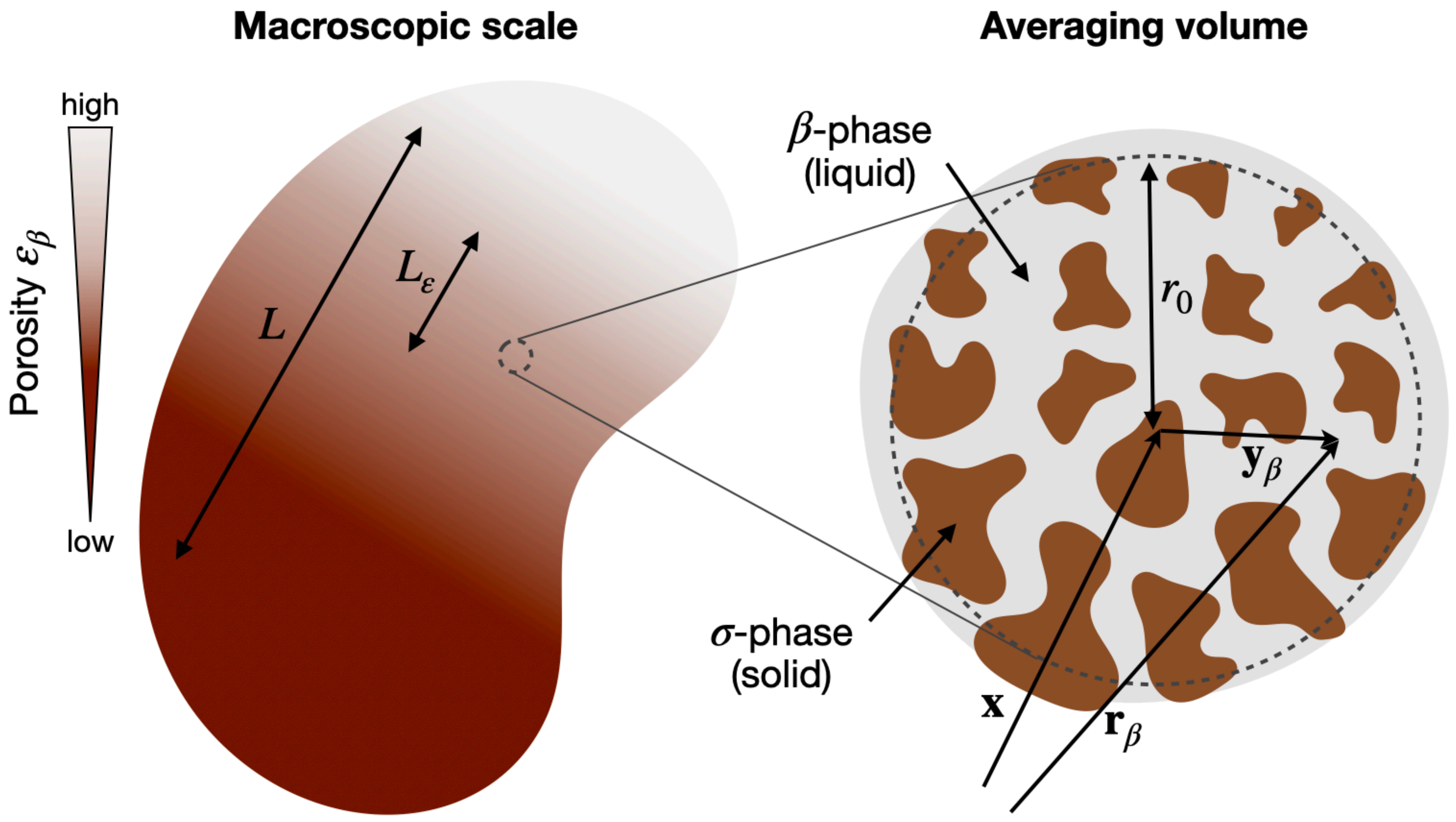
- Develop formal **macroscopic models** in porous media with **porosity gradients** (mass & momentum transport)



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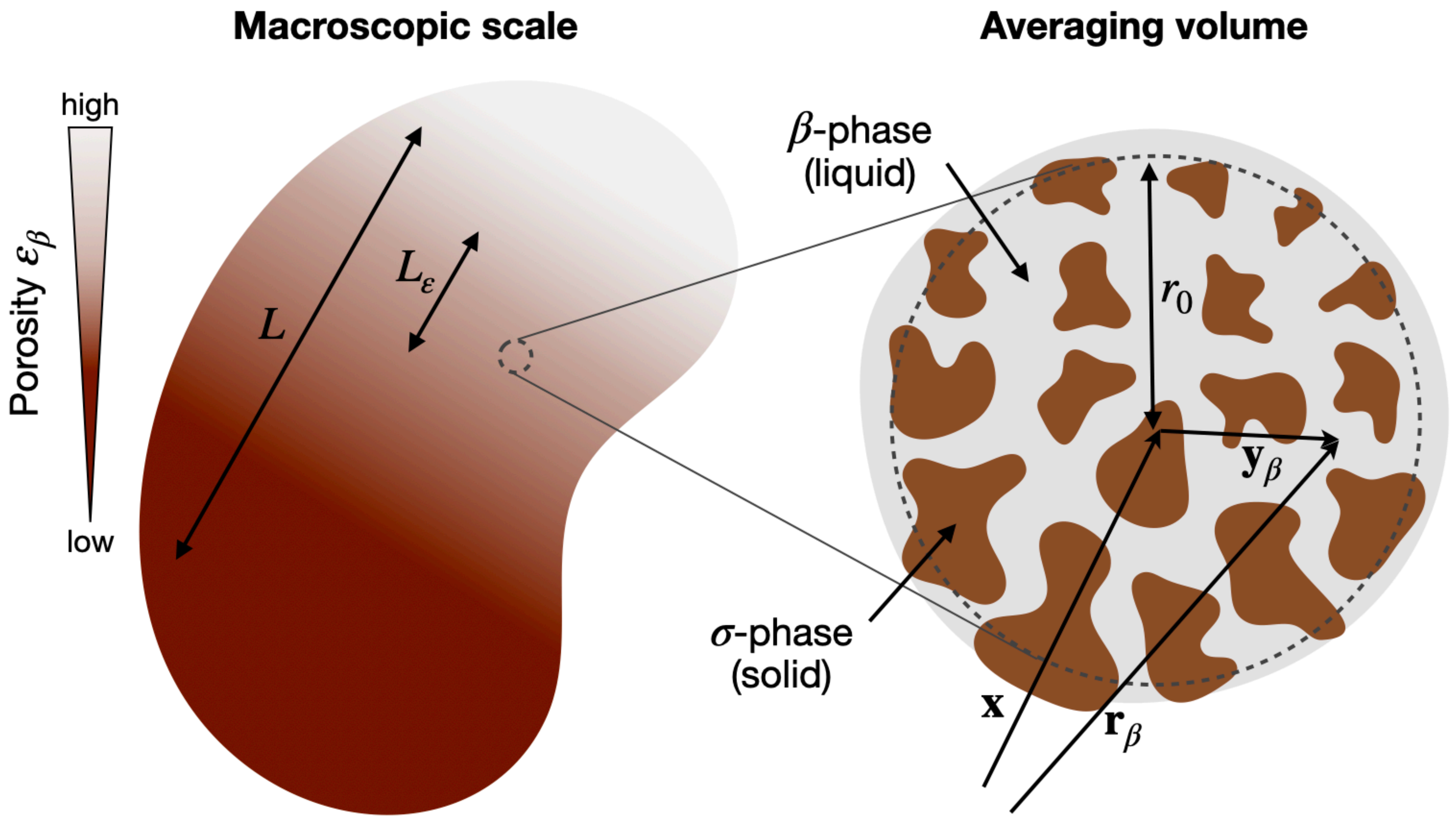

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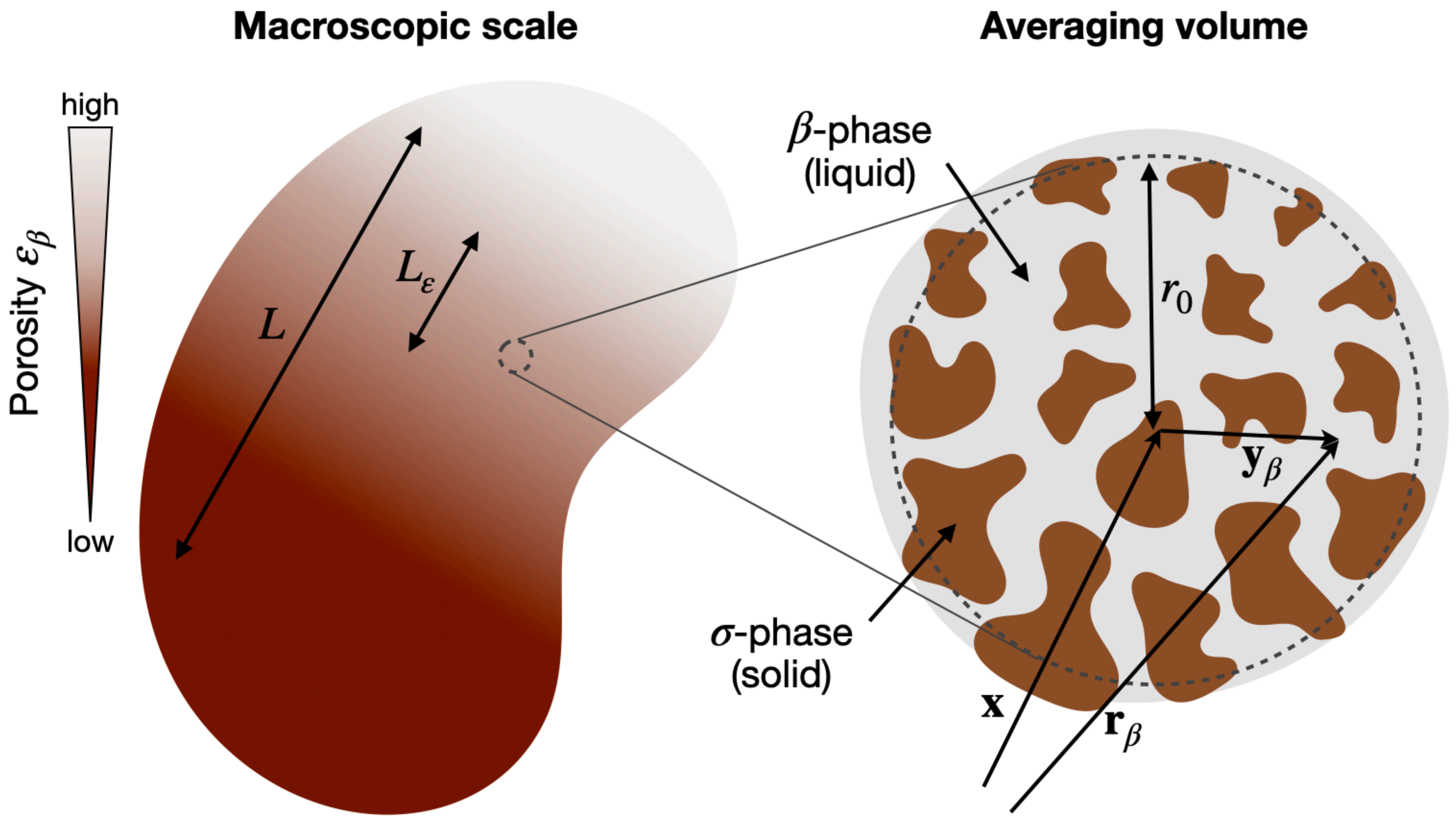

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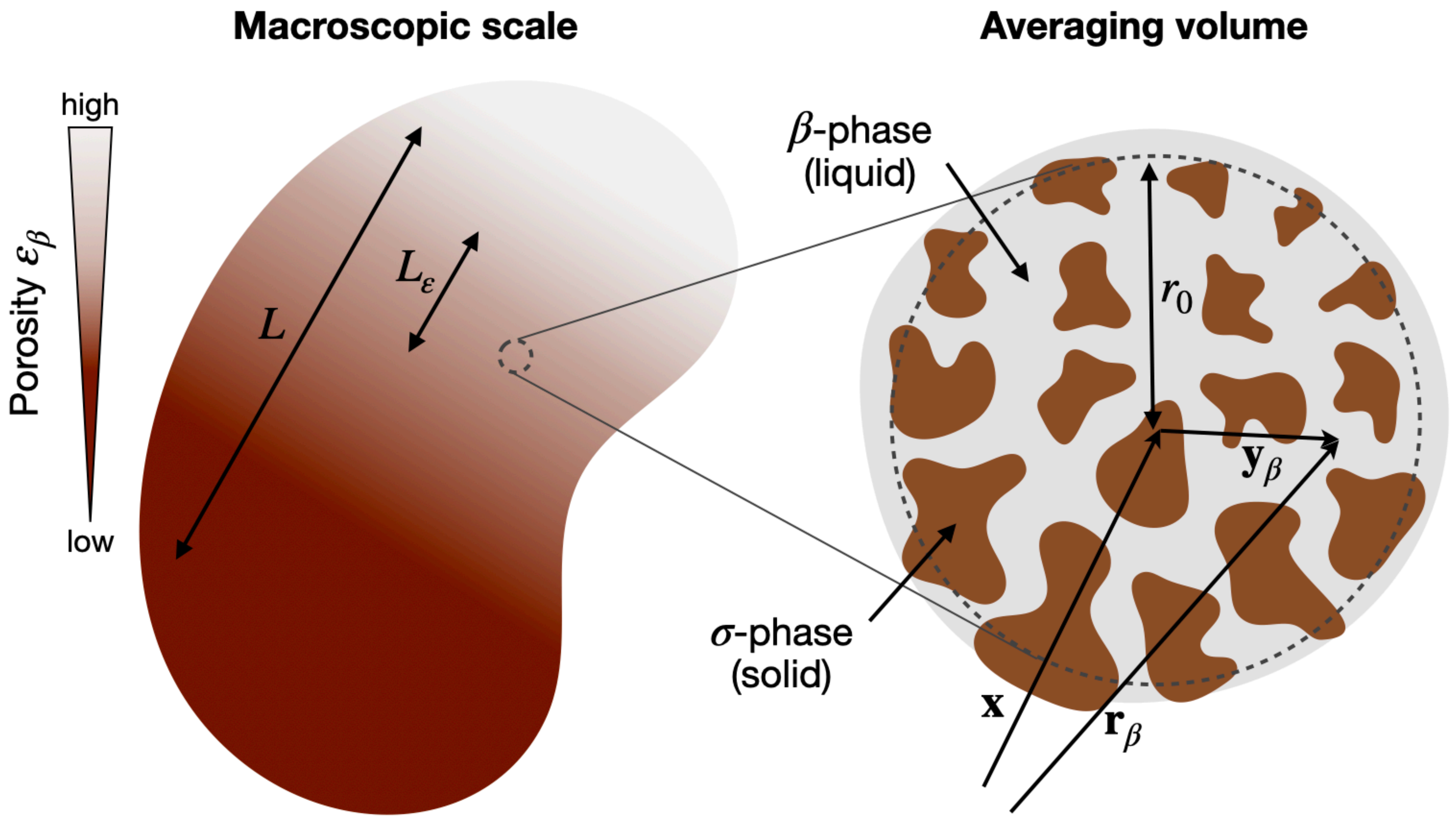
- **Methodology :**
  - Volume averaging method
  - Finite element method



Local problem

- Momentum transport

$$\nabla_y . \mathbf{v}_\beta = 0 \qquad \text{in the } \beta\text{-phase}$$

$$0 = -\nabla_y P_\beta + \rho_\beta \mathbf{g} + \mu_\beta \nabla_y^2 \mathbf{v}_\beta \qquad \text{in the } \beta\text{-phase}$$

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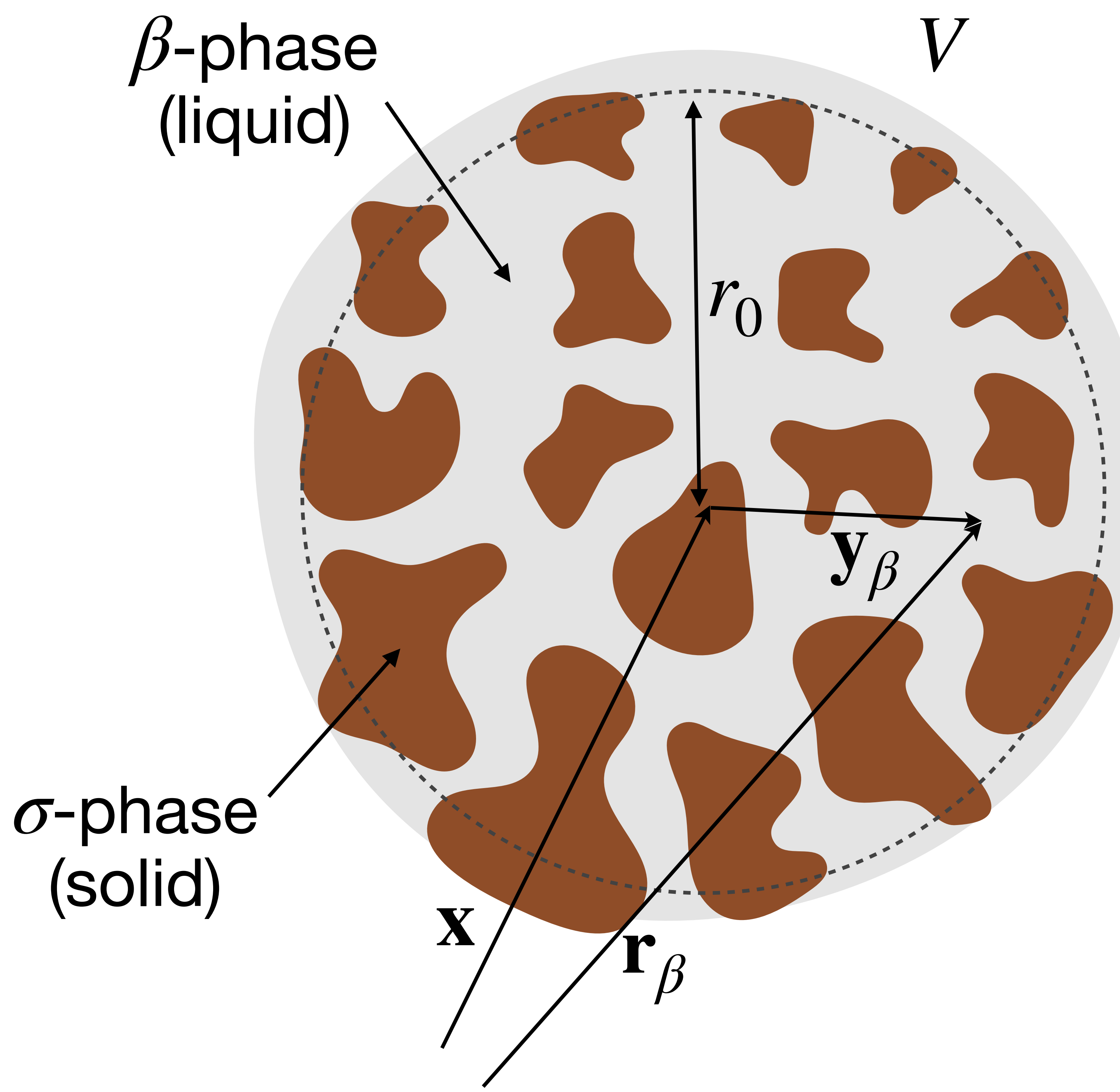
Averaging volume



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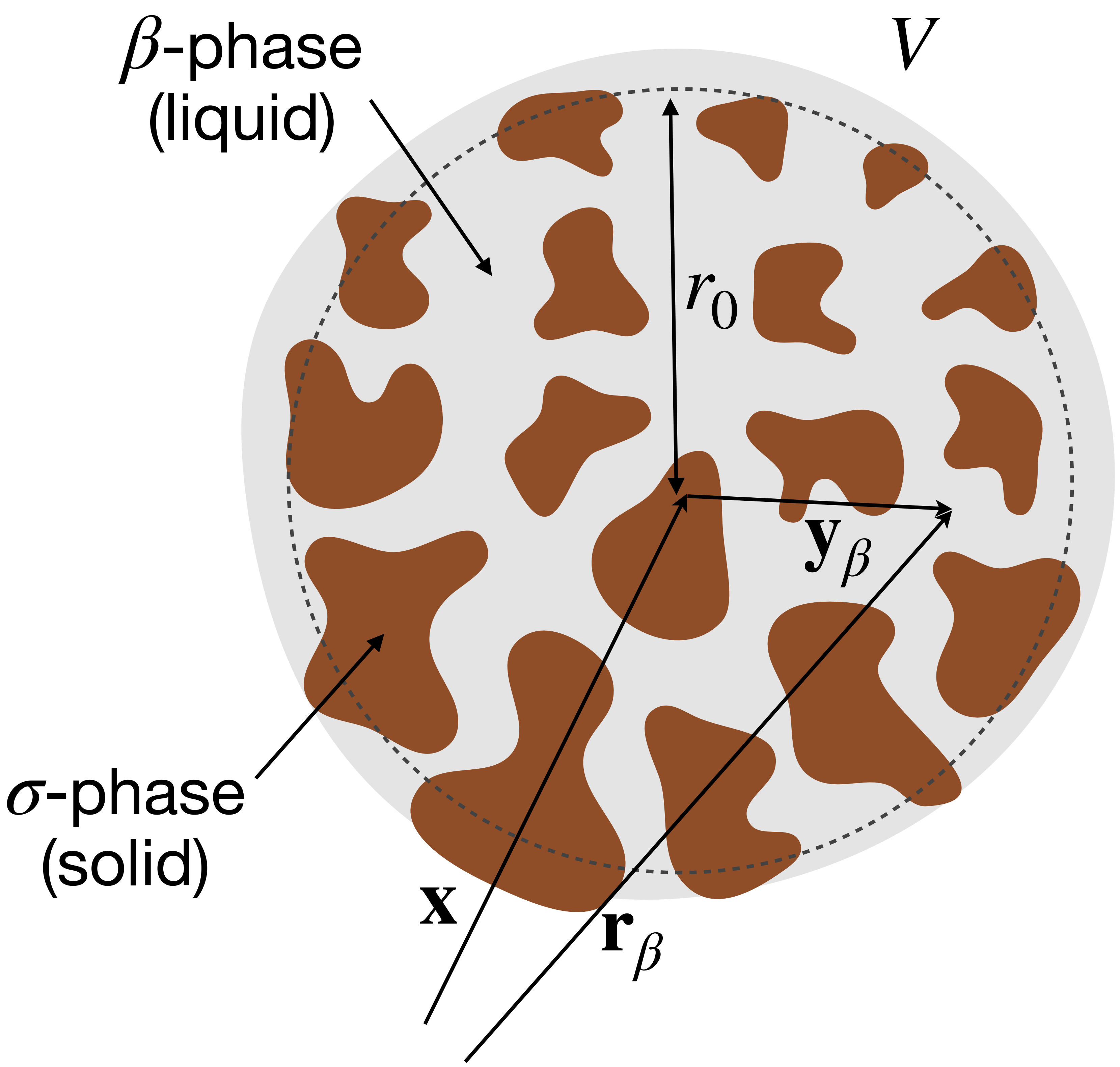

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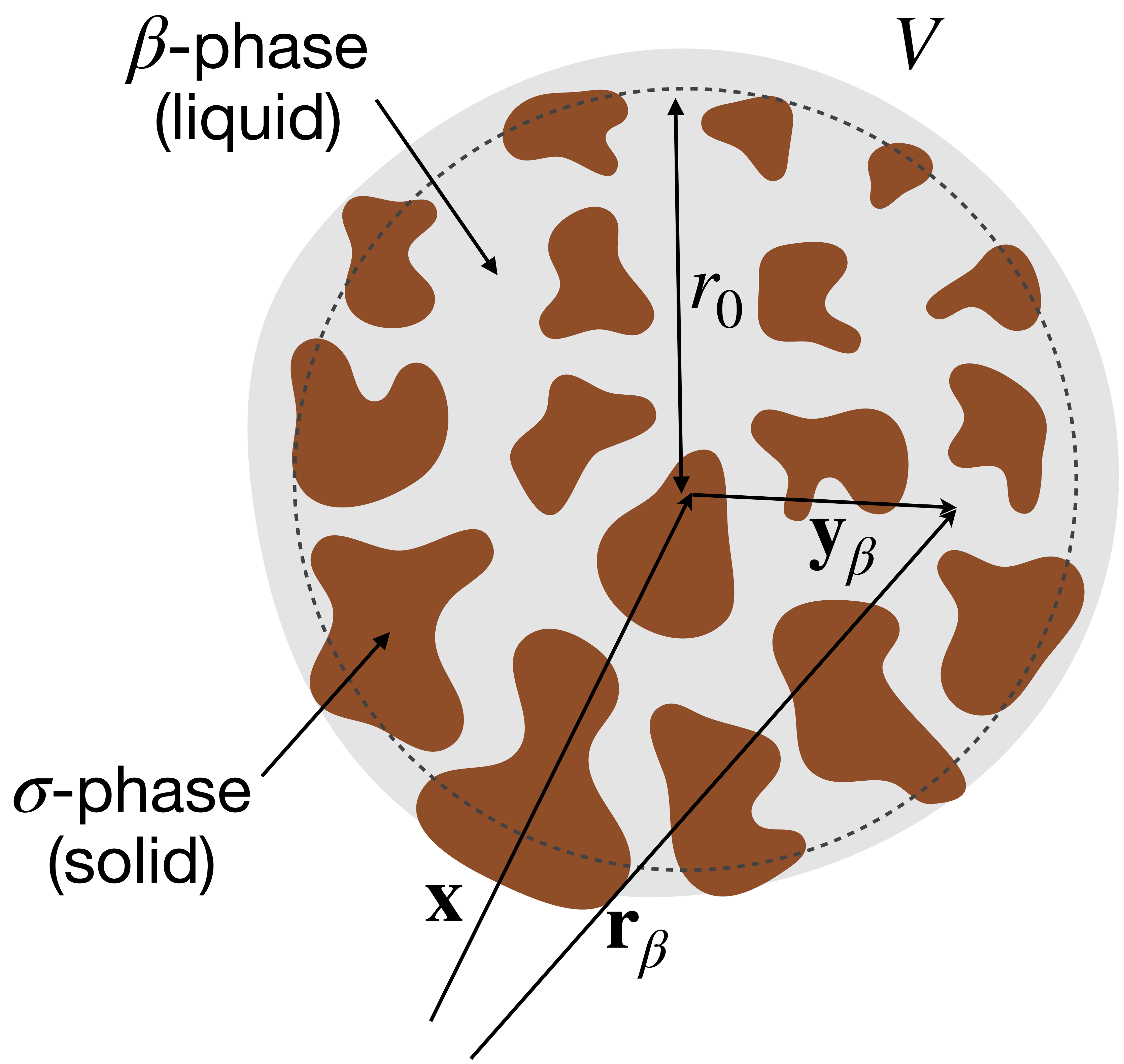
- Volume averaging toolbox: averages, transport theorems, deviations, length scale constraints …

$$\varepsilon_\beta = \frac{V_\beta}{V} \quad ; \quad \langle \psi_\beta \rangle^\beta = \frac{1}{V_\beta} \int_{V_\beta} \psi_\beta \, dV \quad ; \quad \psi_\beta = \langle \psi_\beta \rangle^\beta + \tilde{\psi}_\beta \quad \dots$$

Averaging volume



Upscaling momentum transport

Closed macroscopic model

$$\nabla_x . \langle \mathbf{v}_\beta \rangle^\beta = - \varepsilon_\beta^{-1} \nabla_x \varepsilon_\beta . \langle \mathbf{v}_\beta \rangle^\beta \qquad L_\varepsilon \sim L_v = O(r_0)$$

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With the permeability tensors defined as

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Two closure problems

$$\nabla_y \cdot \mathbf{B}_\beta = \varepsilon_\beta^{-1} \nabla_x \varepsilon_\beta$$

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BC: $\mathbf{B}_\beta = -\, \mathbf{I}$

Outer boundary conditions

$$\nabla_y \cdot \mathscr{C}_\beta = 0$$

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Incompatible with periodic boundary conditions !

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Simplified macro model for momentum transport

$\ell_\beta \ll (L_\varepsilon, L_v) = O(r_o)$ for porous media with spatially evolving heterogeneities [Goyeau et al., TiPM 1997]

Closed macroscopic transport equation

$$\nabla_x . \langle \mathbf{v}_\beta \rangle^\beta = -\, \varepsilon_\beta^{-1} \nabla_x \varepsilon_\beta . \langle \mathbf{v}_\beta \rangle^\beta$$

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Simplified **closure problem** and **permeability** tensor are **identical to homogeneous porous media**

Permeability tensor $$\varepsilon_\beta \mathbf{K}_\beta^{-1} = -\frac{1}{V_\beta} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot \left(-\mathbf{I} \otimes \mathbf{b}'_\beta + \nabla_y \mathbf{B}'_\beta \right) dA$$

$\nabla_y \cdot \mathbf{B}'_\beta = 0$ in the β-phase

$0 = -\nabla_y \mathbf{b}'_\beta + \nabla_y^2 \mathbf{B}'_\beta + \varepsilon_\beta \mathbf{K}_\beta^{-1}$ in the β-phase

BC: $\mathbf{B}'_\beta = -\mathbf{I}$ at $A_{\beta\sigma}$

Periodicity: $\mathbf{B}'_\beta(\mathbf{x} + l_i) = \mathbf{B}'_\beta(\mathbf{x})$; $\mathbf{b}'_\beta(\mathbf{x} + l_i) = \mathbf{b}'_\beta(\mathbf{x})$

Uniqueness: $\langle \mathbf{B}'_\beta \rangle^\beta = 0$; $\langle \mathbf{b}'_\beta \rangle^\beta = 0$

See details in [Chabanon et al., TiPM 2026]

Solute transport

Closed macroscopic transport equation

$$\nabla_x \cdot \left(\varepsilon_\beta \langle \mathbf{v}_\beta \rangle^\beta \langle C_{A\beta} \rangle^\beta \right) = \nabla_x \cdot \left[\mathbf{D}_{eff} \cdot \nabla_x \langle C_{A\beta} \rangle^\beta \right]$$

Diffusion-dispersion tensor

$$\mathbf{D}_{eff} = D_\beta \left(\varepsilon_\beta \mathbf{I} + \frac{1}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \otimes \mathbf{d}_\beta dA \right) - \langle \tilde{\mathbf{v}}_\beta \otimes \mathbf{d}_\beta \rangle$$

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Closure problem

$$\tilde{\mathbf{v}}_\beta + \mathbf{v}_\beta \cdot \nabla_y \mathbf{d}_\beta = D_\beta \nabla_y^2 \mathbf{d}_\beta - \varepsilon_\beta^{-1} \nabla_x \cdot \left(\frac{D_\beta}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \otimes \mathbf{d}_\beta dA \right)$$

BC: $-\mathbf{n}_{\beta\sigma} \cdot D_\beta \nabla_y \mathbf{d}_\beta = \mathbf{n}_{\beta\sigma} D_\beta$ at $A_{\beta\sigma}$

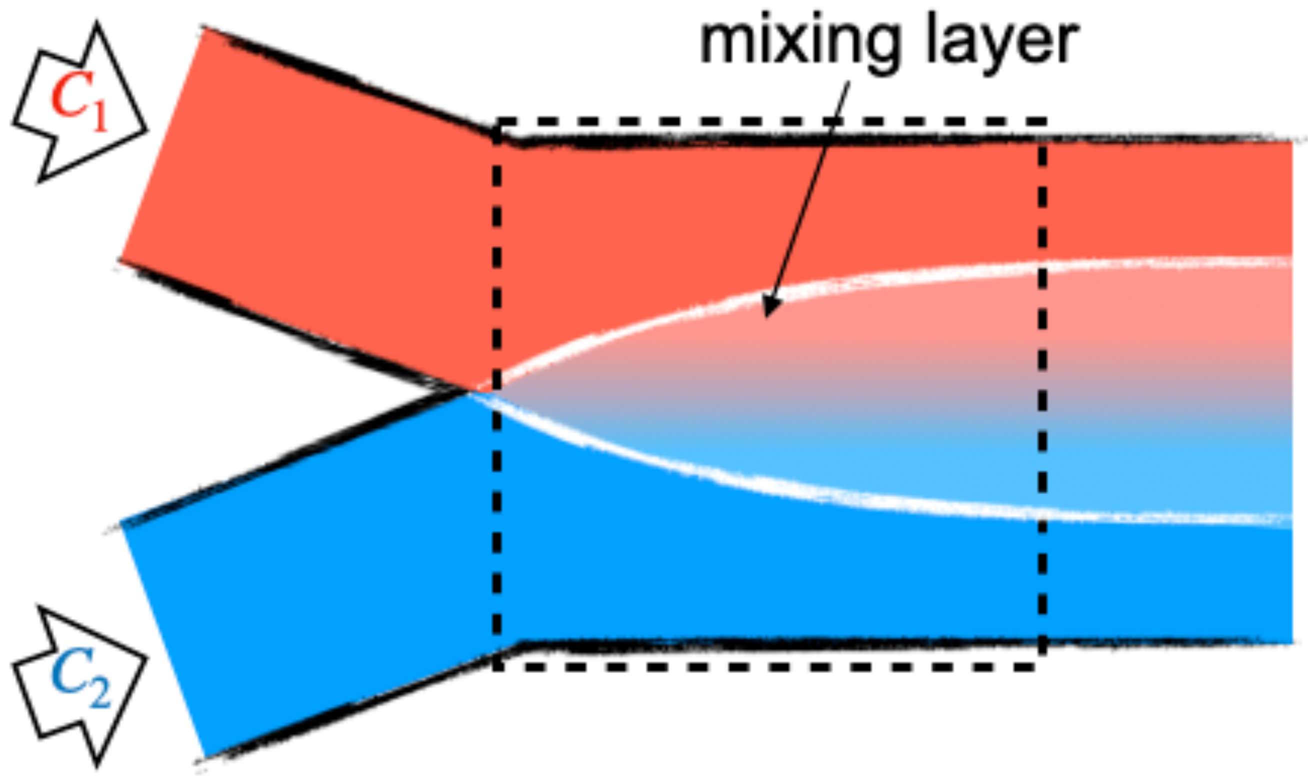
Periodicity: $\mathbf{d}_\beta(\mathbf{x} + l_i) = \mathbf{d}_\beta(\mathbf{x})$ for $i = 1,2,3$

Uniqueness: $\langle \mathbf{d}_\beta \rangle^\beta = 0$

- In its intrinsic average formulation, identical to homogeneous porous media.
- Velocity field influenced by heterogeneities.

Simulation methodology

Application: **mixing chamber filled with a porous medium**



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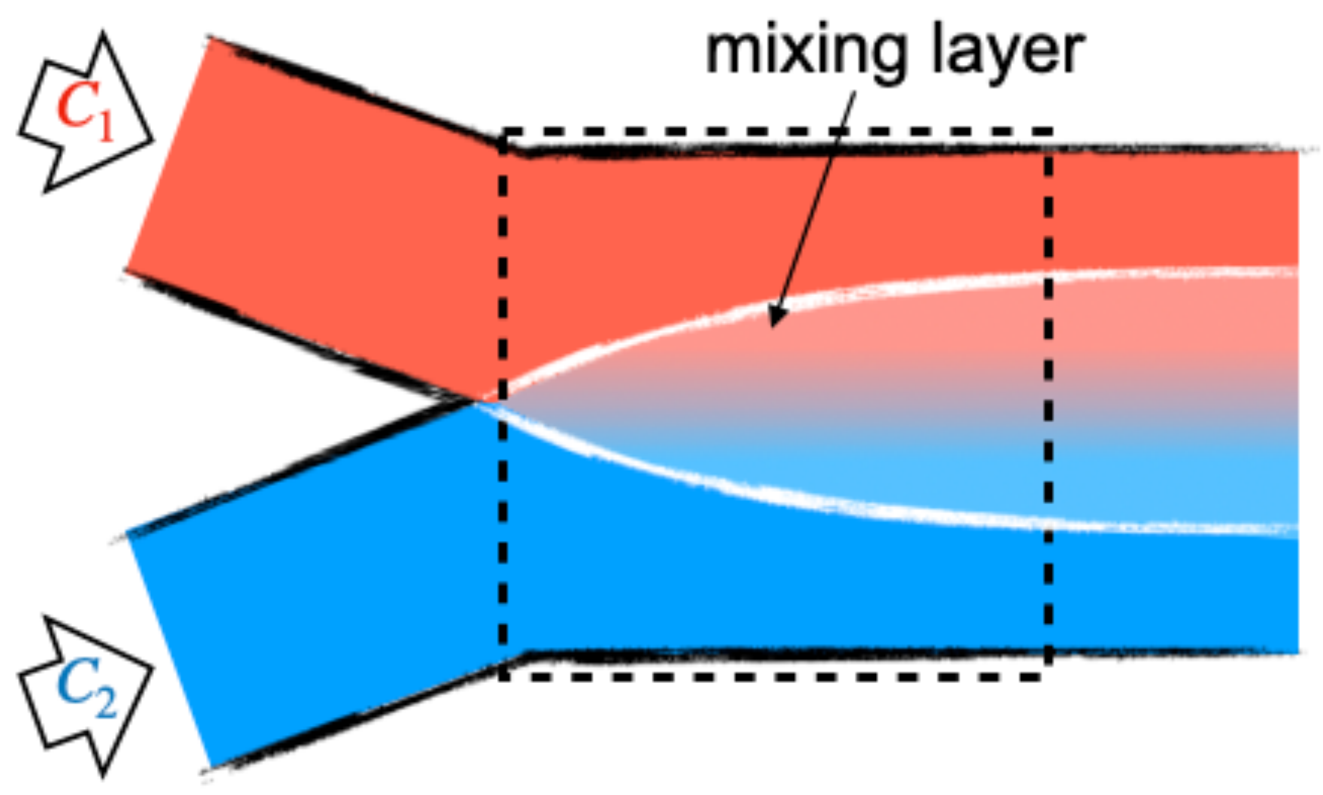

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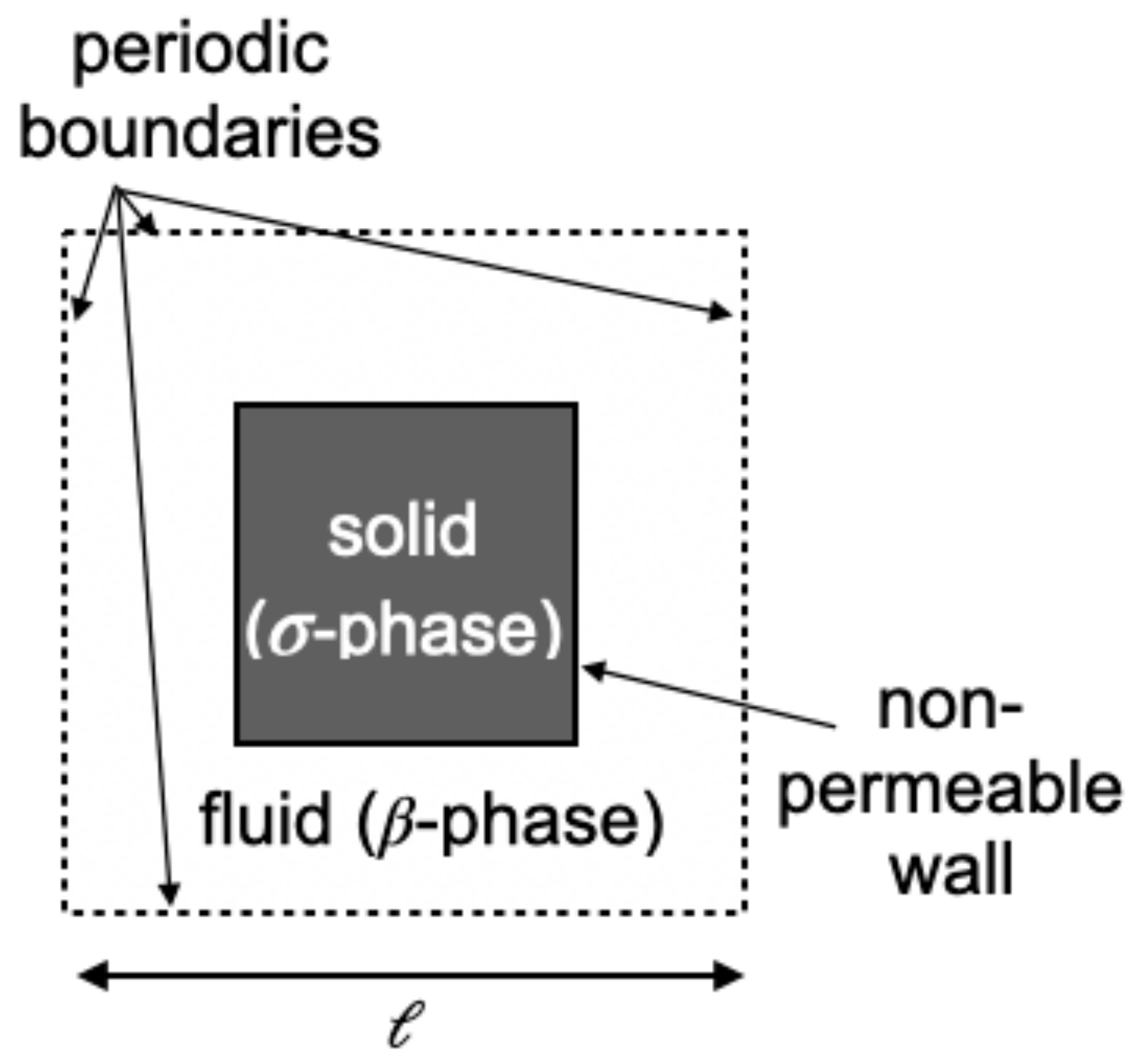
Procedure

- Solve **closure problems** on 2D representative unit cell



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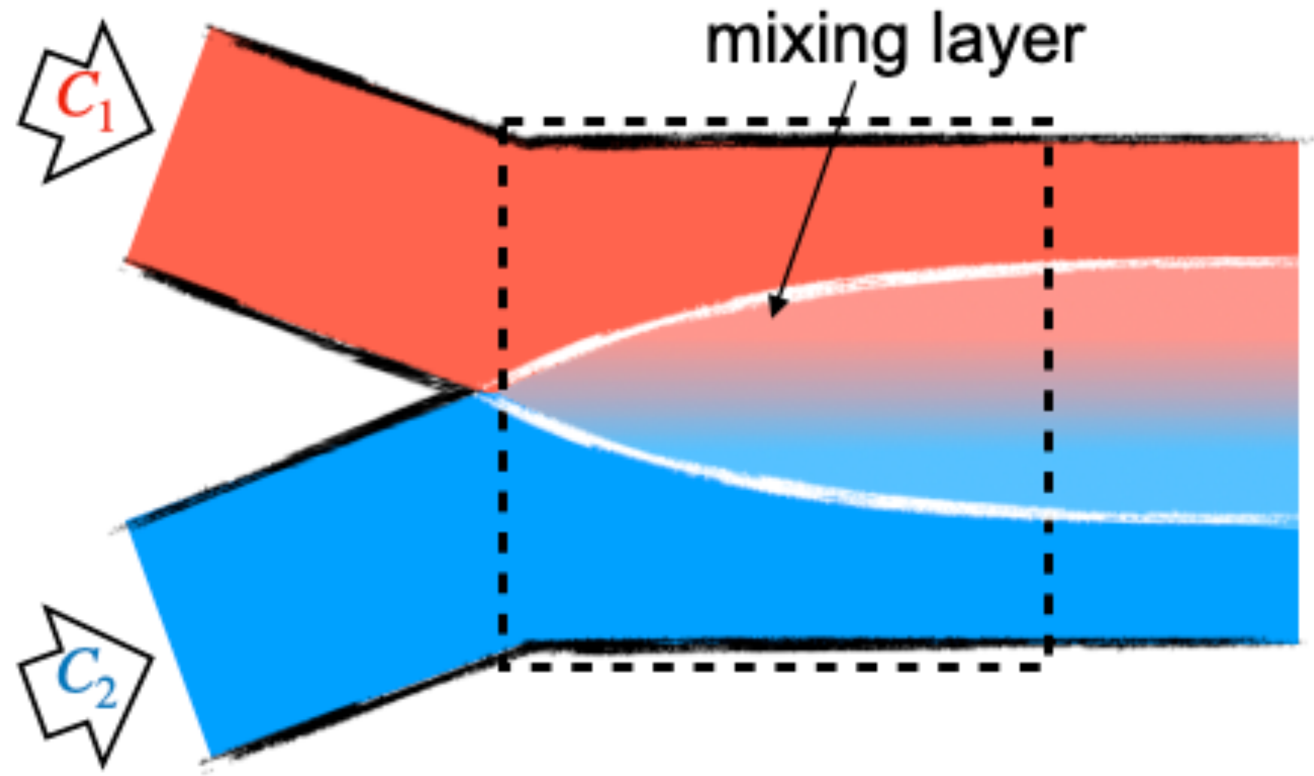

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- Solve **closure problems** on 2D representative unit cell
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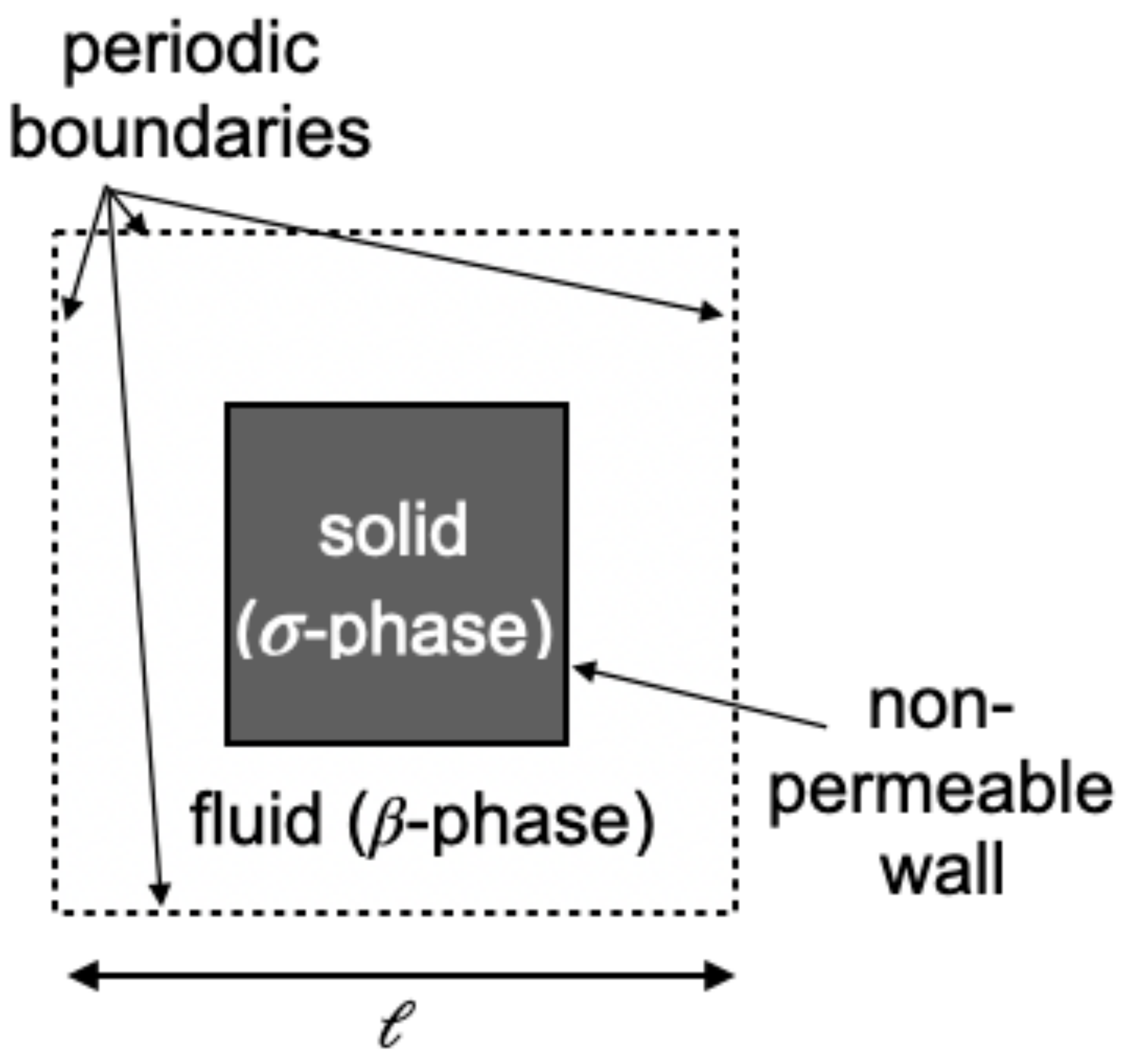

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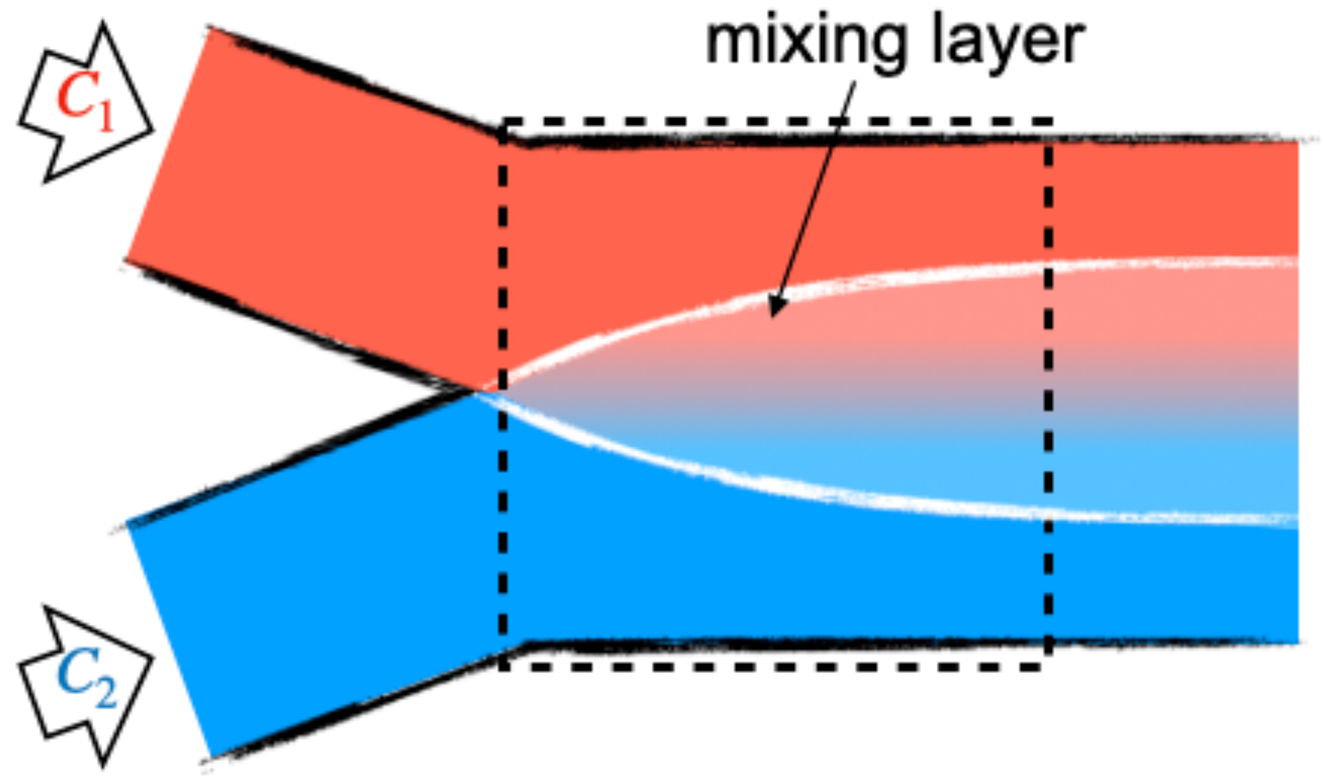

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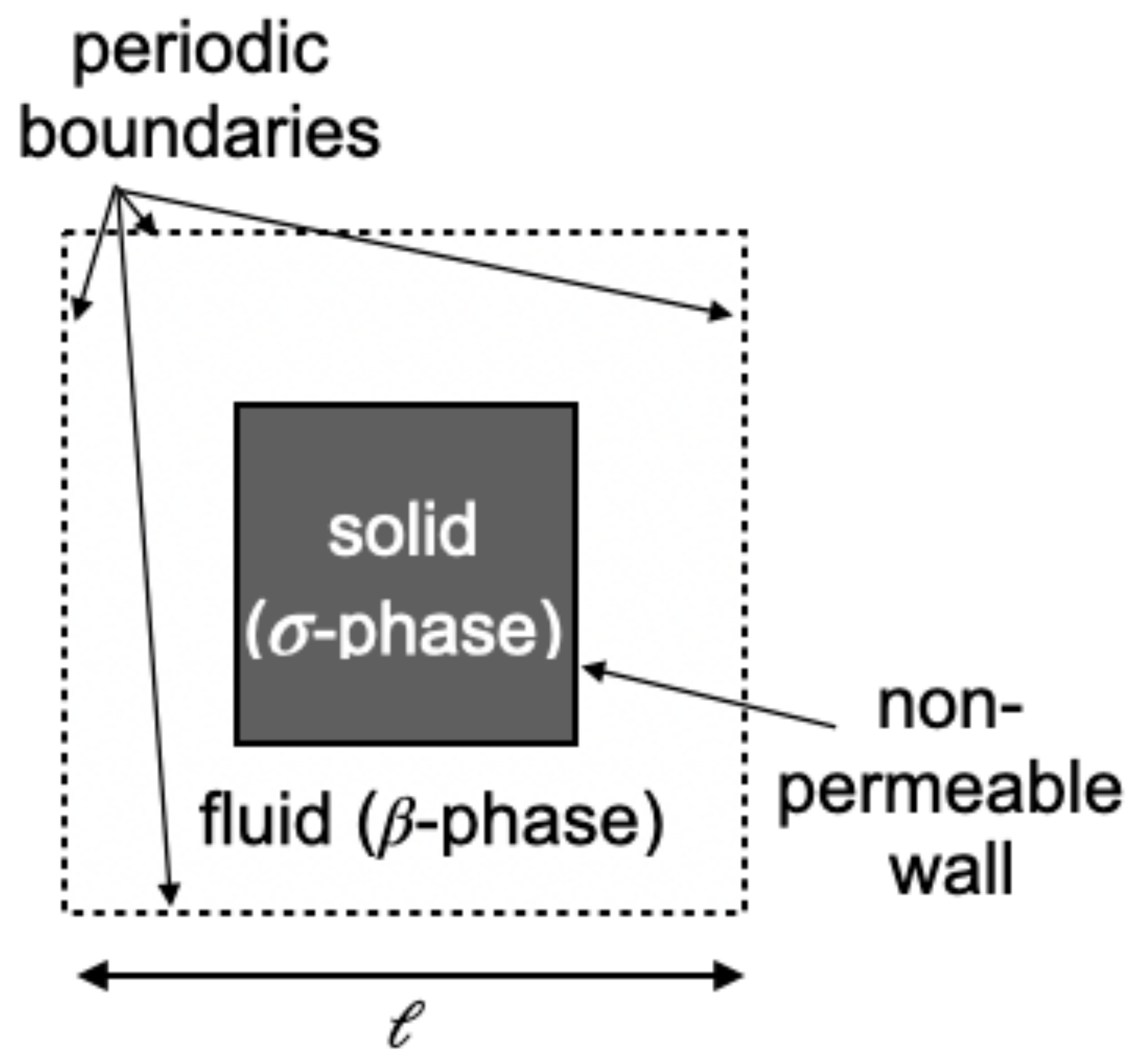

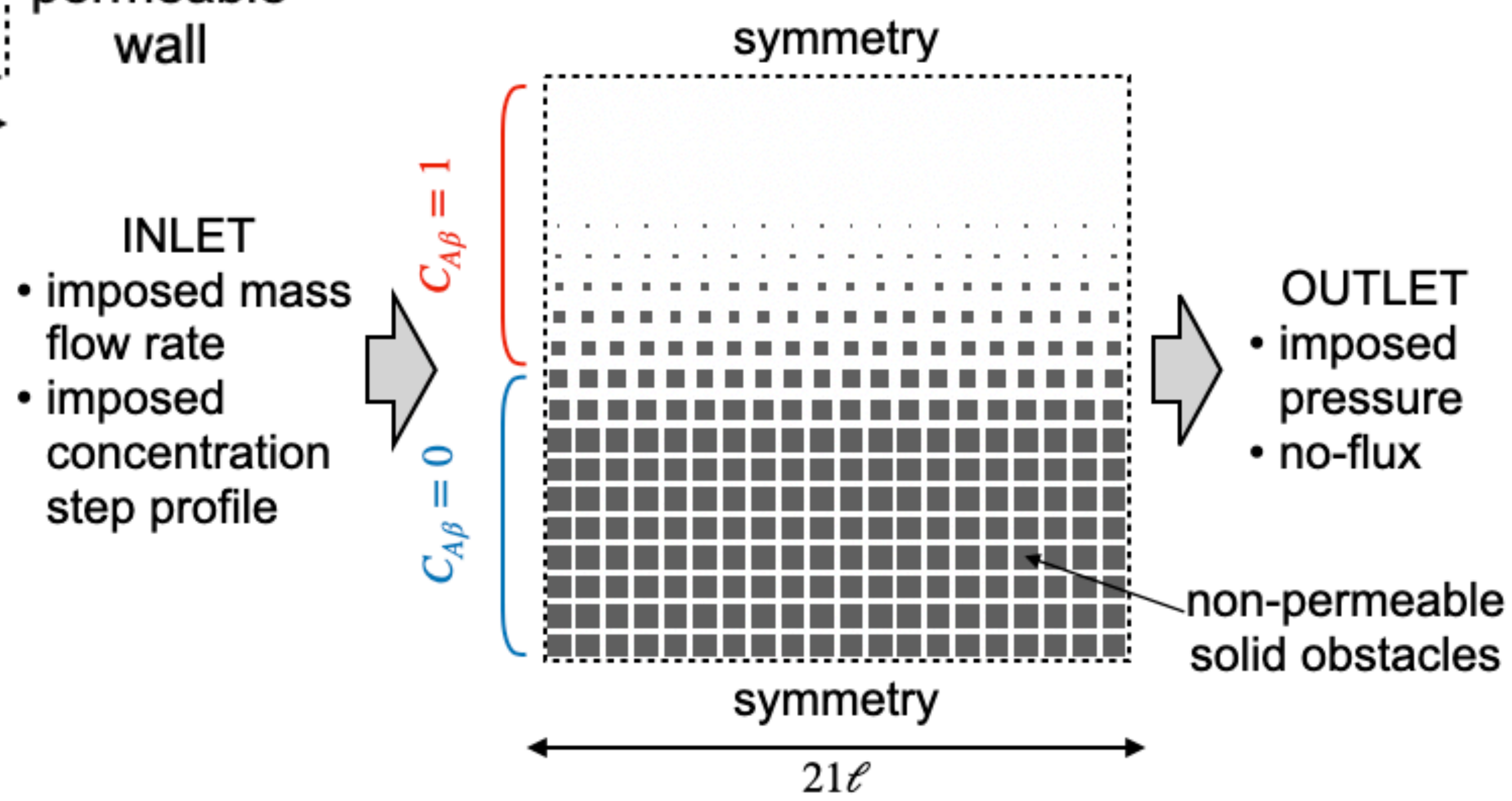

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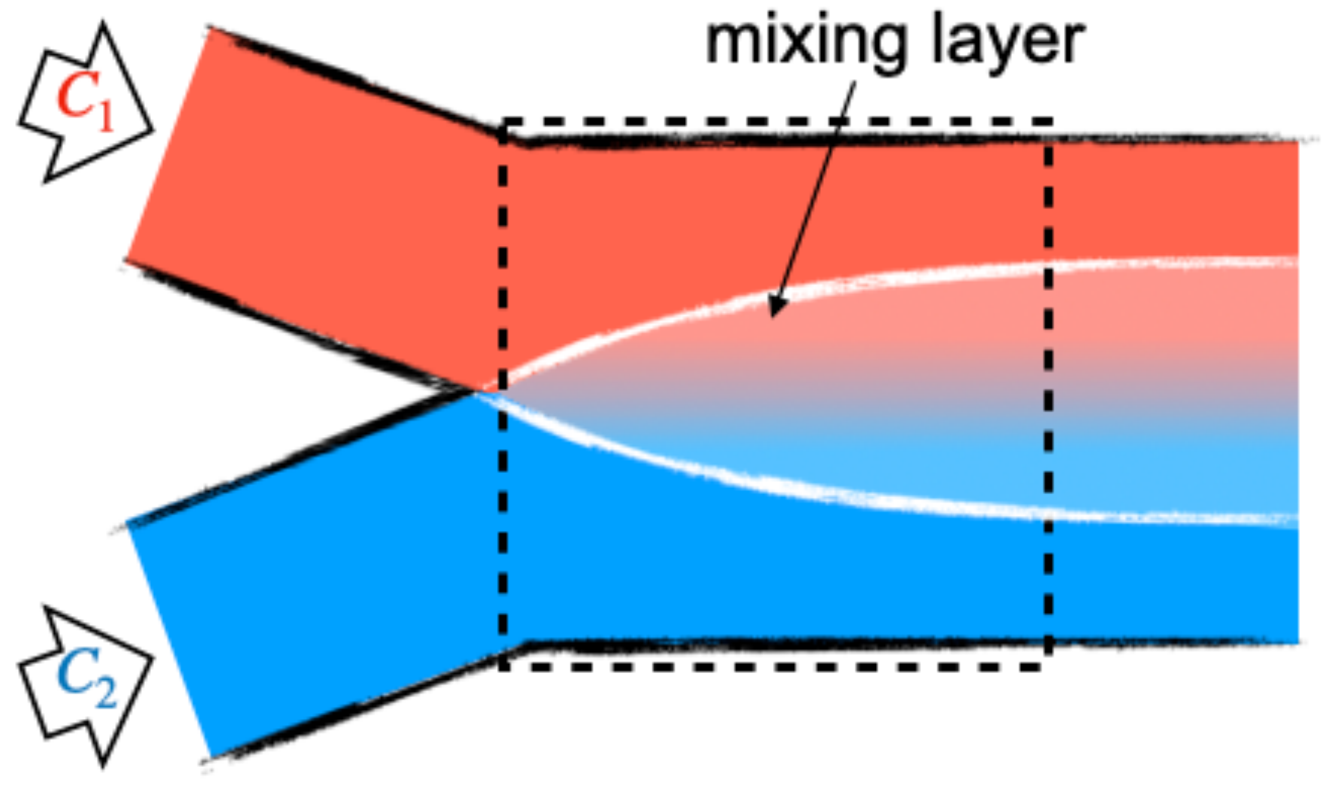

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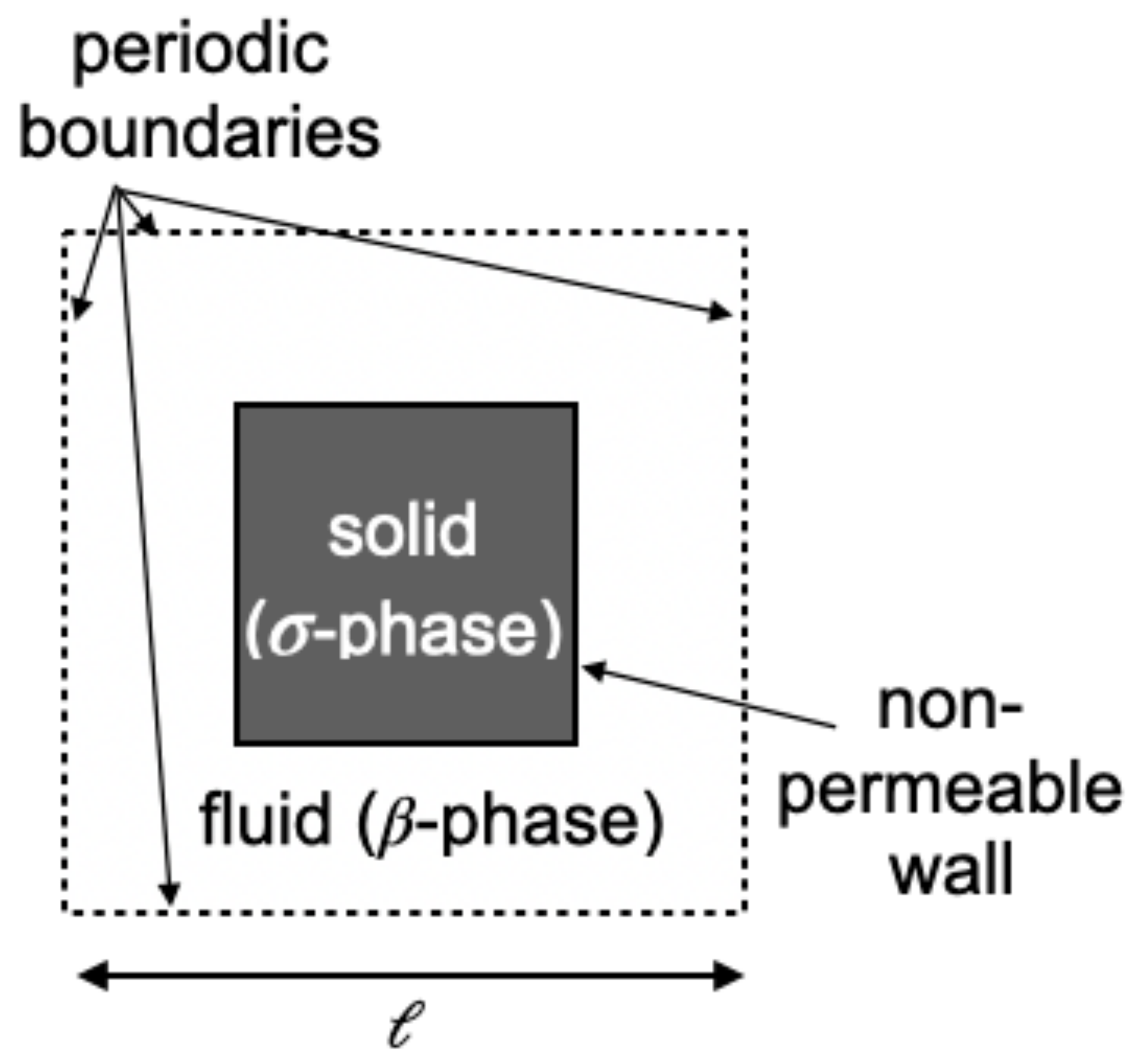
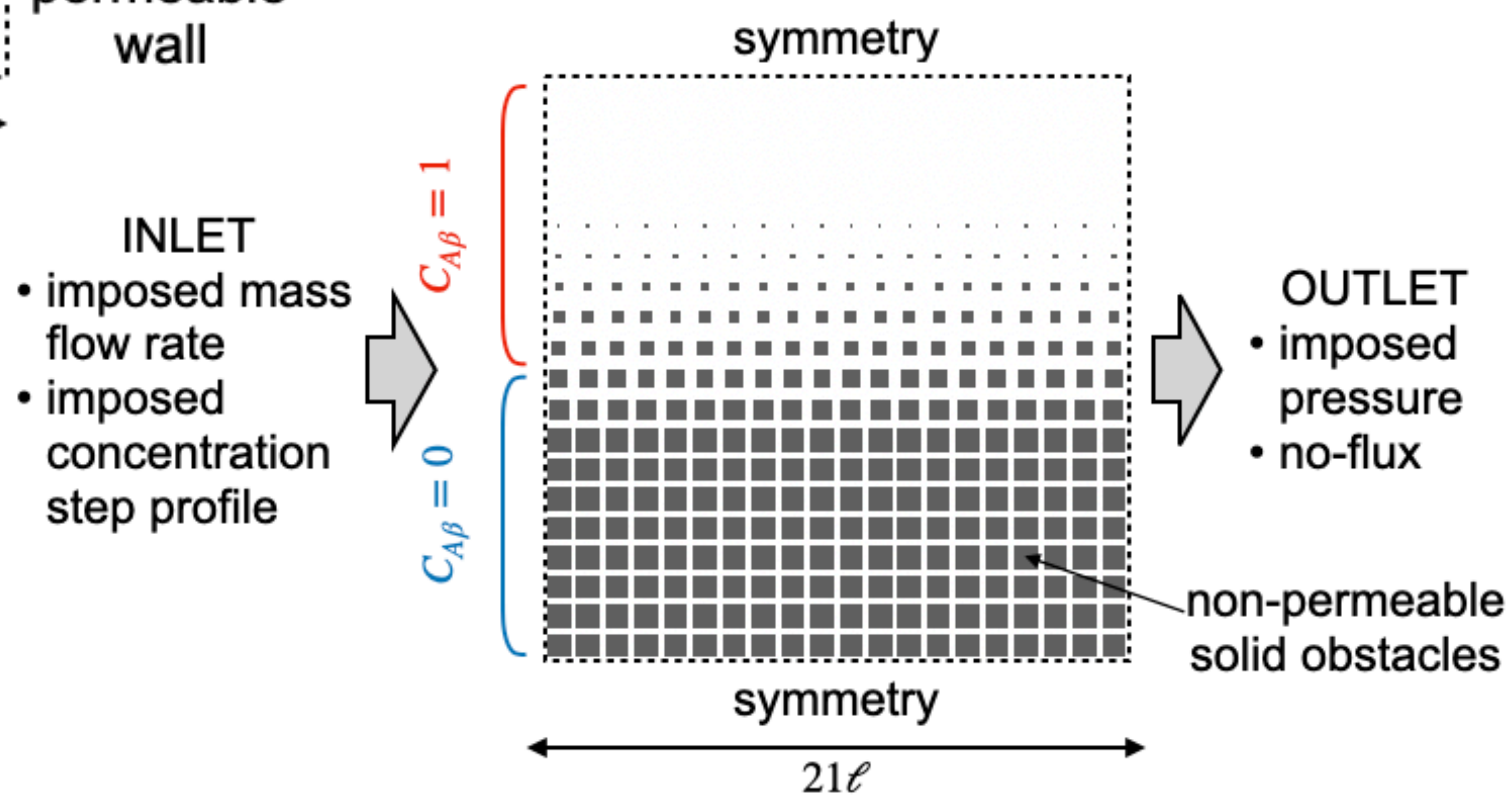
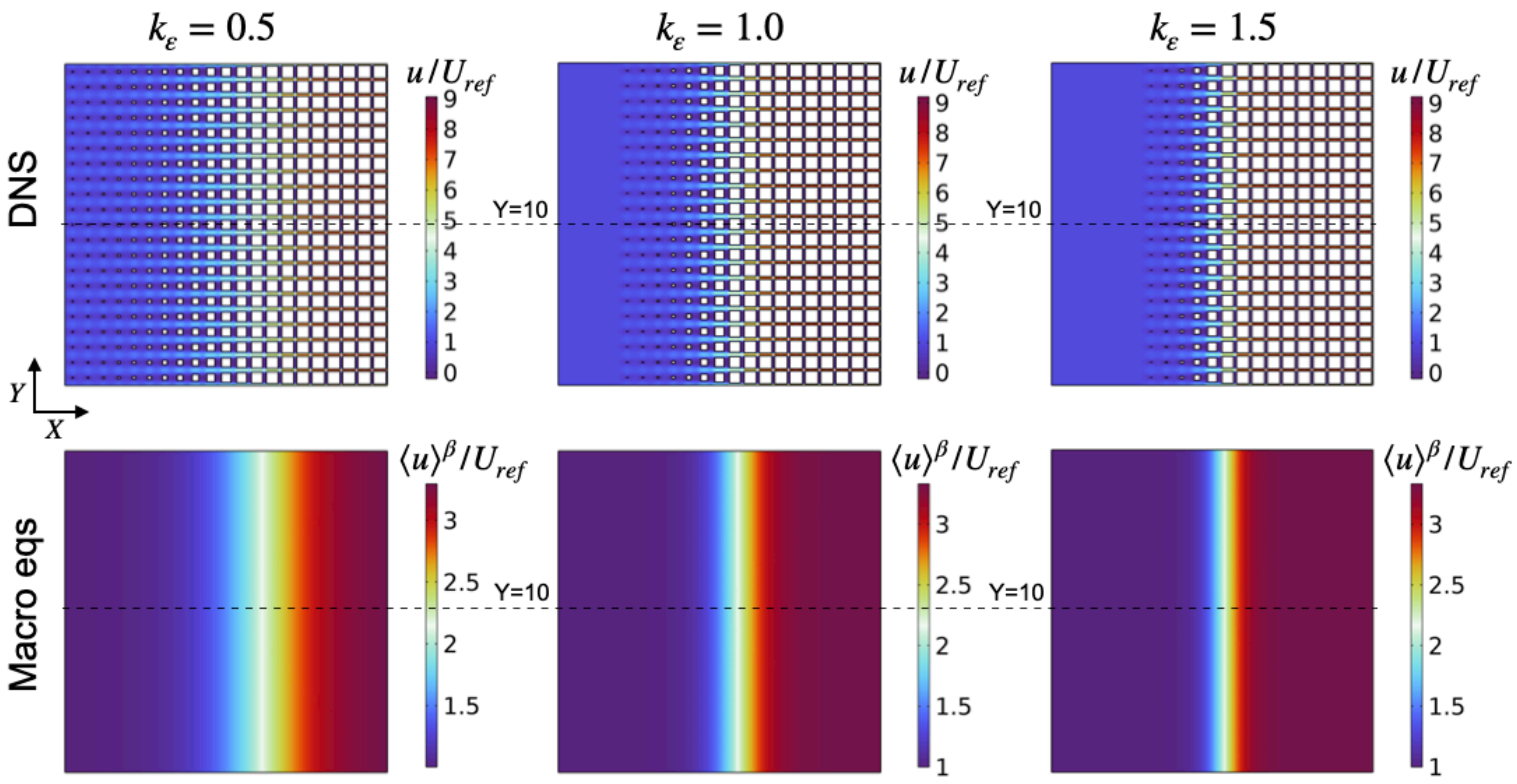
- Tabulate **permeability** and **diffusion-dispersion tensors** for **porosity** and **Péclet** number
- Solve **macroscopic equations** for a **given porosity distribution** and **macroscopic Péclet number**
- Compare to **DNS**





Results : momentum transport (1/2)



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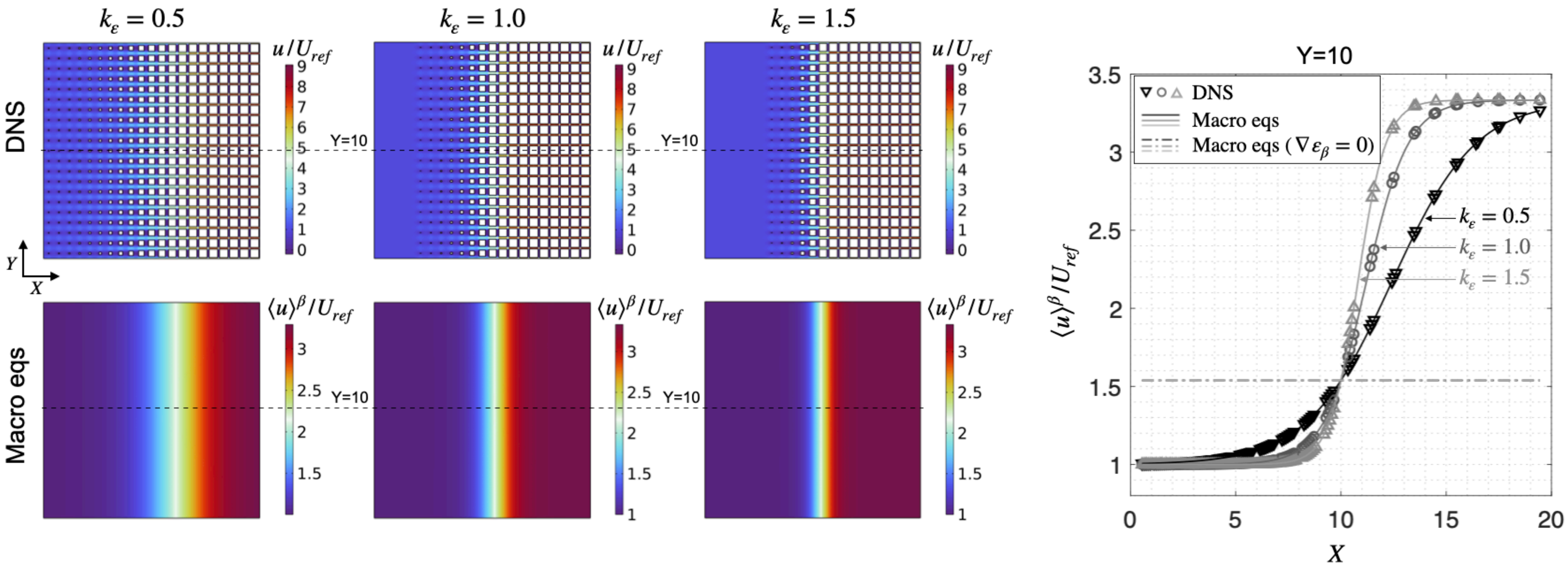

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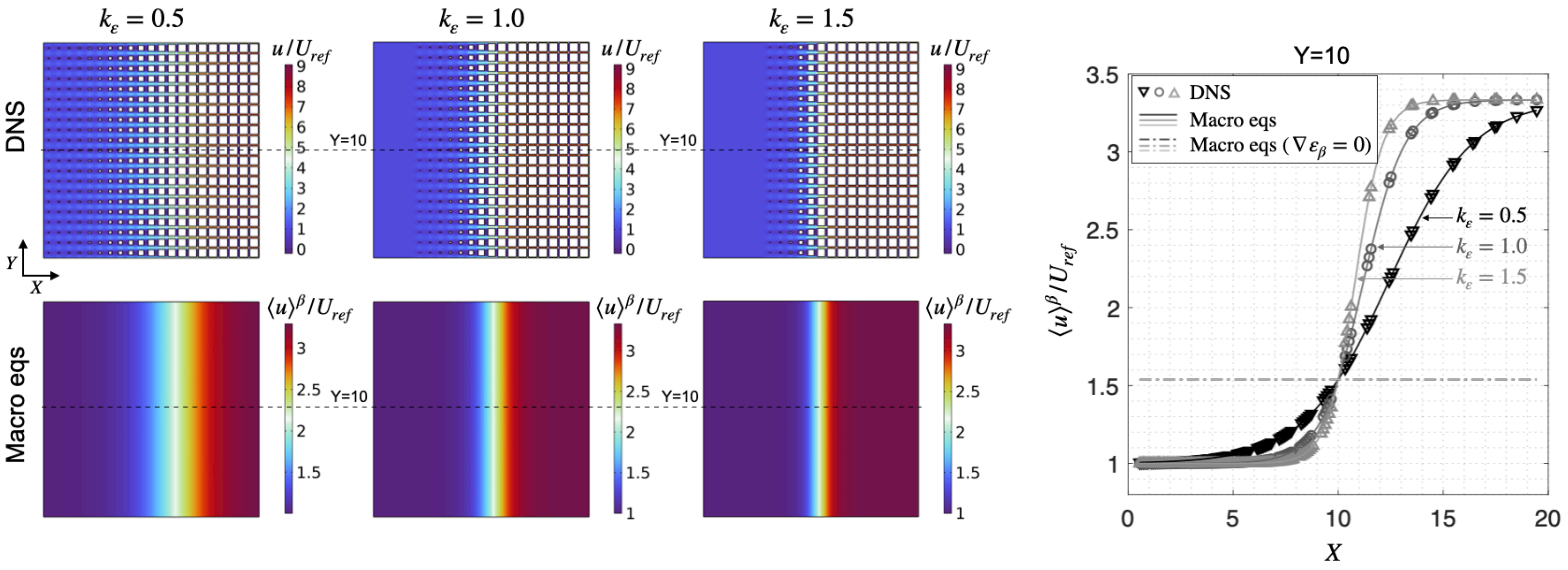
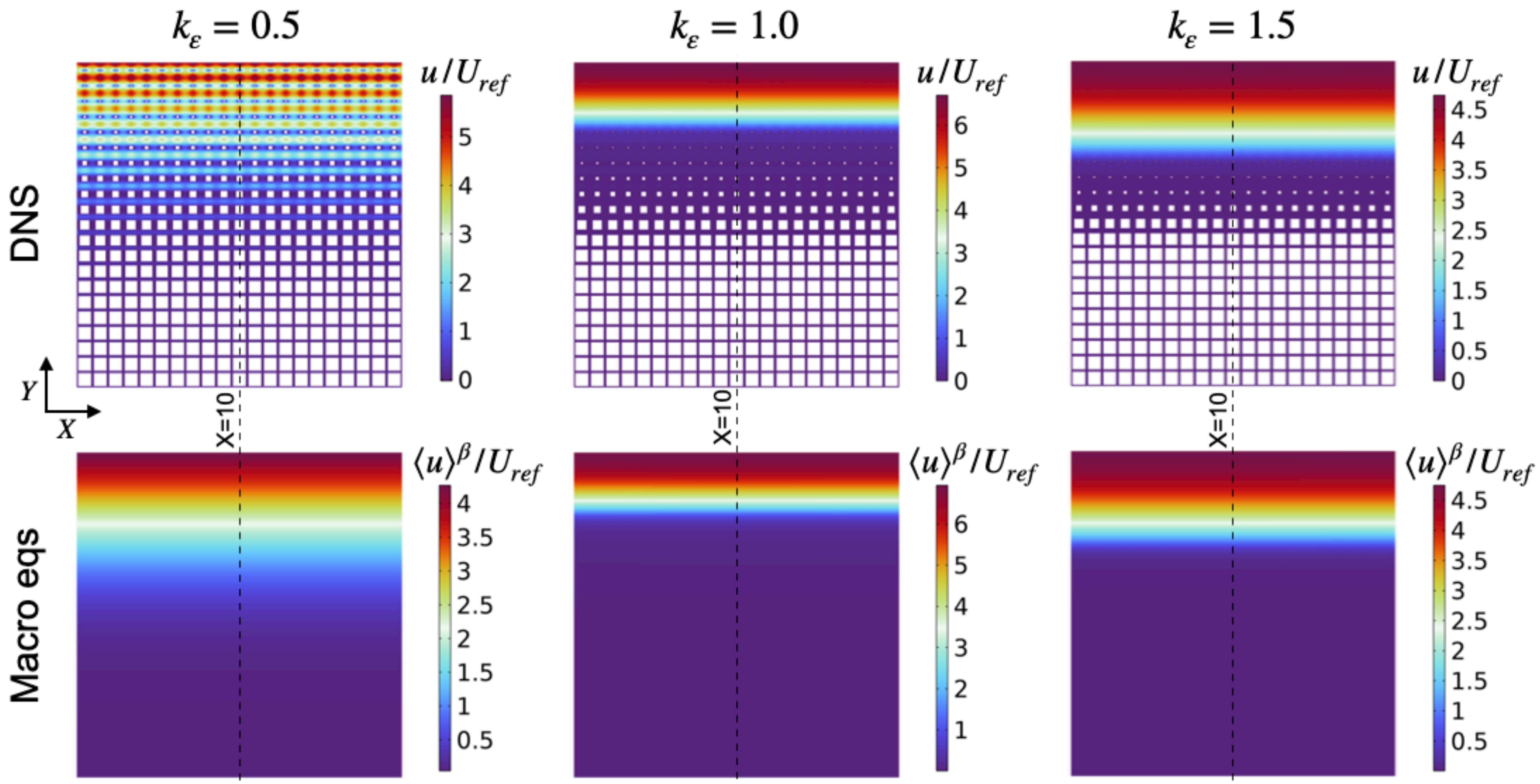
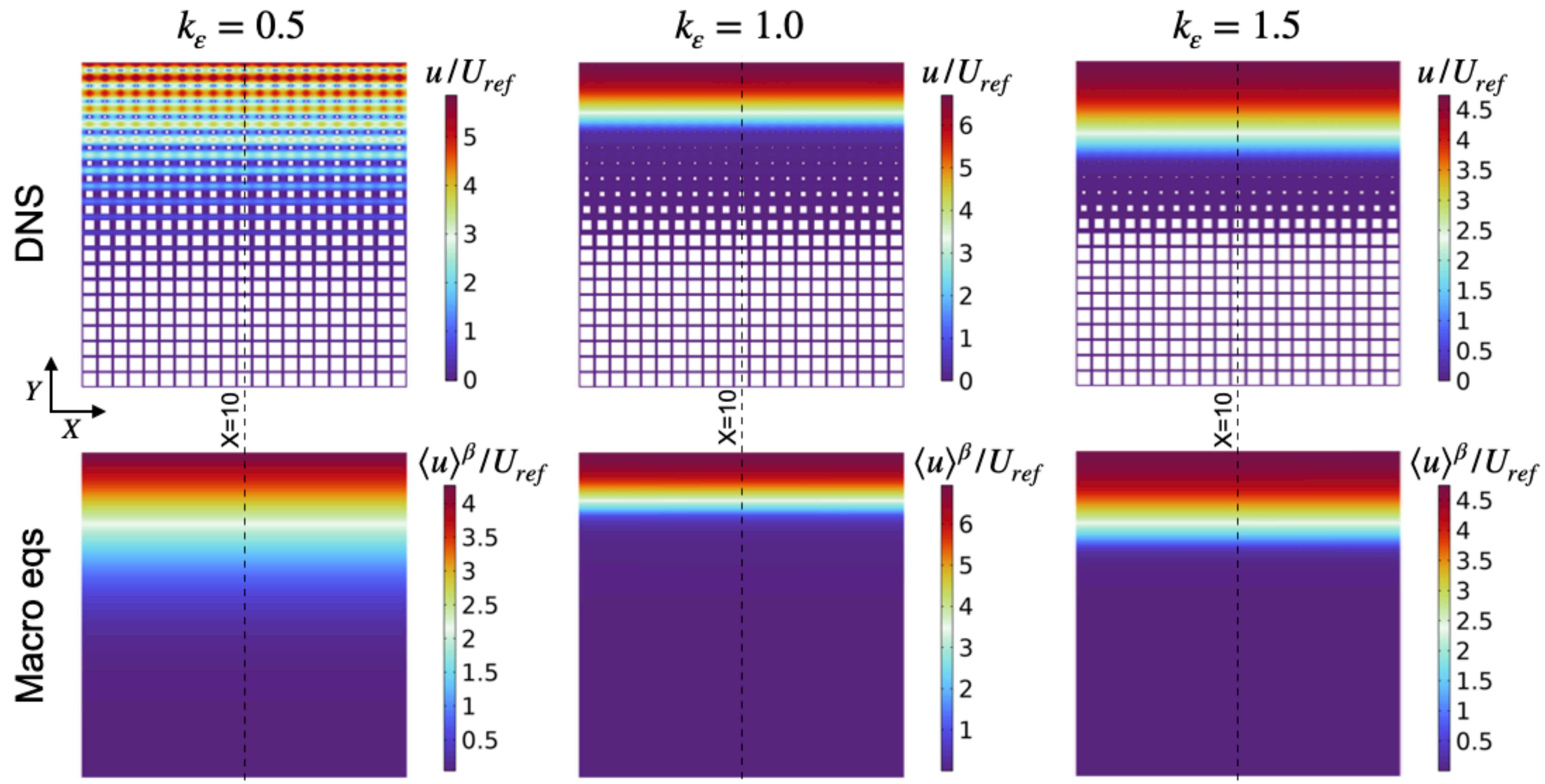


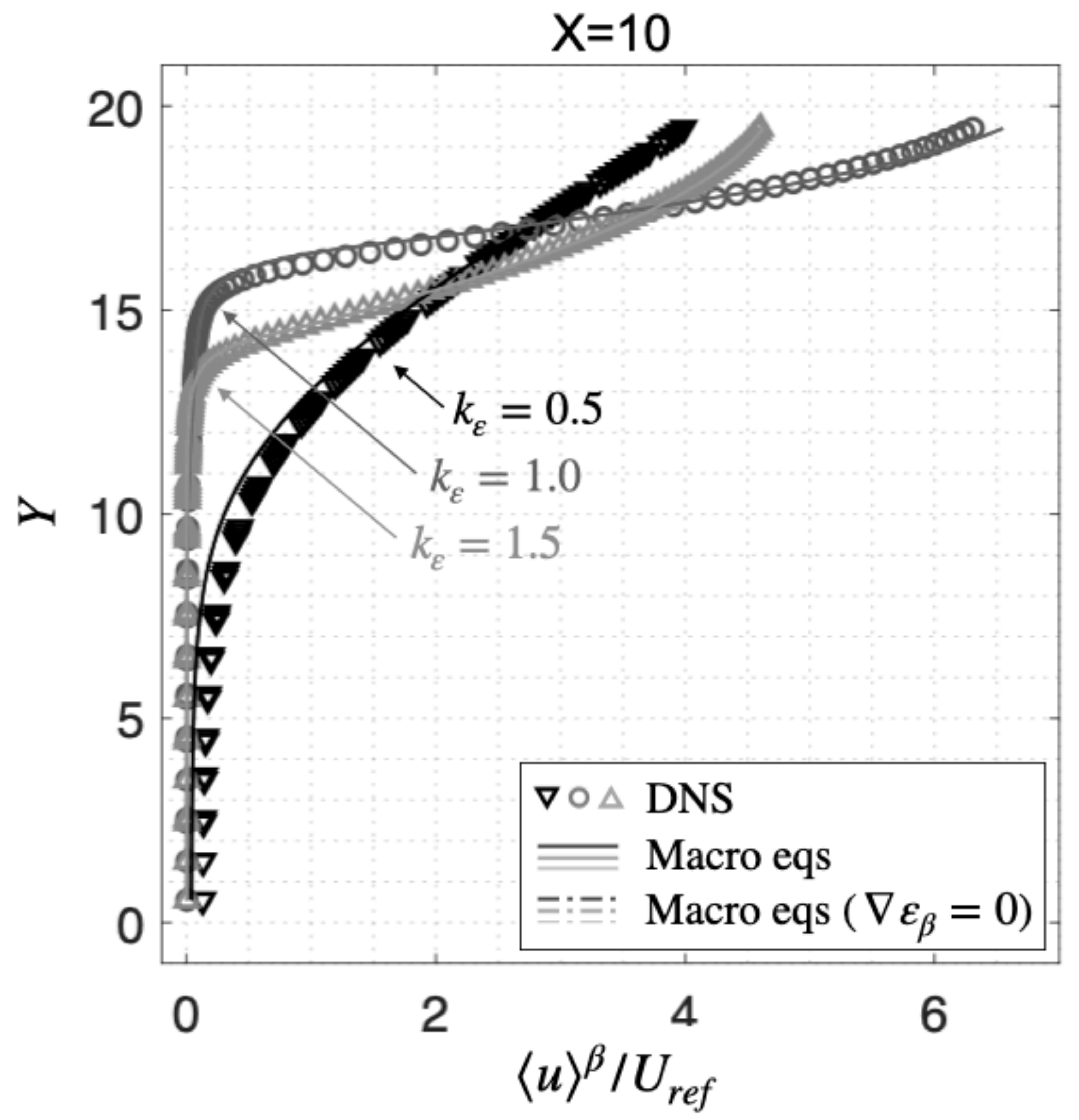
Flow along porosity gradients: extra terms are required!

Results : momentum transport (2/2)



Results : momentum transport (2/2)





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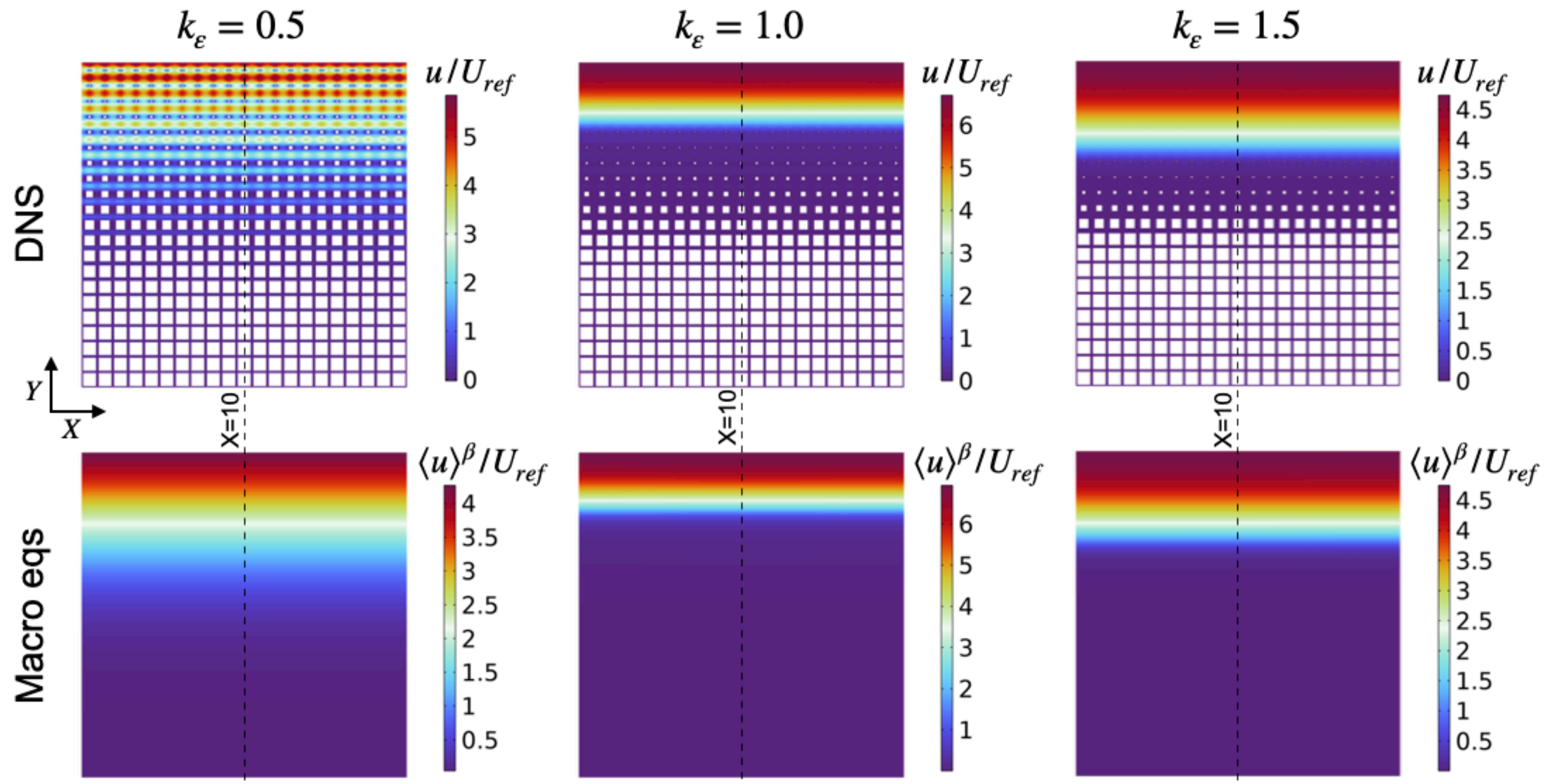
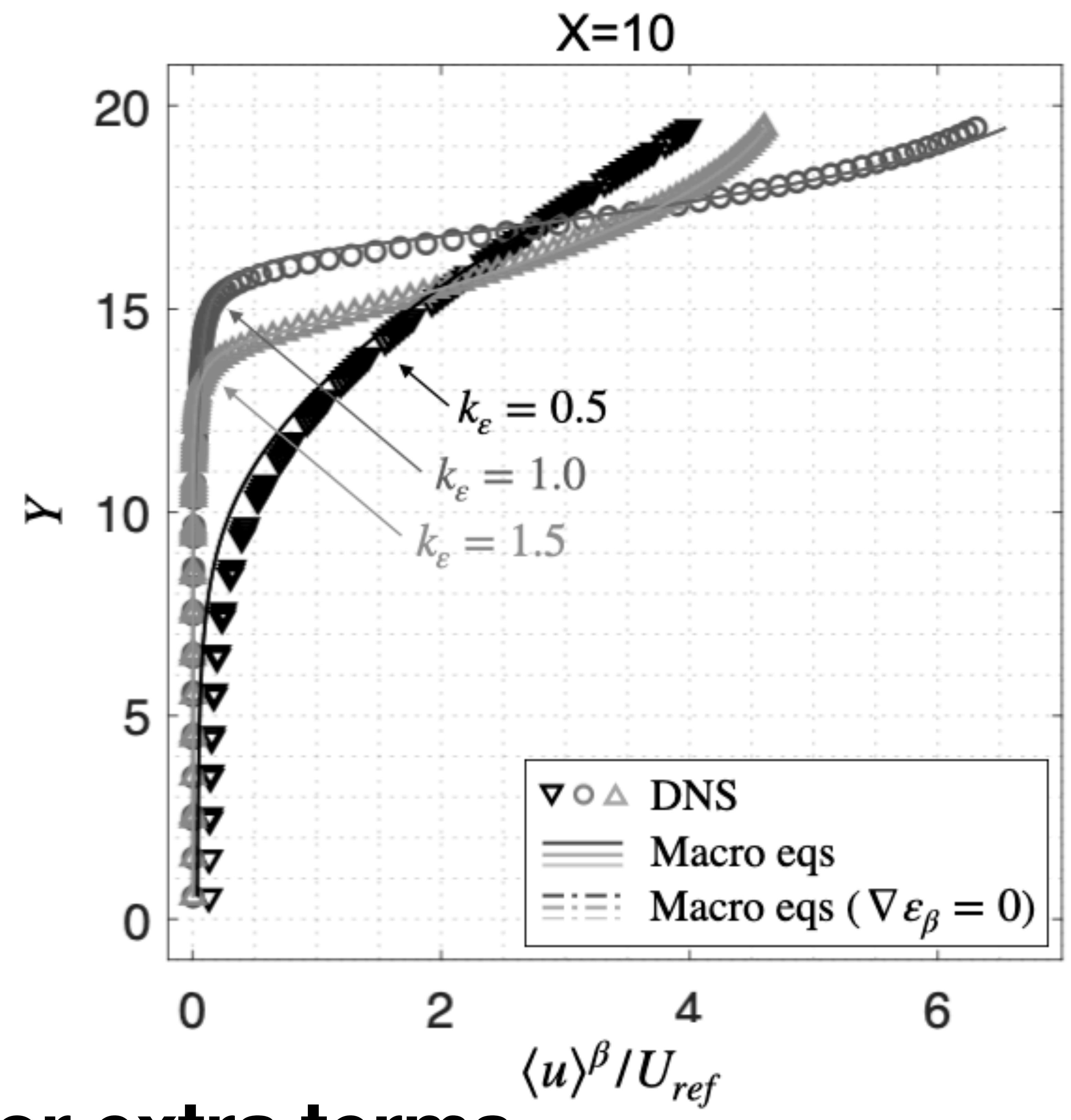


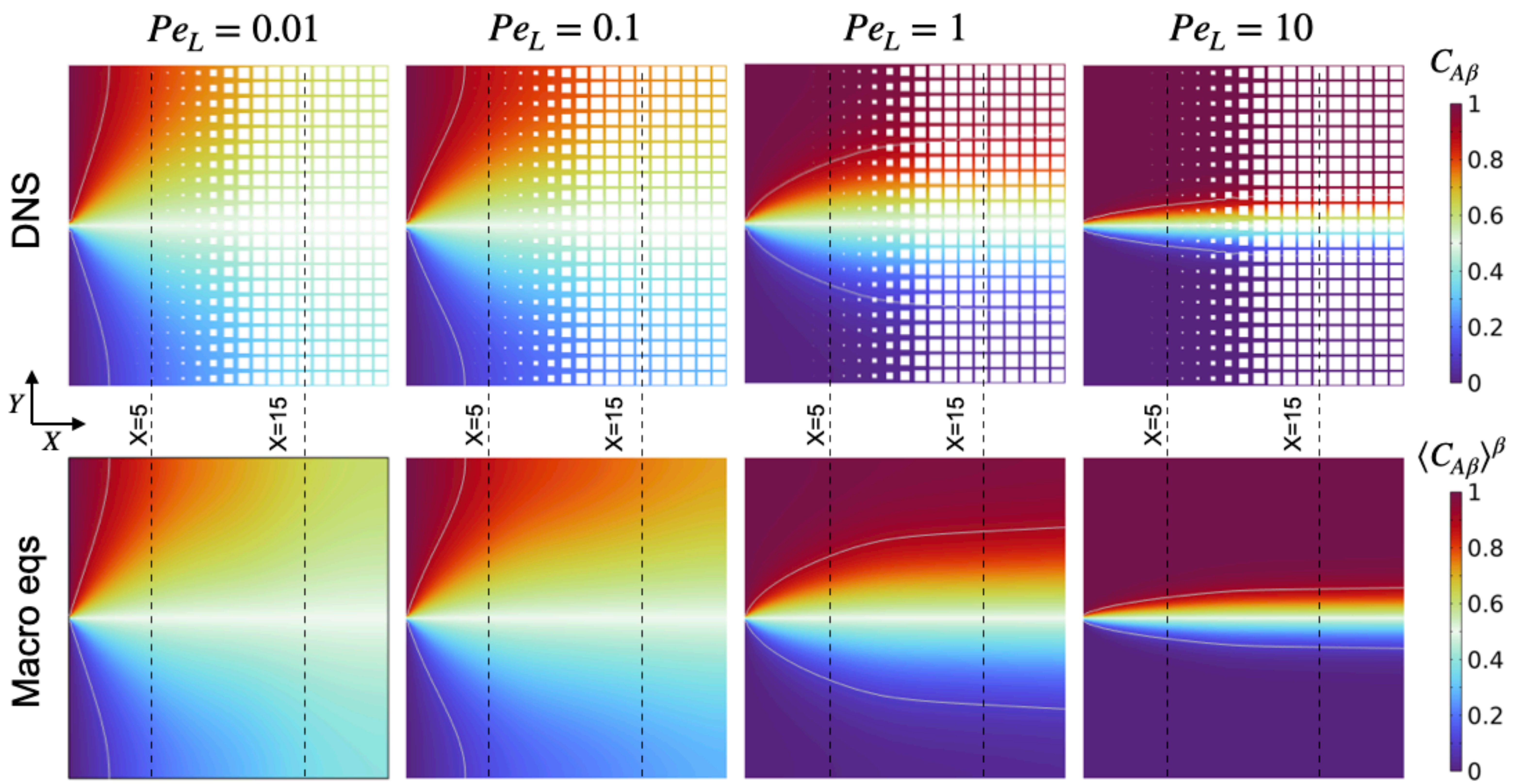


Flow orthogonal to porosity gradients: no need for extra terms

$$\nabla_x . \langle \mathbf{v}_\beta \rangle^\beta = -\varepsilon_\beta^{-1} \nabla_x \varepsilon_\beta . \langle \mathbf{v}_\beta \rangle^\beta$$

$$0 = -\nabla_x \langle P_\beta \rangle^\beta + \rho_\beta \mathbf{g} + \mu_\beta \nabla_x^2 \langle \mathbf{v}_\beta \rangle^\beta - \mu_\beta \left(\varepsilon_\beta \mathbf{K}_\beta^{-1} - \varepsilon_\beta^{-1} \nabla_x^2 \varepsilon_\beta \mathbf{I} \right) \cdot \langle \mathbf{v}_\beta \rangle^\beta + \mu_\beta \varepsilon_\beta^{-1} \nabla_x \varepsilon_\beta \cdot \nabla_x \langle \mathbf{v}_\beta \rangle^\beta$$

Results : dispersive transport (1/2)



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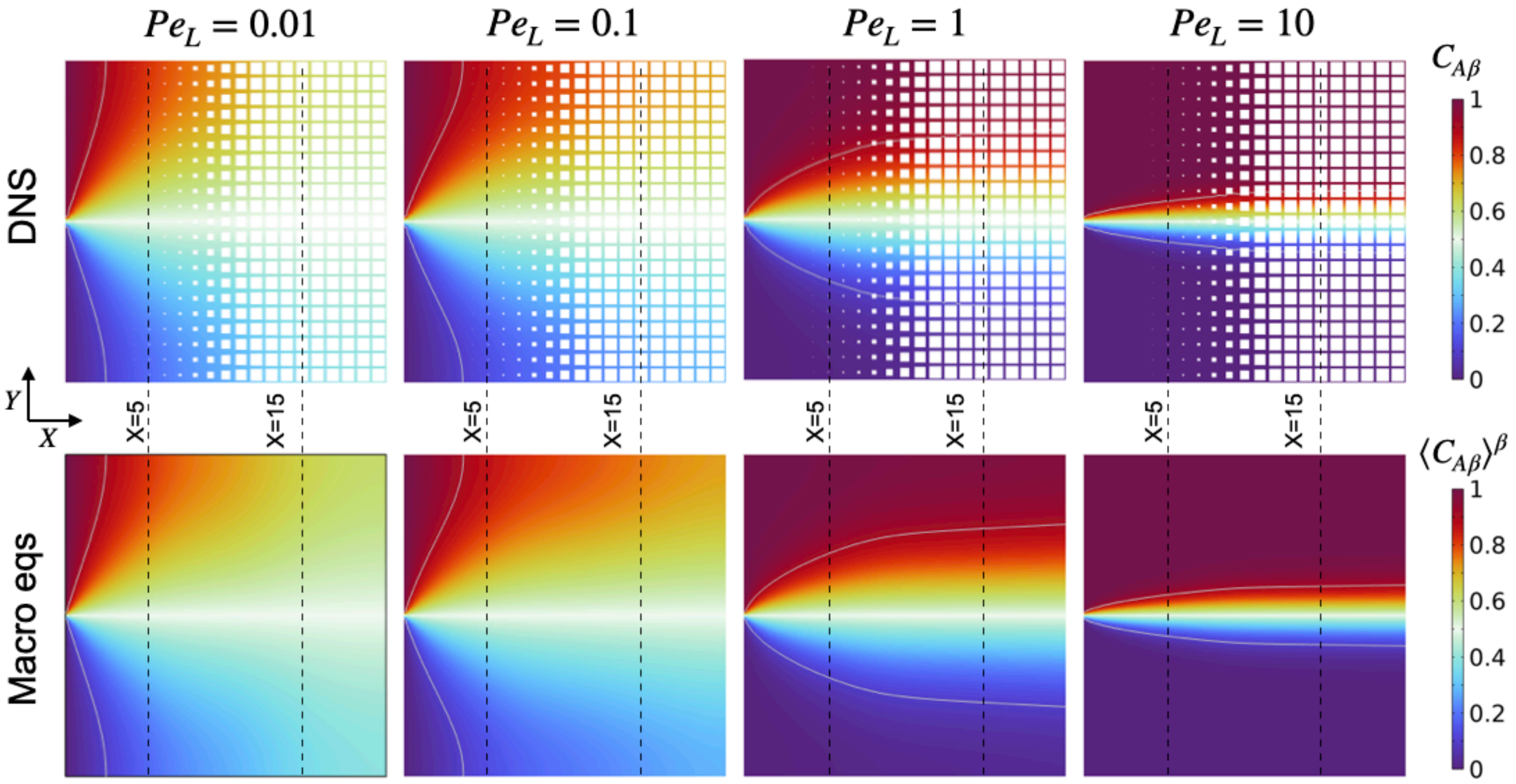
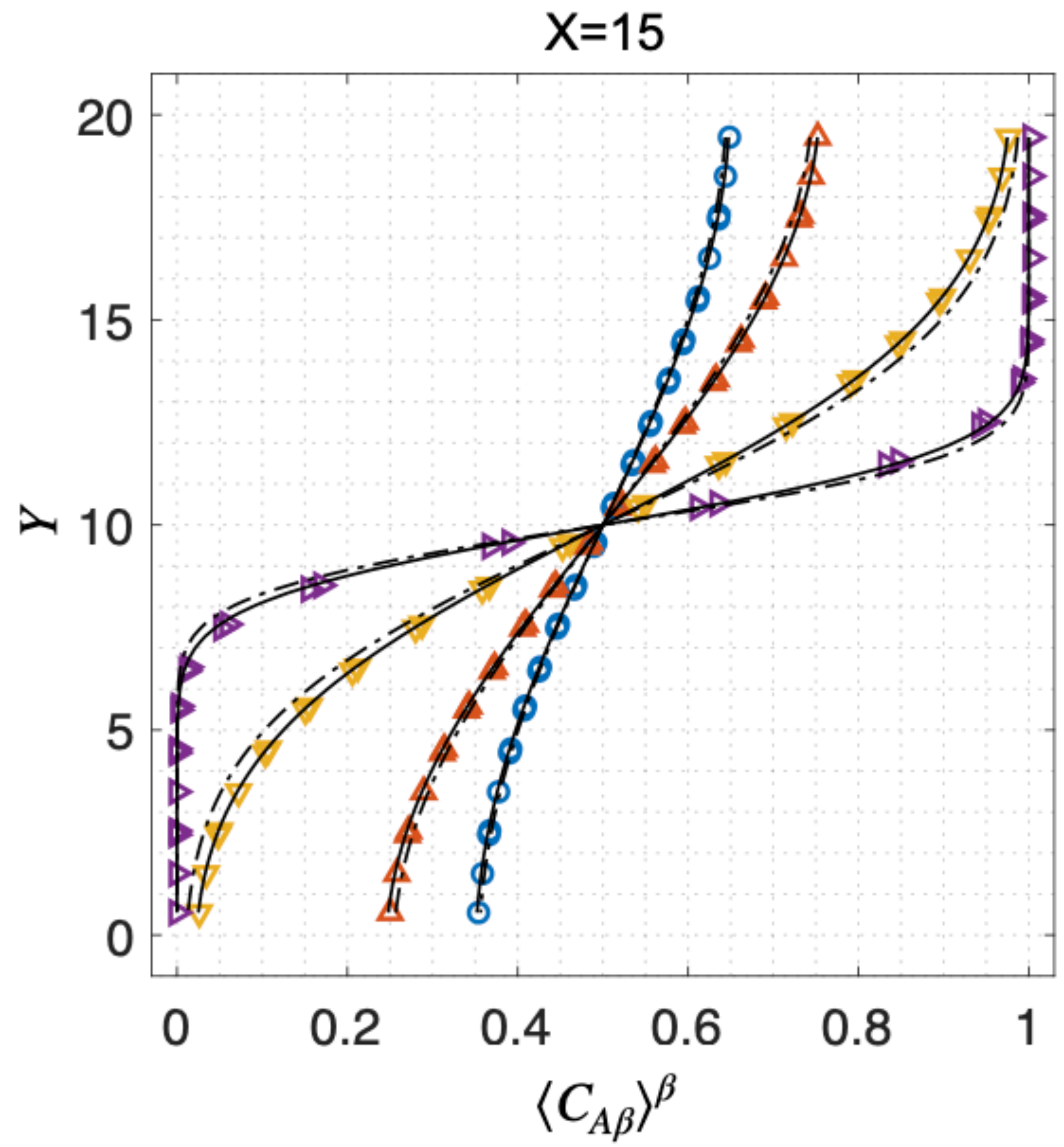
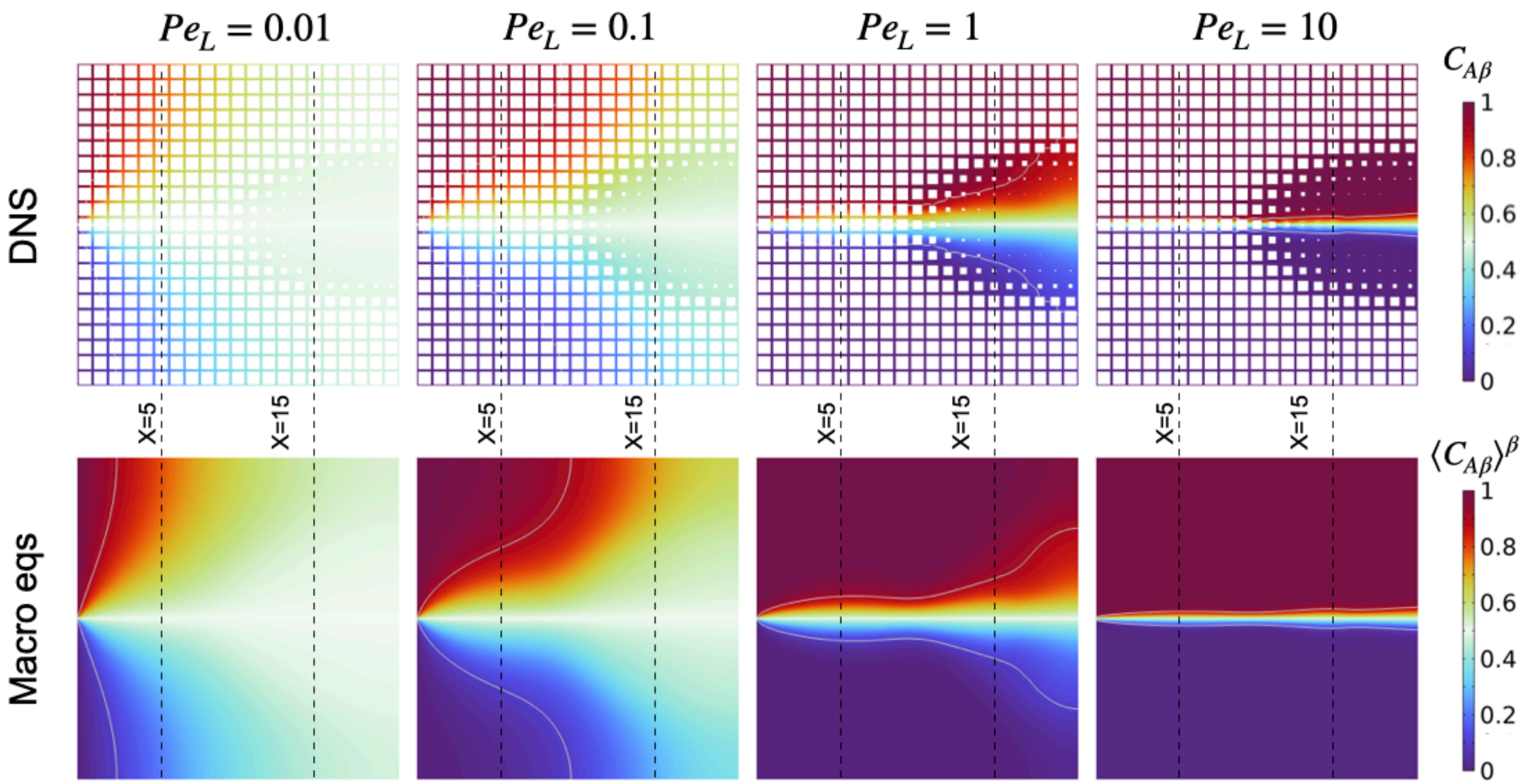
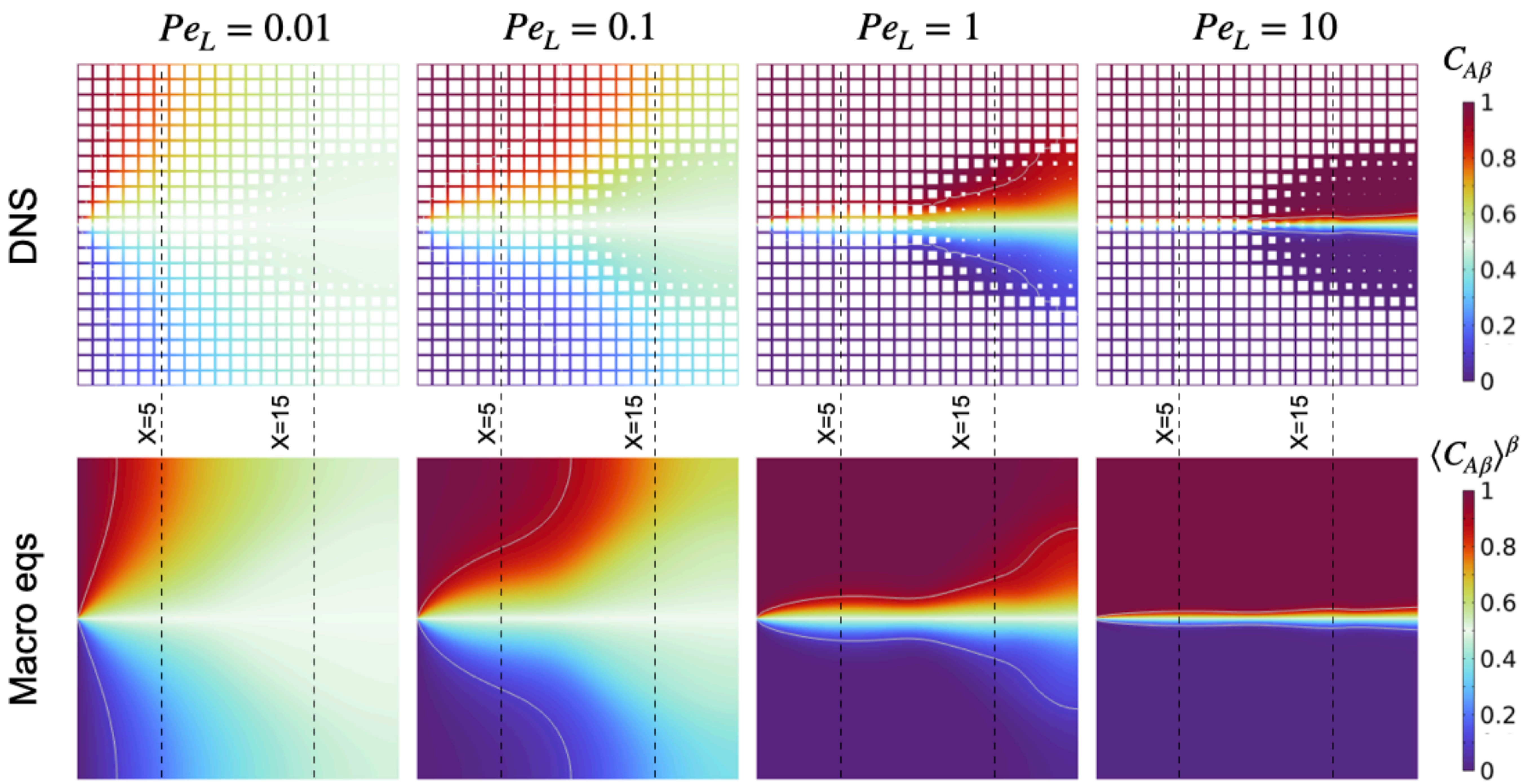


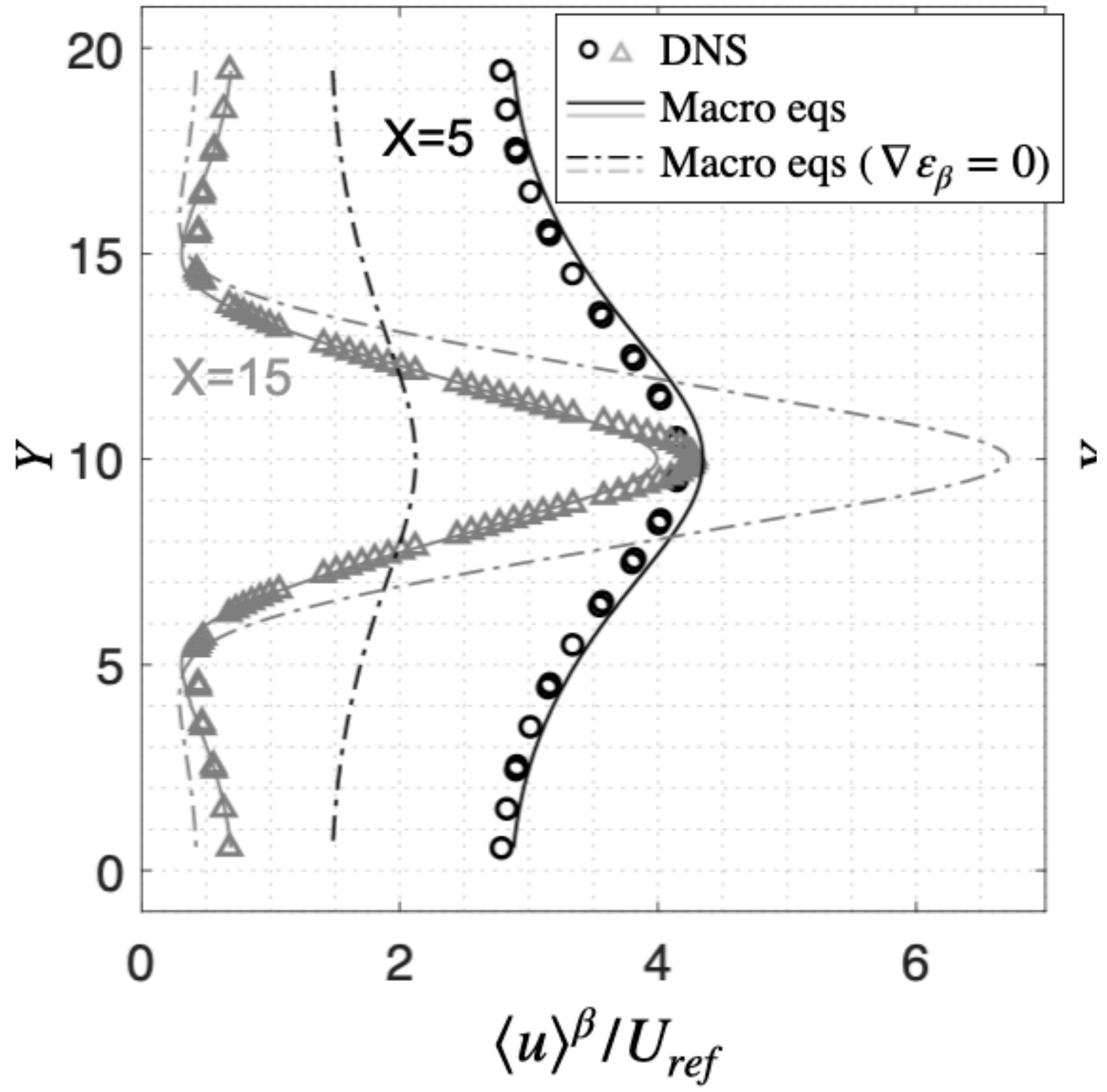


Results : dispersive transport (2/2)

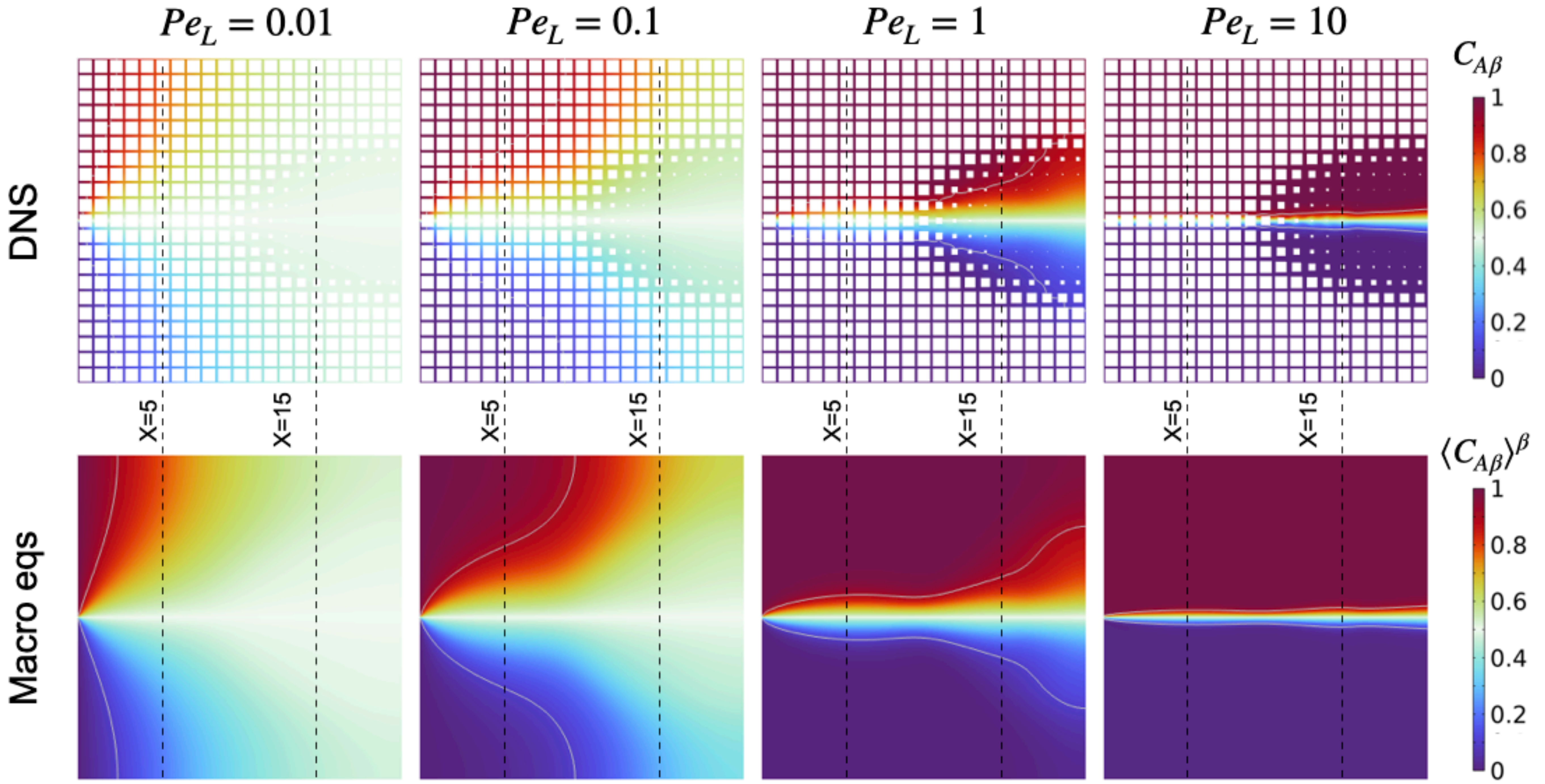


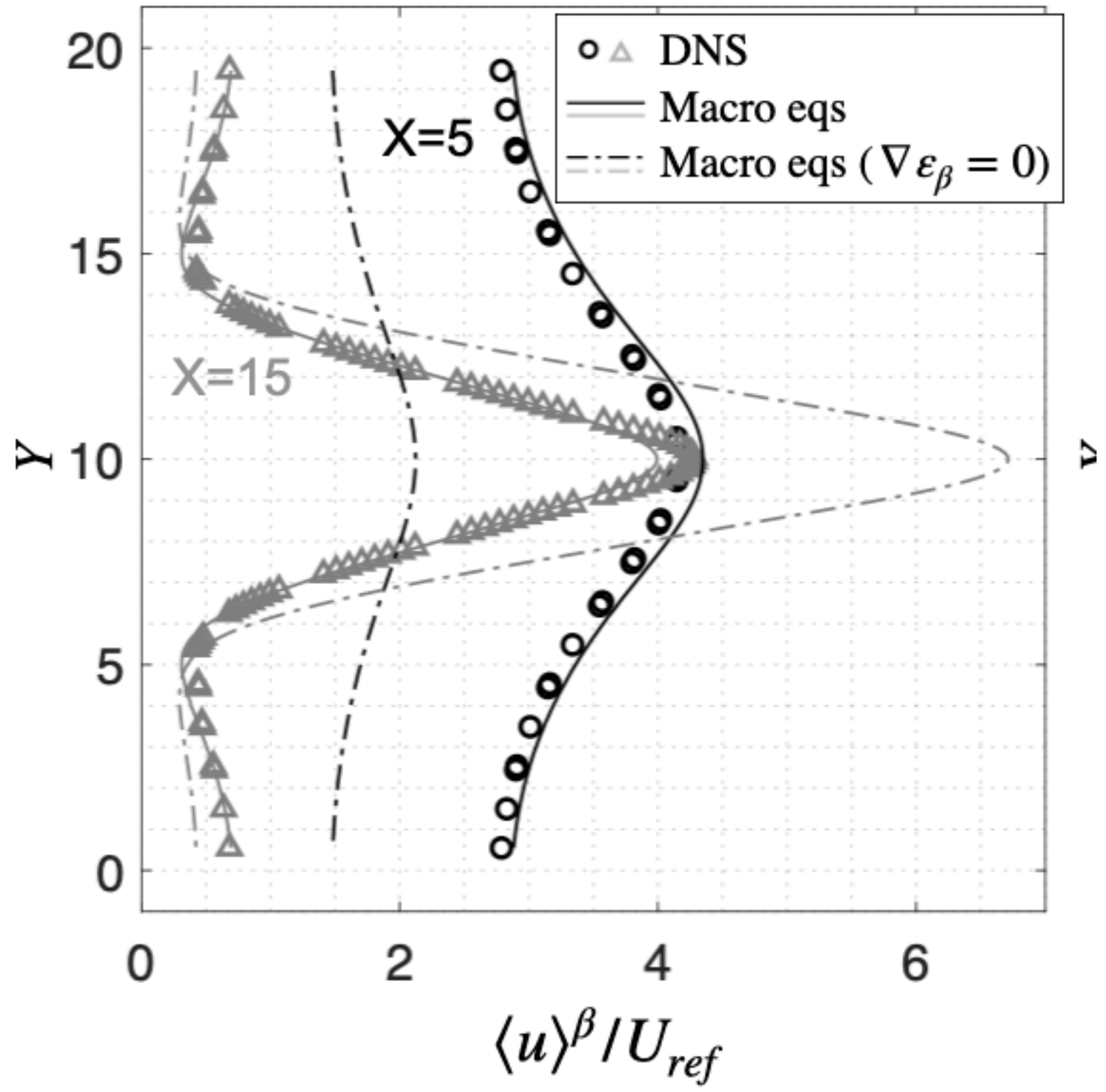
Results : dispersive transport (2/2)

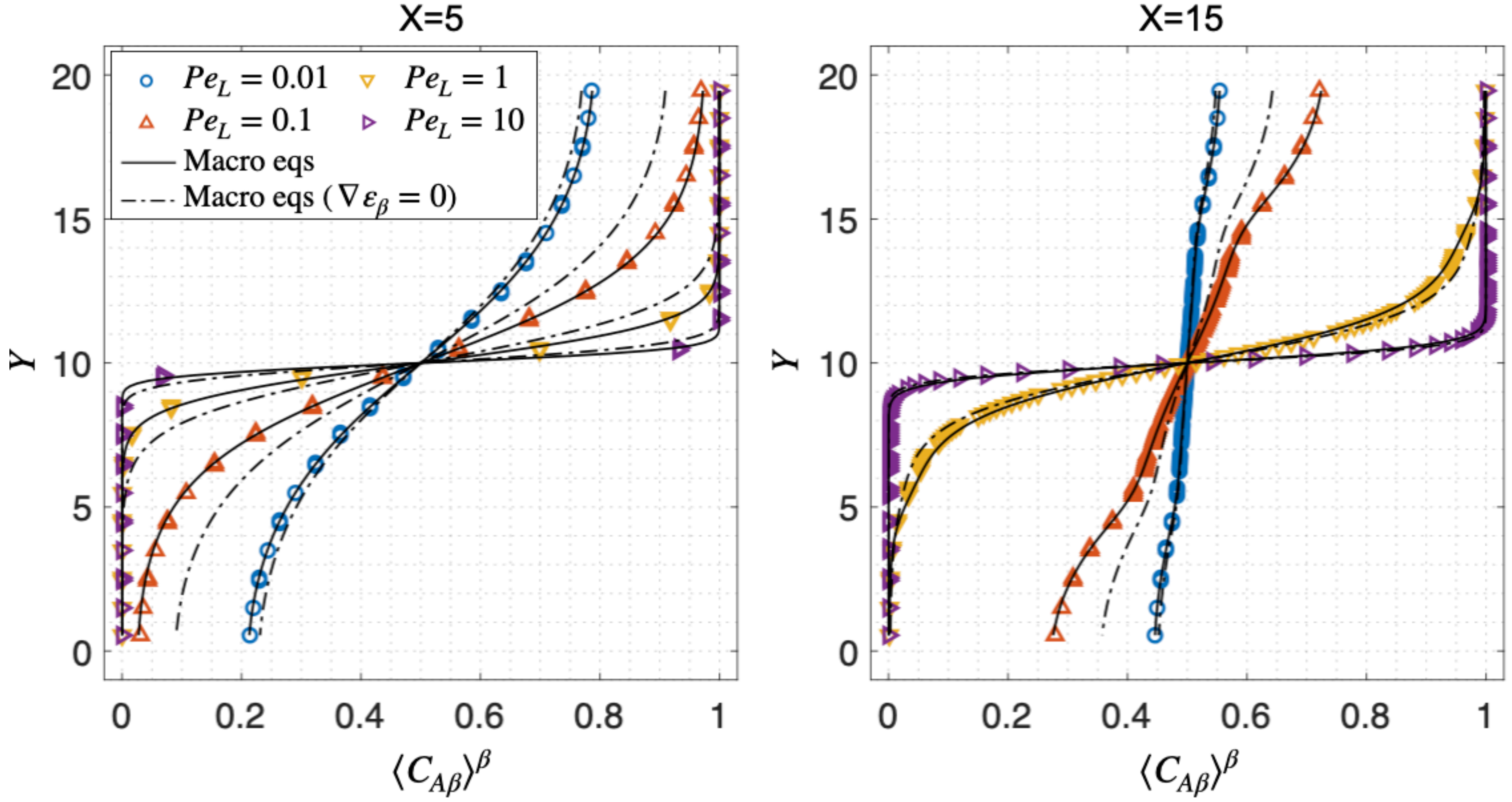




Results : dispersive transport (2/2)







Conclusion

Macroscopic dispersion models work well

- with porosity derivatives only in the macroscopic equation for momentum
- using closure problems for homogeneous porous media
- even with $\nabla \varepsilon$ over short lengths ($\sim \ell$)

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Importance of right choice of average in porosity gradient!

- Mass conservation = conservation of **superficial** velocity

$$\nabla_x \cdot \langle \mathbf{v}_\beta \rangle^\beta = -\,\varepsilon_\beta^{-1} \nabla_x \varepsilon_\beta \cdot \langle \mathbf{v}_\beta \rangle^\beta \iff \nabla_x \cdot \langle \mathbf{v}_\beta \rangle = 0$$

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- Macroscopic dispersion in superficial form has a convective term

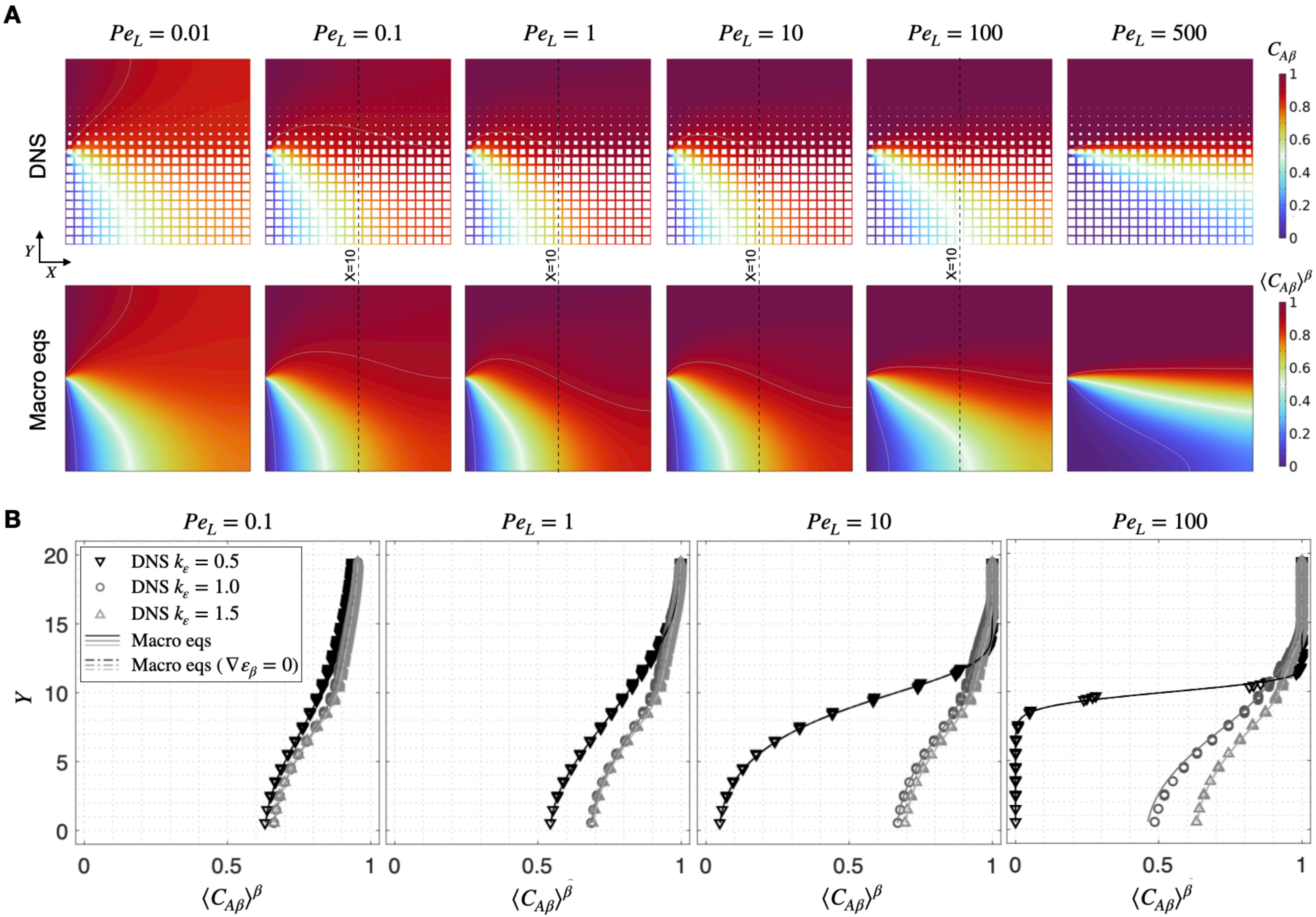
$$\nabla_x \cdot \left(\varepsilon_\beta \langle \mathbf{v}_\beta \rangle^\beta \langle C_{A\beta} \rangle^\beta \right) = \nabla_x \cdot \left[\mathbf{D}_{eff} \cdot \nabla_x \langle C_{A\beta} \rangle^\beta \right]$$

$$\iff \nabla_x \cdot \left[\varepsilon_\beta^{-1} \left(\langle \mathbf{v}_\beta \rangle + \varepsilon_\beta^{-1} \mathbf{D}_{eff} \cdot \nabla_x \varepsilon_\beta \right) \langle C_{A\beta} \rangle \right] = \nabla_x \cdot \left[\varepsilon_\beta^{-1} \mathbf{D}_{eff} \cdot \nabla_x \langle C_{A\beta} \rangle \right]$$

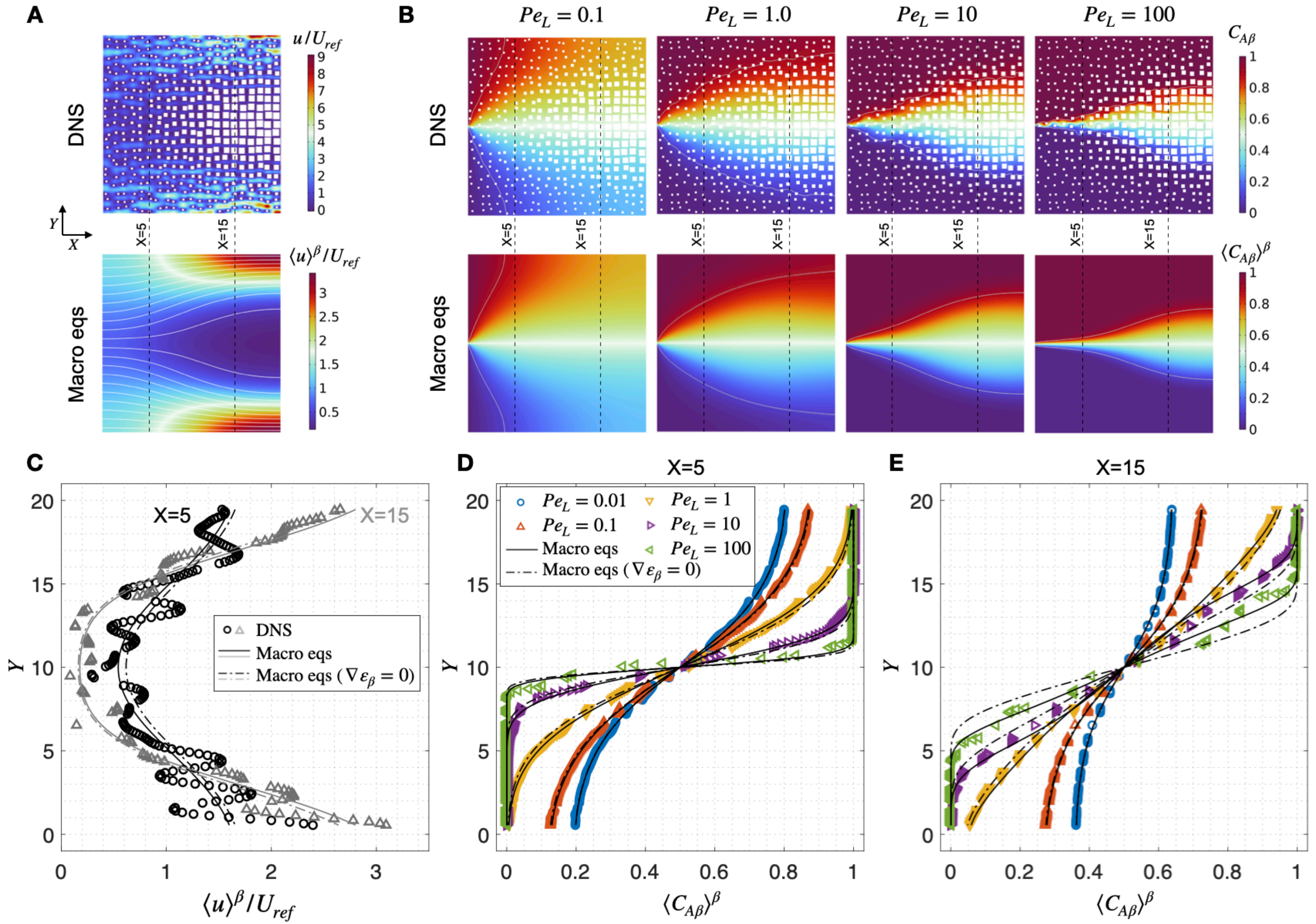
Porosity gradient convective term

Thank you for your attention

Morgan Chabanon, J. Alberto Ochoa-Tapia, & Benoît Goyeau
Dispersion in porous media with porosity gradients
Transport in Porous Media, 153 (59), 2026



A
$Pe_L = 0.01$
$Pe_L = 0.1$
$Pe_L = 1$
$Pe_L = 10$
$Pe_L = 100$
$Pe_L = 500$
DNS
Macro eqs
$C_{A\beta}$
$\langle C_{A\beta} \rangle^\beta$
X=10
Y
X
B
$Pe_L = 0.1$
$Pe_L = 1$
$Pe_L = 10$
$Pe_L = 100$
DNS $k_\varepsilon = 0.5$
DNS $k_\varepsilon = 1.0$
DNS $k_\varepsilon = 1.5$
Macro eqs
Macro eqs ($\nabla \varepsilon_\beta = 0$)
Y
$\langle C_{A\beta} \rangle^\beta$



A
DNS
u/U_{ref}
Macro eqs
$\langle u\rangle^\beta/U_{ref}$
X=5
X=15
B
$Pe_L = 0.1$
$Pe_L = 1.0$
$Pe_L = 10$
$Pe_L = 100$
$C_{A\beta}$
$\langle C_{A\beta}\rangle^\beta$
C
X=5
X=15
DNS
Macro eqs
Macro eqs ($\nabla\varepsilon_\beta = 0$)
Y
$\langle u\rangle^\beta/U_{ref}$
D
X=5
$Pe_L = 0.01$
$Pe_L = 0.1$
$Pe_L = 1$
$Pe_L = 10$
$Pe_L = 100$
Macro eqs
Macro eqs ($\nabla\varepsilon_\beta = 0$)
$\langle C_{A\beta}\rangle^\beta$
E
X=15
$\langle C_{A\beta}\rangle^\beta$

Local problem

- Momentum transport

$$\nabla_y . \mathbf{v}_\beta = 0 \qquad \text{in the } \beta\text{-phase}$$

$$0 = -\nabla_y P_\beta + \rho_\beta \mathbf{g} + \mu_\beta \nabla_y^2 \mathbf{v}_\beta \qquad \text{in the } \beta\text{-phase}$$

$$\mathbf{v}_\beta = 0 \qquad \text{at } A_{\beta\sigma}$$

- Mass transport

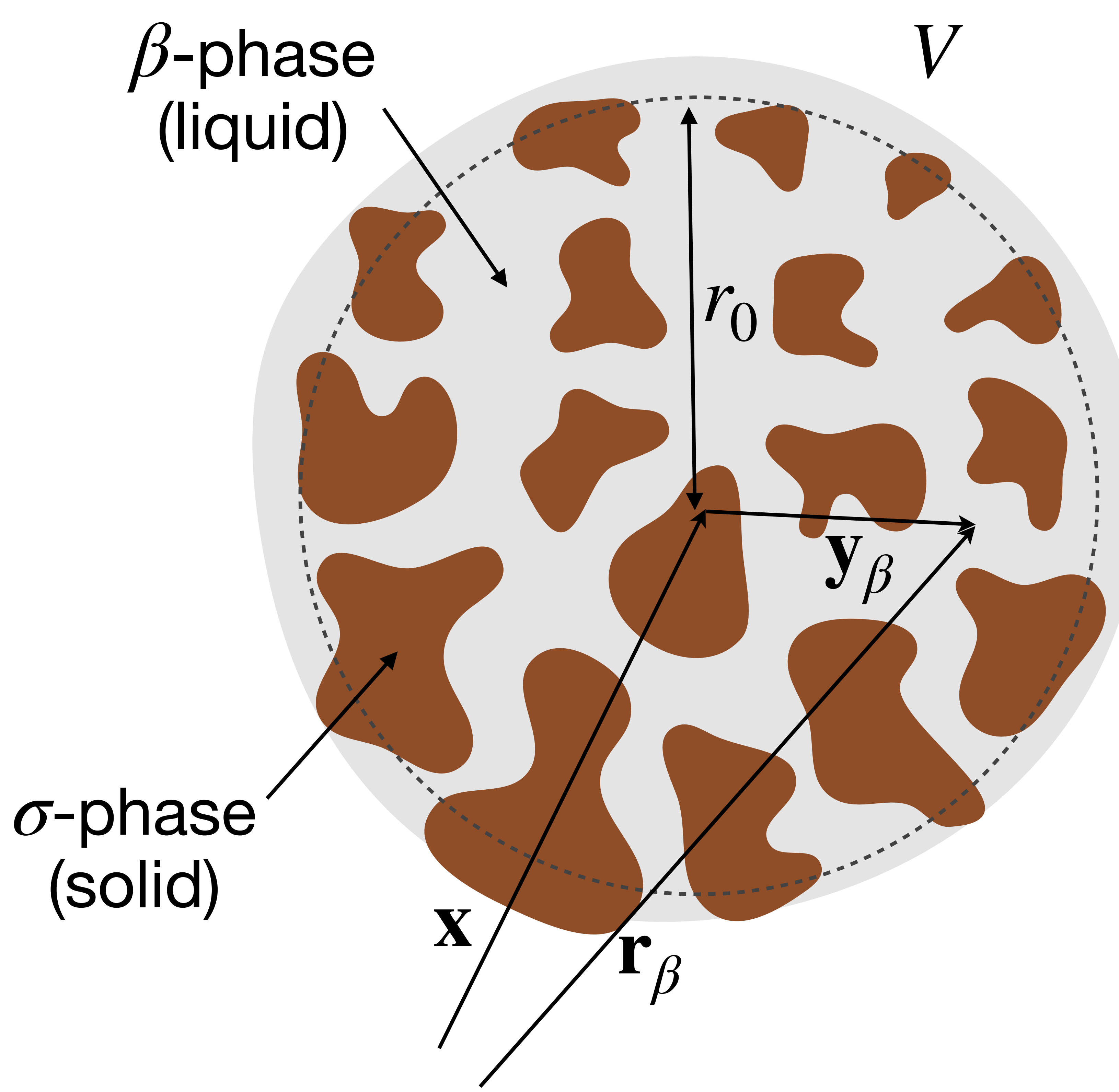
$$\nabla_y \cdot (\mathbf{v}_\beta C_{A\beta}) = \nabla_y \cdot \left(D_\beta \nabla_y C_{A\beta} \right) \qquad \text{in the } \beta\text{-phase}$$

$$\mathbf{n}_{\beta\sigma} \cdot D_\beta \nabla_y C_{A\beta} = 0 \qquad \text{at } A_{\beta\sigma}$$

- Volume averaging toolbox: averages, transport theorems, deviations, length scale constraints …

$$\varepsilon_\beta = \frac{V_\beta}{V} \quad ; \quad \langle \psi_\beta \rangle^\beta = \frac{1}{V_\beta} \int_{V_\beta} \psi_\beta \, dV \quad ; \quad \psi_\beta = \langle \psi_\beta \rangle^\beta + \tilde{\psi}_\beta \quad \dots$$

Averaging volume



Upscaling momentum transport

- Non-closed averaged problem

$$\nabla_x . \langle \mathbf{v}_\beta \rangle^\beta = - \varepsilon_\beta^{-1} \nabla_x \varepsilon_\beta . \langle \mathbf{v}_\beta \rangle^\beta$$

$$L_\varepsilon \sim L_v = O(r_0)$$

$$0 = -\nabla_x \langle P_\beta \rangle^\beta + \rho_\beta \mathbf{g} + \frac{1}{V_\beta} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot \left(-\mathbf{I}\tilde{P}_\beta + \mu_\beta \nabla_y \tilde{\mathbf{v}}_\beta \right) dA$$
$$+\mu_\beta \left(\nabla_x^2 \langle \mathbf{v}_\beta \rangle^\beta + \varepsilon_\beta^{-1} \nabla_x \varepsilon_\beta \cdot \nabla_x \langle \mathbf{v}_\beta \rangle^\beta + \varepsilon_\beta^{-1} \nabla_x^2 \varepsilon_\beta \langle \mathbf{v}_\beta \rangle^\beta \right)$$

- Deviation problem

$$\nabla_y \cdot \tilde{\mathbf{v}}_\beta = \varepsilon_\beta^{-1} \nabla_x \varepsilon_\beta \cdot \langle \mathbf{v}_\beta \rangle^\beta$$

Additional source terms

$$0 = -\nabla_y \tilde{P}_\beta + \mu_\beta \nabla_y^2 \tilde{\mathbf{v}}_\beta - \mu_\beta \varepsilon_\beta^{-1} \nabla_x \varepsilon_\beta \cdot \nabla_x \langle \mathbf{v}_\beta \rangle^\beta - \mu_\beta \varepsilon_\beta^{-1} \nabla_x^2 \varepsilon_\beta \langle \mathbf{v}_\beta \rangle^\beta - \frac{1}{V_\beta} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot \left(-\mathbf{I}\tilde{P}_\beta + \mu_\beta \nabla_y \tilde{\mathbf{v}}_\beta dA \right)$$

BC: $\tilde{\mathbf{v}}_\beta = -\langle \mathbf{v}_\beta \rangle^\beta$

- Closure variables

$$\tilde{P}_\beta = \mu_\beta \mathbf{b}_\beta \cdot \langle \mathbf{v}_\beta \rangle^\beta + \mu_\beta \mathbf{C}_\beta : \nabla_x \langle \mathbf{v}_\beta \rangle^\beta \quad ; \quad \tilde{\mathbf{v}}_\beta = \mathbf{B}_\beta \cdot \langle \mathbf{v}_\beta \rangle^\beta + \mathscr{C}_\beta : \nabla_x \langle \mathbf{v}_\beta \rangle^\beta$$

Upscaling momentum transport

- Closed macroscopic model

$$\nabla_x . \langle \mathbf{v}_\beta \rangle^\beta = - \varepsilon_\beta^{-1} \nabla_x \varepsilon_\beta . \langle \mathbf{v}_\beta \rangle^\beta$$

$$0 = - \nabla_x \langle P_\beta \rangle^\beta + \rho_\beta \mathbf{g} + \mu_\beta \nabla_x^2 \langle \mathbf{v}_\beta \rangle^\beta - \mu_\beta \left(\varepsilon_\beta \mathbf{K}_\varepsilon{}^{-1} - \varepsilon_\beta^{-1} \nabla_x^2 \varepsilon_\beta \mathbf{I} \right) \cdot \langle \mathbf{v}_\beta \rangle^\beta$$
$$- \mu_\beta \left(\varepsilon_\beta \mathscr{K}_\varepsilon^{-1} - \varepsilon_\beta^{-1} \nabla_x \varepsilon_\beta \otimes \mathbf{I} \right) : \nabla_x \langle \mathbf{v}_\beta \rangle^\beta$$

- With the permeability tensors defined as

$$\varepsilon_\beta \mathbf{K}_\varepsilon{}^{-1} = - \frac{1}{V_\beta} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot \left(-\mathbf{I} \otimes \mathbf{b}_\beta + \nabla_y \mathbf{B}_\beta \right) dA$$

$$\varepsilon_\beta \mathscr{K}_\varepsilon^{-1} = - \frac{1}{V_\beta} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot \left(-\mathbf{I} \otimes \mathbf{C}_\beta + \nabla_y \mathscr{C}_\beta \right) dA$$

Upscaling momentum transport

Closure problem 1

$$\nabla_y \cdot \mathbf{B}_\beta = \varepsilon_\beta^{-1} \nabla_x \varepsilon_\beta$$

$$0 = -\nabla_y \mathbf{b}_\beta + \nabla_y^2 \mathbf{B}_\beta + \left(\varepsilon_\beta \mathbf{K}_\varepsilon^{-1} - \varepsilon_\beta^{-1} \nabla_x^2 \varepsilon_\beta \mathbf{I}\right)$$

BC: $\mathbf{B}_\beta = -\mathbf{I}$

Outer boundary conditions

Closure problem 2

$$\nabla_y \cdot \mathscr{C}_\beta = 0$$

$$0 = -\nabla_y \mathbf{C}_\beta + \nabla_y^2 \mathscr{C}_\beta + \left(\varepsilon_\beta \mathscr{K}_\varepsilon^{-1} - \varepsilon_\beta^{-1} \nabla_x \varepsilon_\beta \otimes \mathbf{I}\right)$$

BC: $\mathscr{C}_\beta = 0$

Outer boundary conditions

To be solved on a **representative elementary volume (REV)**

“Mass production term” is incompatible with periodic boundary conditions !

Simplification of the closure problem

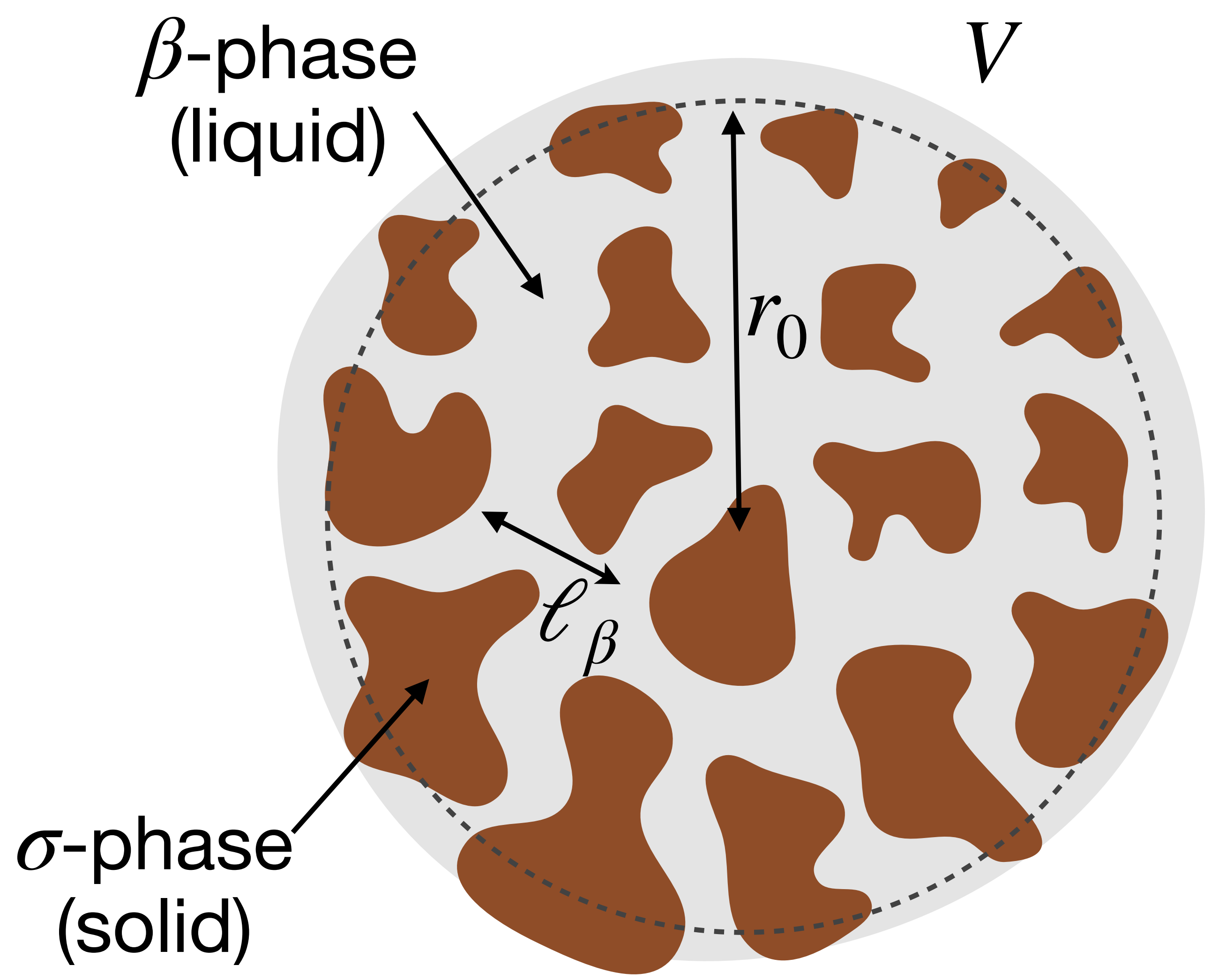
Back to the deviation problem

Source terms

$$0 = -\nabla_y \tilde{P}_\beta + \mu_\beta \nabla_y^2 \tilde{\mathbf{v}}_\beta - \mu_\beta \varepsilon_\beta^{-1} \nabla_x \varepsilon_\beta \cdot \nabla_x \langle \mathbf{v}_\beta \rangle^\beta - \mu_\beta \varepsilon_\beta^{-1} \nabla_x^2 \varepsilon_\beta \langle \mathbf{v}_\beta \rangle^\beta - \frac{1}{V_\beta} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot \left(-\mathbf{I}\tilde{P}_\beta + \mu_\beta \nabla_y \tilde{\mathbf{v}}_\beta dA \right)$$

$$O\left(\mu_\beta \frac{\langle \mathbf{v}_\beta \rangle^\beta}{l_\beta^2} \right) \gg O\left(\mu_\beta \frac{\langle \mathbf{v}_\beta \rangle^\beta}{L_\varepsilon L_v} ; \mu_\beta \frac{\langle \mathbf{v}_\beta \rangle^\beta}{L_\varepsilon^2} \right)$$

$\ell_\beta \ll (L_\varepsilon, L_v) = O(r_o)$ for porous media
with spatially evolving heterogeneities
[Goyeau et al., TiPM 1997]



Simplified closure variables

$$\tilde{P}_\beta = \mu_\beta \mathbf{b}'_\beta \cdot \langle \mathbf{v}_\beta \rangle^\beta \quad ; \quad \tilde{\mathbf{v}}_\beta = \mathbf{B}'_\beta \cdot \langle \mathbf{v}_\beta \rangle^\beta$$

Simplified macro model for momentum transport

$\ell_\beta \ll (L_\varepsilon, L_v) = O(r_o)$ for porous media with spatially evolving heterogeneities [Goyeau et al., TiPM 1997]

Closed macroscopic transport equation

$$\nabla_x . \langle \mathbf{v}_\beta \rangle^\beta = - \varepsilon_\beta^{-1} \nabla_x \varepsilon_\beta . \langle \mathbf{v}_\beta \rangle^\beta$$

$$0 = -\nabla_x \langle P_\beta \rangle^\beta + \rho_\beta \mathbf{g} + \mu_\beta \nabla_x^2 \langle \mathbf{v}_\beta \rangle^\beta - \mu_\beta \left(\varepsilon_\beta \mathbf{K}_\beta^{-1} - \varepsilon_\beta^{-1} \nabla_x^2 \varepsilon_\beta \mathbf{I} \right) \cdot \langle \mathbf{v}_\beta \rangle^\beta + \mu_\beta \varepsilon_\beta^{-1} \nabla_x \varepsilon_\beta \cdot \nabla_x \langle \mathbf{v}_\beta \rangle^\beta$$

Simplified **closure problem** and **permeability** tensor are **identical to homogeneous porous media**

Permeability tensor $\quad \varepsilon_\beta \mathbf{K}_\beta^{-1} = -\frac{1}{V_\beta} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot \left(-\mathbf{I} \otimes \mathbf{b}'_\beta + \nabla_y \mathbf{B}'_\beta \right) dA$

$\nabla_y \cdot \mathbf{B}'_\beta = 0$ in the β-phase

$0 = -\nabla_y \mathbf{b}'_\beta + \nabla_y^2 \mathbf{B}'_\beta + \varepsilon_\beta \mathbf{K}_\beta^{-1}$ in the β-phase

BC: $\mathbf{B}'_\beta = -\mathbf{I}$ at $A_{\beta\sigma}$

Periodicity: $\mathbf{B}'_\beta(\mathbf{x} + l_i) = \mathbf{B}'_\beta(\mathbf{x})$; $\quad \mathbf{b}'_\beta(\mathbf{x} + l_i) = \mathbf{b}'_\beta(\mathbf{x})$

Uniqueness: $\langle \mathbf{B}'_\beta \rangle^\beta = 0$; $\quad \langle \mathbf{b}'_\beta \rangle^\beta = 0$

See details in [Chabanon et al., TiPM 2026]