Weierstrass Institute for
Applied Analysis and Stochastics

Effective model for a reaction-diffusion system in strongly heterogeneous media

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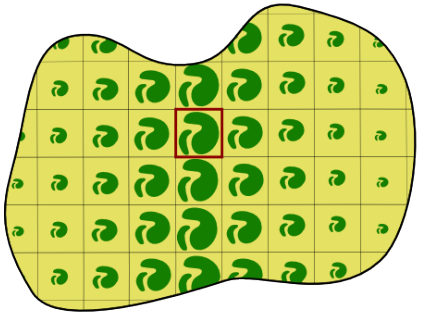
Content

Given: original, macroscopic model depending on $\varepsilon = \frac{\text{micro-length}}{\text{macro-length}} \ll 1$

$$\begin{aligned} \dot{u}_\varepsilon &= \operatorname{div}(D_1^\varepsilon \nabla u_\varepsilon) + F_1^\varepsilon(u_\varepsilon, v_\varepsilon) \\ \dot{v}_\varepsilon &= \operatorname{div}(\varepsilon^2 D_2^\varepsilon \nabla v_\varepsilon) + F_2^\varepsilon(u_\varepsilon, v_\varepsilon) \end{aligned} \quad \text{in } [0,T] \times \Omega \qquad (P_\varepsilon)$$

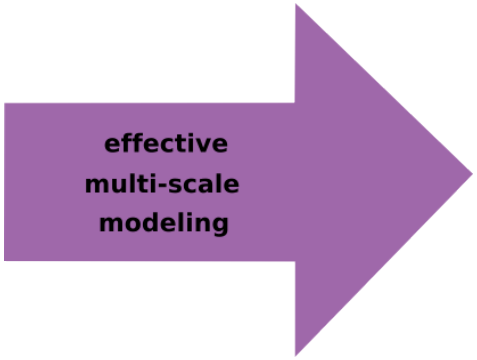
Difficulty: Coupling via nonlinear reaction terms + slow diffusion (degeneracy) in v_ε-equation

Model with ε-periodic microstructure (P_ε).

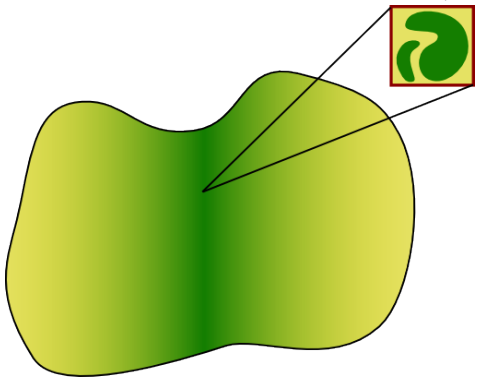


E.g. $D_i^\varepsilon(x) := D_i(x, \frac{x}{\varepsilon})$
$F_i^\varepsilon(x,u,v) := F_i(x, \frac{x}{\varepsilon}, u, v)$
(periodic in $y = \frac{x}{\varepsilon}$, $i = 1, 2$)

What happens for $\varepsilon \to 0$?



Effective two-scale model (P_0).



x = macroscopic scale
y = microscopic scale.

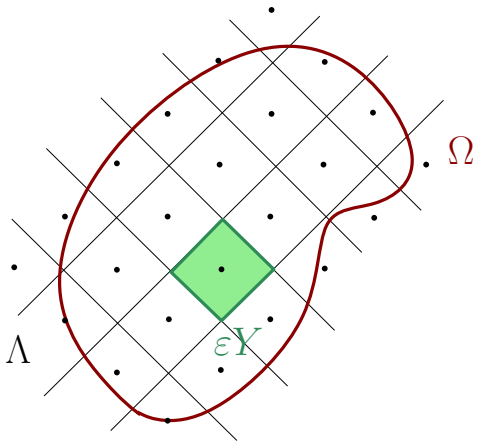
Original definition of two-scale convergence

Definition [Nguetseng'89, Allaire'92]

We say $u_\varepsilon \rightharpoonup U$ in the two-scale sense, if

$$\int_\Omega u_\varepsilon(x)\Phi(x, \tfrac{x}{\varepsilon})\,\mathrm{d}x \to \int_{\Omega\times Y} U(x,y)\Phi(x,y)\,\mathrm{d}x\,\mathrm{d}y \quad \text{for all } \Phi \in C_c^\infty(\Omega \times Y_{\text{per}}).$$

- This is a weak convergence.
- Nonlinearity requires strong convergence.
- Strong two-scale convergence formulation via periodic unfolding operator $\mathcal{T}_\varepsilon$.



Notation:

$\Omega \subset \mathbb{R}^d$: macroscopic domain

Λ : lattice in $\mathbb{R}^d$

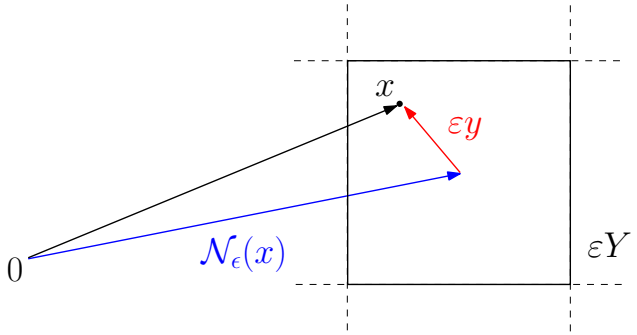
$Y = (0,1)^d$: unit-cell

$Y_{\text{per}} = \mathbb{R}^d/\Lambda$: torus

We decompose every point $x \in \mathbb{R}^d$ as follows

$$x = \mathcal{N}_\varepsilon(x) + \varepsilon y,$$

where $y \in Y$ and $\mathcal{N}_\varepsilon(x) = \varepsilon[\frac{x}{\varepsilon}]$ is the closest lattice point to x (node of lattice Λ).



The **periodic unfolding operator** $\mathcal{T}_\varepsilon : L^2(\Omega) \to L^2(\Omega \times Y_{\text{per}})$ is defined via

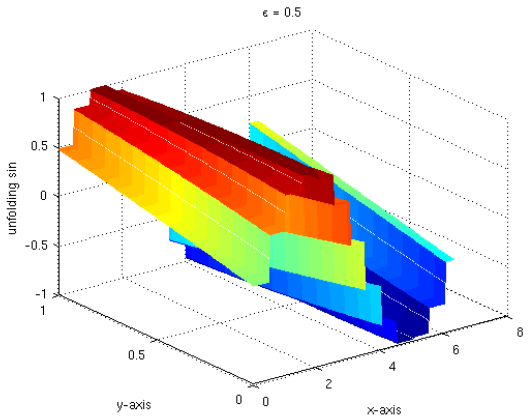
$$(\mathcal{T}_\varepsilon\, u)(x,y) = u(\mathcal{N}_\varepsilon(x) + \varepsilon y).$$

[Cioranescu/Damlamian/Griso'02]

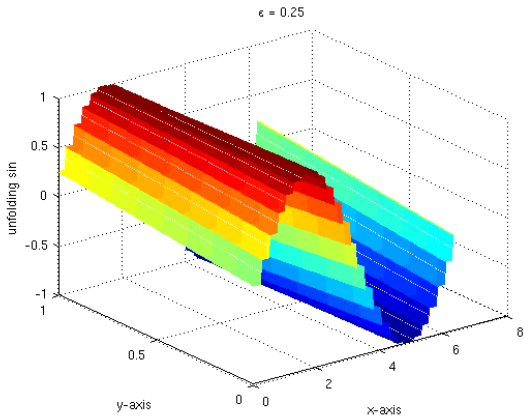
$$\boxed{(\mathcal{T}_\varepsilon\, u)(x,y) = u(\mathcal{N}_\varepsilon(x) + \varepsilon y)}$$

Example 1: micro-macro decomposition

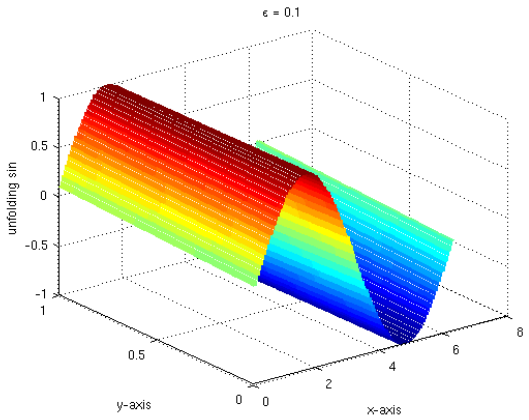
- $\Omega = (0, 2\pi)$, $Y = (0,1)$, and $\Lambda = \{\ldots, -\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \ldots\}$
- $u(x) = \sin(x)$
- $(\mathcal{T}_\varepsilon\, u)(x,y) = \sin(\mathcal{N}_\varepsilon(x) + \varepsilon y) \to \sin(x)$



$\varepsilon = 0.5$



$\varepsilon = 0.25$

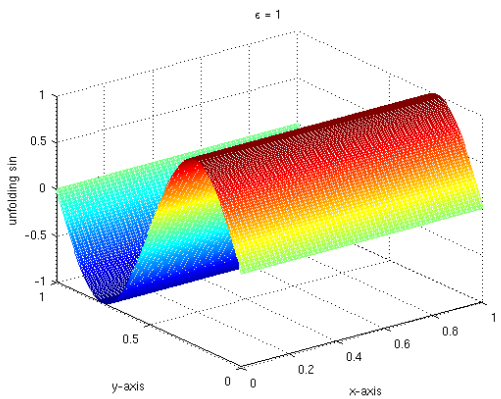


$\varepsilon = 0.1$

No gain in using periodic unfolding, if $u_\varepsilon \to u$!

Example 2: benefit of periodic unfolding in periodic case

- $\Omega = Y = (0,1)$, $\Lambda = \{\ldots, -\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \ldots\}$
- $u_\varepsilon(x) = \sin(2\pi \frac{x}{\varepsilon})$
- $u_\varepsilon \rightharpoonup 0$ in $L^2(\Omega)$, but $u_\varepsilon \nrightarrow 0$ in $L^2(\Omega)$
- $(\mathcal{T}_\varepsilon\, u_\varepsilon)(x,y) = \sin\left(2\pi \frac{\mathcal{N}_\varepsilon(x)+\varepsilon y}{\varepsilon}\right) = \sin(2\pi y)$



Definition (weak and strong two-scale convergence) [Mielke/Timofte'07, Visintin'04'06]

Let $(u_\varepsilon)_{\varepsilon>0}$ be a sequence in $L^2(\Omega)$.

$$u_\varepsilon \xrightarrow{2\mathrm{w}} U \quad \text{in } L^2(\Omega \times Y_{\mathrm{per}}) \quad :\overset{\mathrm{Def}}{\Longleftrightarrow} \quad \mathcal{T}_\varepsilon\, u_\varepsilon \rightharpoonup U \quad \text{in } L^2(\Omega \times Y_{\mathrm{per}})$$
$$u_\varepsilon \xrightarrow{2\mathrm{s}} U \quad \text{in } L^2(\Omega \times Y_{\mathrm{per}}) \quad :\overset{\mathrm{Def}}{\Longleftrightarrow} \quad \mathcal{T}_\varepsilon\, u_\varepsilon \to U \quad \text{in } L^2(\Omega \times Y_{\mathrm{per}})$$

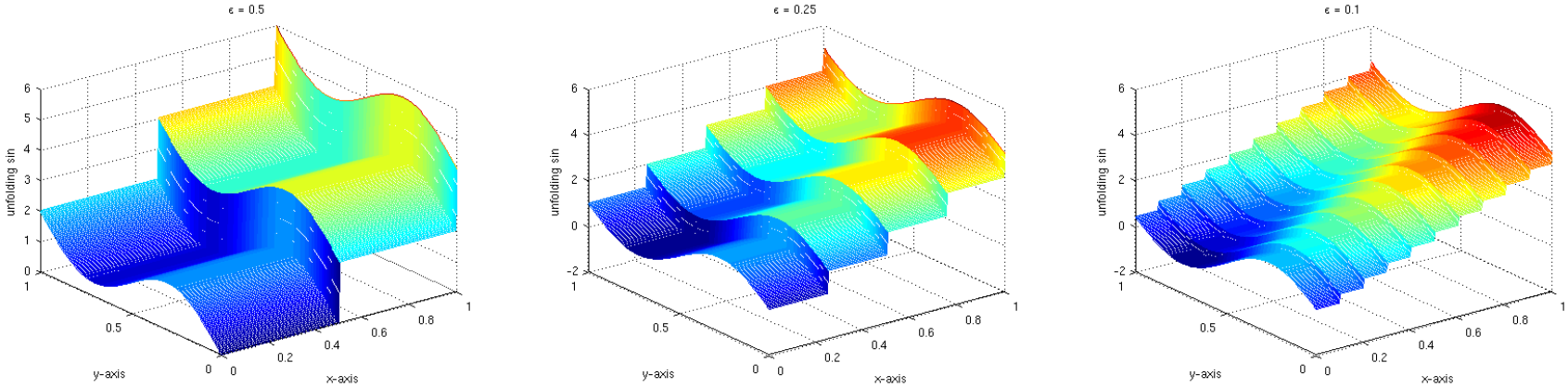
In Example 2: $\mathcal{T}_\varepsilon\, u_\varepsilon \xrightarrow{2\mathrm{s}} U$, where $U(x,y) = \sin(2\pi y)$

Strong two-scale convergence of (ε-periodic) oscillations

$\Psi : \Omega \times Y_{\mathrm{per}} \to \mathbb{R}$ suff. smooth, $\quad \psi_\varepsilon(x) := \Psi(x, \frac{x}{\varepsilon}) \quad \Longrightarrow \quad \psi_\varepsilon \xrightarrow{2\mathrm{s}} \Psi$

Example 3: two-scale limit is Y-periodic

- $\Omega = Y = (0,1)$, $\Lambda = \{\ldots, -\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \ldots\}$
- $u_\varepsilon(x) = \sin(2\pi \frac{x}{\varepsilon}) + 4x$
- $(\mathcal{T}_\varepsilon\, u_\varepsilon)(x,y) = \sin(2\pi y) + 4(\mathcal{N}_\varepsilon(x) + \varepsilon y)$ is not Y-periodic



$\varepsilon = 0.5$ $\qquad$ $\varepsilon = 0.25$ $\qquad$ $\varepsilon = 0.1$

- Limit $\lim_{\varepsilon\to 0}(\mathcal{T}_\varepsilon\, u_\varepsilon)(x,y) = \sin(2\pi y) + 4x$ is Y-periodic

We call this $\mathcal{T}_\varepsilon$**-property of recovered periodicity:**
for $u_\varepsilon \in H^1(\Omega) : \mathcal{T}_\varepsilon\, u_\varepsilon \in L^2(\Omega; H^1(Y))$, but $\lim_{\varepsilon\to 0} \mathcal{T}_\varepsilon\, u_\varepsilon \in L^2(\Omega; H^1(Y_{\text{per}}))$

$$\begin{aligned} \dot{u}_\varepsilon &= \operatorname{div}(D_1^\varepsilon \nabla u_\varepsilon) + F_1^\varepsilon(u_\varepsilon, v_\varepsilon) \\ \dot{v}_\varepsilon &= \operatorname{div}(\varepsilon^2 D_2^\varepsilon \nabla v_\varepsilon) + F_2^\varepsilon(u_\varepsilon, v_\varepsilon) \\ &\quad + \text{homog. Neumann bound. cond. on } \partial\Omega \end{aligned} \qquad \text{in } [0,T]\times\Omega \qquad (P_\varepsilon)$$

Solutions of (P_ε):

- $u_\varepsilon : [0,T]\times\Omega \to \mathbb{R}$
  "classically" diffusing variable
- $v_\varepsilon : [0,T]\times\Omega \to \mathbb{R}$
  slowly diffusing variable

Assumptions on the given data $(i = 1, 2)$:

- $D_i^\varepsilon : \Omega \to \mathbb{R}^{d\times d}$ uniformly elliptic and bounded
- $F_i^\varepsilon : \Omega \times \mathbb{R} \times \mathbb{R} \to \mathbb{R}$ differentiable and globally Lipschitz-continuous
- suitable choice of initial data: $u_\varepsilon^0, v_\varepsilon^0 \in L^2(\Omega)$ and $\operatorname{div}(D_1^\varepsilon \nabla u_\varepsilon^0), \operatorname{div}(\varepsilon^2 D_2^\varepsilon \nabla v_\varepsilon^0) \in L^2(\Omega)$

Theorem (Existence and improved time-regularity)

For given $T > 0$, $\varepsilon > 0$, there exists a unique (weak) solution $(u_\varepsilon, v_\varepsilon) \in C^1([0,T]; L^2(\Omega))$ with $(\nabla u_\varepsilon, \varepsilon \nabla v_\varepsilon) \in C^0([0,T]; L^2(\Omega))$.

Boundedness & a priori weak convergence

For all $t \in [0,T]$, $\varepsilon > 0$, we have

$$\max_{0\le t\le T} \|u_\varepsilon(t)\|_{L^2(\Omega)} + \|\nabla u_\varepsilon(t)\|_{L^2(\Omega)} \le C,$$
$$\max_{0\le t\le T} \|v_\varepsilon(t)\|_{L^2(\Omega)} + \varepsilon\|\nabla v_\varepsilon(t)\|_{L^2(\Omega)} \le C.$$

The boundedness implies (for a subsequ.)

$$u_\varepsilon(t) \to u(t) \quad \text{and} \quad \nabla u_\varepsilon(t) \rightharpoonup \nabla u(t) \quad \text{in } L^2(\Omega),$$
$$v_\varepsilon(t) \xrightarrow{2\mathrm{w}} V(t) \quad \text{and} \quad \varepsilon\nabla v_\varepsilon(t) \xrightarrow{2\mathrm{w}} \nabla_y V(t) \quad \text{in } L^2(\Omega\times Y_{\text{per}}).$$

Existing results:

- nondegenerating and nonlinear: $\dot u_\varepsilon = \operatorname{div}(D^\varepsilon \nabla u_\varepsilon) + f^\varepsilon(u_\varepsilon)$
  [Bensoussan/Lions/Papanicolaou'78, Murat/Tarar'97, etc.] (G-convergence is applicable)
- degenerating and linear: $\dot v_\varepsilon = \operatorname{div}(\varepsilon^2 D^\varepsilon \nabla v_\varepsilon) + f^\varepsilon \cdot v_\varepsilon$ (also $f^\varepsilon = \nabla\Phi$, Φ convex)
  [Hornung/Jäger/Mikelić'94, Peter/Böhm'08, Visintin'07, Hanke'11, etc.]
- degenerating and nonlinear: asymp. expansion + conv. rates for suff. smooth data [Eck'04]

Our task (rigorous proof):

- degenerating and nonlinear: $\dot v_\varepsilon = \operatorname{div}(\varepsilon^2 D^\varepsilon \nabla v_\varepsilon) + f^\varepsilon(v_\varepsilon)$

Therefore we need to prove $v_\varepsilon \xrightarrow{2\mathrm{s}} V$.

Theorem (Mielke/R/Thomas'13 (WIAS Preprint Nr. 1834))

We assume $\mathcal{T}_\varepsilon D_i^\varepsilon \to D_i \in L^\infty(\Omega \times Y_{per})$ *pointwise,* $F_i^\varepsilon(\cdot, u, v) \xrightarrow{2s} F_i(\cdot, \cdot, u, v)$ *and* $v_\varepsilon^0 \xrightarrow{2s} V^0$ *in* $L^2(\Omega \times Y_{per})$ *and* $u_\varepsilon^0 \to u^0$ *in* $L^2(\Omega)$.

Then we have for all $t \in [0, T]$*:*

$$u_\varepsilon(t) \to u(t) \text{ in } L^2(\Omega) \quad \text{and} \quad v_\varepsilon(t) \xrightarrow{2s} V(t) \text{ in } L^2(\Omega \times Y_{per}),$$

where (u, V) *solves the* ***effective two-scale model*** (P_0).

Macroscopic equation on $[0, T] \times \Omega$:

$$\dot{u}(t,x) = \underbrace{\operatorname{div}(D_{\text{eff}}(x)\nabla u(t,x))}_{\text{macro-diffusion}} + \underbrace{\int_Y F_1(x, y, u(t,x), V(t,x,y))\,\mathrm{d}y}_{\text{macro-reaction}},$$

Two-scale equation on $[0, T] \times Y_{\text{per}}$, $\quad \Omega \sim$ "set of parameter": $\qquad (P_0)$

$$\dot{V}(t,x,y) = \underbrace{\operatorname{div}_y(D_2(x,y)\nabla_y V(t,x,y))}_{\text{micro-diffusion}} + \underbrace{F_2(x, y, u(t,x), V(t,x,y))}_{\text{two-scale reaction}}.$$

1. Consider $\dot{v}_\varepsilon = \operatorname{div}(\varepsilon^2 D^\varepsilon \nabla v_\varepsilon) + F^\varepsilon(v_\varepsilon)$ in Ω
   and $\dot{V} = \operatorname{div}_y(D\nabla_y V) + F(V)$ in $\Omega \times Y_{\text{per}}$

Aim: Gronwall-estimate for the difference $W_\varepsilon = \mathcal{T}_\varepsilon v_\varepsilon - V$:

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|W_\varepsilon(t)\|^2 \leq L\|W_\varepsilon(t)\|^2 + \Delta^\varepsilon(t)$$

(then $\|W_\varepsilon(t)\|^2 \leq c(\|W_\varepsilon(0)\|^2 + \Delta^\varepsilon(t))$ and show $\Delta^\varepsilon = \Delta_1^\varepsilon + \Delta_2^\varepsilon + \Delta_3^\varepsilon$ vanishes)

Therefore

- Given $\mathcal{T}_\varepsilon$ and folding operator $\mathcal{F}_\varepsilon : L^2(\Omega \times Y_{\text{per}}) \to L^2(\Omega)$ with $\mathcal{F}_\varepsilon \mathcal{T}_\varepsilon = \mathrm{id}_{L^2(\Omega)}$, $\mathcal{F}_\varepsilon = \mathcal{T}_\varepsilon{}'$, and $\mathcal{F}_\varepsilon V \xrightarrow{2s} V$ for all $V \in L^2(\Omega \times Y_{\text{per}})$
- Gradient folding operator $\mathcal{G}_\varepsilon : L^2(\Omega; H^1(Y_{\text{per}})) \to H^1(\Omega)$ (= recovery operator) with $\mathcal{G}_\varepsilon V \xrightarrow{2s} V$ and $\varepsilon\nabla(\mathcal{G}_\varepsilon V) \xrightarrow{2s} \nabla_y V$ for all $V \in L^2(\Omega; H^1(Y_{\text{per}}))$
- Desirable test functions

$$w_\varepsilon = v_\varepsilon - \mathcal{G}_\varepsilon V \text{ resp. } \mathcal{T}_\varepsilon w_\varepsilon \quad \text{and} \quad W_\varepsilon = \mathcal{T}_\varepsilon v_\varepsilon - V \text{ resp. } \mathcal{F}_\varepsilon W_\varepsilon = v_\varepsilon - \mathcal{F}_\varepsilon V$$

not admissible $\Rightarrow$ test limit equation only with V and create error Δ_2^ε

- Δ_1^ε : mismatch between folding operators $\mathcal{F}_\varepsilon$ and $\mathcal{G}_\varepsilon$
- Δ_2^ε : $\mathcal{T}_\varepsilon$-property of recovered periodicity
- Δ_3^ε : $\mathcal{T}_\varepsilon\, D_2^\varepsilon \to D_2$ pointwise and $F^\varepsilon \xrightarrow{2s} F$ by assumption

2. Coupling with u_ε-equation

End of proof.

Corollary

- We have $\nabla u_\varepsilon \xrightarrow{2s} \nabla u + \nabla_y U$ and $\varepsilon \nabla v_\varepsilon \xrightarrow{2s} \nabla_y V$ in $L^2(\Omega \times Y_{\text{per}})$ a.e. in $[0,T]$.
- For $D_i, F_i \in C^1$ and $u, V \in C^2$, we have

$$\max_{0\le t\le T} \{\| \mathcal{T}_\varepsilon\, v_\varepsilon(t) - V(t)\|_{L^2(\Omega\times Y_{\text{per}})} + \|u_\varepsilon(t) - u(t)\|_{L^2(\Omega)}\} \le \varepsilon^{1/2} C.$$

Possible generalizations:

- Nonhomogenous Dirichlet/Neumann boundary conditions.
- Indeed $D^\varepsilon = \mathcal{F}_\varepsilon D$ and $F^\varepsilon = \mathcal{F}_\varepsilon F$ (instead of Example on p. 4).
- Without improved time-regularity, i.e. $(\dot u_\varepsilon, \dot v_\varepsilon) \notin L^2(\Omega)$ (work in progress).

Thank you for your attention.