Hierarchical Model Reduction for Advection-Diffusion-Reaction Problems

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Abstract Some engineering problems ranging from blood flow to river flow, from internal combustion engines to electronic devices have been recently modelled by coupling problems with different space dimensions (geometrical multiscale method). In this paper we focus on a new approch, where different levels of detail of the problem at hand stem from a different selection of the dimension of a suitable function space. The coarse and fine models are thus identified in a straightforward way. Moreover this approach lends itself to an automatic model adaptive strategy. The approach is addressed on a 2D linear advection-diffusion reaction problem.

1 Motivations

Many engineering problems of practical interest, even though formulated in 3D, exhibit a spatial dimension predominant over the others. This is the case, for instance, of river dynamics, blood flow problems or internal combustion engines. In these cases, it is sometimes possible to resort to downscaled models where only the dominant space dependence is considered (e.g., the Euler equations come from a 1D approximation of blood flows). Nevertheless the simplifying assumptions at the basis of these models can fail locally, essentially where "transversal" dynamics are relevant (e.g., a lake in a river network, an aneurysm in a blood vessel). Ideally, in correspondence with these configurations, one would like to locally enhance the 1D approximation via a proper higher-dimensional enrichment. In the so-called geometrical multiscale approach these enrichments consist of 2D or 3D models. Here

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we follow a different strategy. We simplify the reference problem (the *full model*) by tackling in a different manner the dependence of the solution on the leading direction and on the transverse ones. The former is spanned by a classical piecewise polynomial basis. The latter are expanded into a *modal basis*. We end up with a real *hierarchy* of simplified models (the *reduced models*), distinguishing one another for the different number of modal transversal functions. From a computational viewpoint, independently of the dimension of the full problem, the reduced formulation leads us to a system of 1D problems (associated with the leading direction), coupled by the transversal information. In this work we present preliminary results of this approach applied to a 2D elliptic framework.

A similar approach can be found in [1, 2, 4, 5], though confined to a thin domain setting. Our proposal is potentially more effective than these approaches, as our reduced model is a system of 1D (rather than 2D) problems, also for a 3D full problem.

2 The Full Problem

Let us consider a linear advection diffusion reaction (ADR) problem. For the sake of simplicity we assume the computational domain Ω in $\mathbb{R}^2$ and homogeneous Dirichlet boundary conditions.

Let $\mu \in L^\infty(\Omega)$, with $\mu \geq \mu_0 > 0$, the diffusivity coefficient, $\mathbf{b} = (b_1, b_2)^T \in [L^\infty(\Omega)]^2$ the convective field and $\sigma \in L^\infty(\Omega)$ the reaction coefficient. We assume $\nabla \cdot \mathbf{b} \in L^\infty(\Omega)$. Moreover for the well-posedness of the problem we assume $-\frac{1}{2}\nabla \cdot \mathbf{b} + \sigma \geq 0$ a.e. in Ω. Finally, let $f \in L^2(\Omega)$ be the forcing term. Standard notation for the Sobolev spaces as well as for the spaces of functions bounded a.e. in Ω is adopted.

The weak formulation of the problem reads: find $u \in V = H_0^1(\Omega)$ s.t.

$$\int_\Omega \mu \nabla u \cdot \nabla v \, dxdy + \int_\Omega \left(\mathbf{b} \cdot \nabla u + \sigma u\right) v \, dxdy = \int_\Omega f v \, dxdy \quad \forall v \in V. \tag{1}$$

Furthermore we assume that the domain Ω can be represented as a 2D *fiber bundle*, i.e.

$$\Omega = \bigcup_{x \in \Omega_{1D}} \gamma_x, \tag{2}$$

where Ω_{1D} is a supporting one-dimensional domain, while $\gamma_x \subset \mathbb{R}$ represents the 1D (transversal) *fiber* associated with $x \in \Omega_{1D}$. In practice we distinguish in Ω a *leading direction*, associated with Ω_{1D}, and a secondary *transversal direction*, represented by the fibers γ_x. This choice finds its justification in the hydrodynamic as well as haemodynamic applications we are interested in, where the dominant direction is provided by the blood or the water main stream, respectively (see Fig. 1, left).

We map domain Ω into a reference domain $\widehat{\Omega}$, where the analysis is easier. For this purpose, for any $x \in \Omega_{1D}$, we introduce the map $\psi_x : \gamma_x \to \widehat{\gamma}_1$ between the generic fiber $\gamma_x \subset \mathbb{R}$ and a 1D reference fiber $\widehat{\gamma}_1$. The domain $\widehat{\Omega}$ is identified as the rectangle

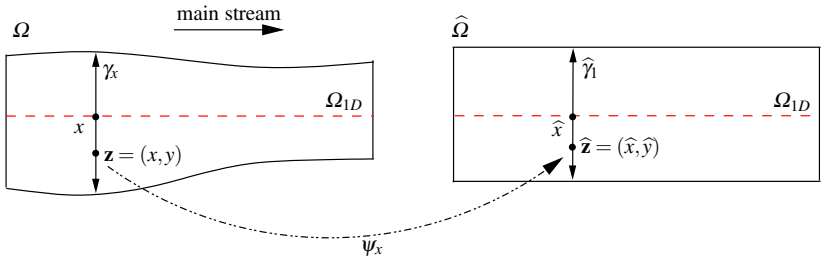

Fig. 1 The map ψ_x

with sides of length $|\Omega_{1D}|$ and $|\widehat{\gamma}_1|$. The map ψ_x thus simply acts on the fiber length (see Fig. 1). Throughout the paper we denote with $\mathbf{z}=(x,y)$ and $\widehat{\mathbf{z}}=(\widehat{x},\widehat{y})$ the generic point in Ω and the corresponding point in $\widehat{\Omega}$ via the map ψ_x, respectively, where $x\equiv\widehat{x}\in\Omega_{1D}$ while $\widehat{y}=\psi_x(y)\in\widehat{\gamma}_1$, with $y\in\gamma_x$.

A predominant role in the applications of our interest is played by the so-called *affine map*, given by $\widehat{y}=\psi_x(y)=L(x)^{-1}\left[y-g\right]$, where $L(x)=|\gamma_x|$ is the length fiber while g is a suitable shift factor. In particular when $L(x)=L=$ constant, the physical domain Ω itself coincides with a rectangle.

3 The Reduced Setting

The fiber structure introduced on the domain Ω is the starting point in defining the dimensional reduction. We resort to different function spaces along the supporting fiber Ω_{1D} rather than the transversal ones γ_x, in the spirit of a *model anisotropy*.
In more detail, we associate with Ω_{1D} the function space $V_{1D}\equiv H^1_0(\Omega_{1D})$, whose functions account for the homogeneous Dirichlet boundary conditions on $\partial\Omega_{1D}$. On the transversal reference fiber we introduce a *modal basis* $\{\varphi_k\}$, with $k\in\mathbb{N}$, where $\varphi_k:\widehat{\gamma}_1\to\mathbb{R}$ and $\{\varphi_k\}$ is assumed $L^2(\widehat{\gamma}_1)$-orthonormal. The functions φ_k take into account the boundary conditions on $\partial\Omega_\gamma=\bigcup_{x\in\Omega_{1D}}\partial\gamma_x$. The transversal function space is therefore given by $V_{\widehat{\gamma}_1}=span\{\varphi_k\}$.

Different choices can be pursued for the modal functions φ_k (see [3], Remark 1). Here we adopt trigonometric functions, according to a classical Fourier expansion.

By properly combining the space V_{1D} with the modal basis $\{\varphi_k\}_k$, we define the *reduced space*, for any fixed a priori $m\in\mathbb{N}$,

$$V_m=\left\{v_m(x,y)=\sum_{k=0}^{m}\varphi_k(\psi_x(y))\,\widetilde{v}_k(x),\ \text{with}\ \widetilde{v}_k\in V_{1D}\right\}. \tag{3}$$

The $L^2(\widehat{\gamma}_1)$-orthogonality of the modal functions implies that the frequency coefficients $\widetilde{v}_k$ in (3) are

$$\widetilde{v}_k(x) = \int_{\widehat{\gamma}_1} v_m(x, \psi_x^{-1}(\widehat{y}))\varphi_k(\widehat{y})\, d\widehat{y}, \quad \text{with} \quad k = 0, \ldots, m. \tag{4}$$

Convergence of an approximation u_m to (1) stems essentially from the following assumptions: *i)* the *conformity* of the reduced space V_m in V, i.e. that $V_m \subset V$, $\forall m \in \mathbb{N}$; *ii)* the *spectral approximability* of V_m in V, namely that $\lim_{m\to+\infty} \left(\inf_{v_m \in V_m} \|v - v_m\|_V \right) = 0$, for any $v \in V$. These two requirements basically lead to proper regularity assumptions on the map ψ_x as well as on the spaces V_{1D} and $V_{\widehat{\gamma}_1}$ (for further details, see [3]). Throughout the paper we assume that these two hypotheses are fulfilled.

3.1 The ADR Reduced Form

The reduced formulation of the ADR equation (1) entails solving such a problem on the subspace V_m of V in (3).

Thus, for any $m \in \mathbb{N}$, we can state the so-called ADR *reduced problem*: find $u_m \in V_m$ such that

$$\int_\Omega \mu \nabla u_m \cdot \nabla v_m \, dxdy + \int_\Omega \left(\mathbf{b} \cdot \nabla u_m + \sigma u_m \right) v_m \, dxdy = \int_\Omega f v_m \, dxdy \quad \forall v_m \in V_m. \tag{5}$$

The well-posedness as well as the strong consistency of this formulation are guaranteed by assumption *i)* above.

Actually the reduced formulation (5) amounts to solving a system of $(m+1)$ coupled 1D problems, with coefficients computed on the reference fiber $\widehat{\gamma}_1$. For this purpose we introduce the Jacobian $\mathscr{J}(\widehat{y}) = \left(\partial \psi_x(y)/\partial y\right)|_{y=\psi_x^{-1}(\widehat{y})}$ associated with the map ψ_x. Moreover we define $\mathscr{D}(\widehat{y}) = \left(\partial \psi_x(y)/\partial x\right)|_{y=\psi_x^{-1}(\widehat{y})}$, representing a *deformation index* of the current domain Ω with respect to the reference one.

Let us exploit in (5) the representation $u_m(x,y) = \sum_{j=0}^m \widetilde{u}_j(x)\, \varphi_j(\psi_x(y))$ of u_m as a function of V_m and identify the test function v_m with $v_m(x,y) = \vartheta(x)\, \varphi_k(\psi_x(y))$, for any $\vartheta \in V_{1D}$ and any $k = 0, \ldots, m$, to get

$$\begin{aligned} &\sum_{j=0}^m \Big[\int_\Omega \mu(x,y) \nabla\left(\widetilde{u}_j(x)\, \varphi_j(\psi_x(y))\right) \cdot \nabla\left(\vartheta(x)\, \varphi_k(\psi_x(y))\right) dxdy \\ &+ \int_\Omega \Big(\mathbf{b}(x,y) \cdot \nabla\left(\widetilde{u}_j(x)\, \varphi_j(\psi_x(y))\right) + \sigma(x,y) \widetilde{u}_j(x)\, \varphi_j(\psi_x(y)) \Big) \vartheta(x)\, \varphi_k(\psi_x(y))\, dxdy \Big] \\ &= \int_\Omega f(x,y)\, \vartheta(x)\, \varphi_k(\psi_x(y))\, dxdy. \end{aligned} \tag{6}$$

We analyze separately the different terms. Moving from the gradient expansion

$$\nabla\left(w(x)\, \varphi_s(\psi_x(y))\right) = \varphi_s(\psi_x(y)) \begin{bmatrix} \frac{dw(x)}{dx} \\ 0 \end{bmatrix} + w(x)\, \varphi_s'(\psi_x(y)) \begin{bmatrix} \frac{\partial \psi_x(y)}{\partial x} \\ \frac{\partial \psi_x(y)}{\partial y} \end{bmatrix}, \tag{7}$$

with $\varphi_s'(\psi_x(y)) = d\varphi_s(\psi_x(y))/d\psi_x(y)$, for $s = 0,\dots,m$, and $w \in V_{1D}$, we rewrite the diffusive contribution in (6) as the sum of 1D diffusive-, convective-, and reactive-terms with respect to the unknowns $\widetilde{u}_j$, since

$$\begin{aligned}
&\int_{\Omega_{1D}} \Big\{ \Big(\int_{\gamma_x} \mu(x,y)\, \varphi_j(\psi_x(y))\, \varphi_k(\psi_x(y))\, dy \Big) \frac{d\widetilde{u}_j(x)}{dx}\, \frac{d\vartheta(x)}{dx} \\
&+ \Big(\int_{\gamma_x} \mu(x,y)\, \varphi_j(\psi_x(y))\, \varphi_k'(\psi_x(y))\, \frac{\partial \psi_x(y)}{\partial x}\, dy \Big) \frac{d\widetilde{u}_j(x)}{dx}\, \vartheta(x) \\
&+ \Big(\int_{\gamma_x} \mu(x,y)\, \varphi_j'(\psi_x(y))\, \varphi_k(\psi_x(y))\, \frac{\partial \psi_x(y)}{\partial x}\, dy \Big) \widetilde{u}_j(x)\, \frac{d\vartheta(x)}{dx} \\
&+ \Big(\int_{\gamma_x} \mu(x,y)\, \varphi_j'(\psi_x(y))\, \varphi_k'(\psi_x(y)) \Big\{ \Big[\frac{\partial \psi_x(y)}{\partial x} \Big]^2 + \Big[\frac{\partial \psi_x(y)}{\partial y} \Big]^2 \Big\} dy \Big) \widetilde{u}_j(x)\, \vartheta(x) \Big\}\, dx.
\end{aligned} \tag{8}$$

Similarly, we recast the convective term in (6) as the sum of a 1D convective and a 1D reactive term:

$$\begin{aligned}
&\int_{\Omega_{1D}} \Big\{ \Big(\int_{\gamma_x} b_1(x,y)\, \varphi_j(\psi_x(y))\, \varphi_k(\psi_x(y))\, dy \Big) \frac{d\widetilde{u}_j(x)}{dx}\, \vartheta(x) \\
&+ \Big(\int_{\gamma_x} \varphi_j'(\psi_x(y)) \varphi_k(\psi_x(y)) \Big[b_1(x,y) \frac{\partial \psi_x(y)}{\partial x} + b_2(x,y) \frac{\partial \psi_x(y)}{\partial y} \Big] dy \Big) \widetilde{u}_j(x)\, \vartheta(x) \Big\}\, dx.
\end{aligned} \tag{9}$$

Finally the reactive contribution in (6) leads to a reactive term with respect to the $\widetilde{u}_j$'s:

$$\int_{\Omega_{1D}} \Big(\int_{\gamma_x} \sigma(x,y) \varphi_j(\psi_x(y))\, \varphi_k(\psi_x(y))\, dy \Big) \widetilde{u}_j(x)\, \vartheta(x)\, dx. \tag{10}$$

In practice all the integrals above on γ_x, as well as the forcing term in (6), are computed on the reference fiber $\widehat{\gamma}_1$, by properly exploiting the map ψ_x (i.e. both the Jacobian $\mathscr{J}(\widehat{y})$ and the deformation index $\mathscr{D}(\widehat{y})$). A straightforward arrangement of the terms in (8), (9) and (10) allows us to reformulate problem (5) as follows: for $j = 0,\dots,m$, find $\widetilde{u}_j \in V_{1D}$ such that, $\forall \vartheta \in V_{1D}$,

$$\begin{aligned}
&\sum_{j=0}^{m} \Big\{ \int_{\Omega_{1D}} \Big[\underbrace{\widehat{r}_{kj}^{1,1}(x) \frac{d\widetilde{u}_j(x)}{dx} \frac{d\vartheta(x)}{dx}}_{\text{(I)}} + \underbrace{\widehat{r}_{kj}^{1,0}(x) \frac{d\widetilde{u}_j(x)}{dx} \vartheta(x) + \widehat{r}_{kj}^{0,1}(x) \widetilde{u}_j(x) \frac{d\vartheta(x)}{dx}}_{\text{(II)}} \\
&+ \underbrace{\widehat{r}_{kj}^{0,0}(x) \widetilde{u}_j(x)\, \vartheta(x)}_{\text{(III)}} \Big] dx \Big\} = \int_{\Omega_{1D}} \Big[\int_{\widehat{\gamma}_1} f(x, \psi_x^{-1}(\widehat{y})) \varphi_k(\widehat{y}) \big| \mathscr{J}^{-1}(\widehat{y}) \big| d\widehat{y} \Big] \vartheta(x)\, dx,
\end{aligned} \tag{11}$$

with $k = 0,\dots,m$, where

$$\widehat{r}_{kj}^{s,t}(x) = \int_{\widehat{\gamma}_1} r_{kj}^{s,t}(x,\widehat{y}) \big| \mathscr{J}^{-1}(\widehat{y}) \big| d\widehat{y}, \quad \text{for} \quad s,t = 0,1, \tag{12}$$

and

$$r_{kj}^{1,1}(x,\widehat{y}) = \mu\left(x,\psi_x^{-1}(\widehat{y})\right)\varphi_j(\widehat{y})\,\varphi_k(\widehat{y}),$$
$$r_{kj}^{0,1}(x,\widehat{y}) = \mu\left(x,\psi_x^{-1}(\widehat{y})\right)\varphi_j'(\widehat{y})\,\varphi_k(\widehat{y})\,\mathscr{D}(\widehat{y}),$$
$$r_{kj}^{1,0}(x,\widehat{y}) = \mu\left(x,\psi_x^{-1}(\widehat{y})\right)\varphi_j(\widehat{y})\,\varphi_k'(\widehat{y})\,\mathscr{D}(\widehat{y}) + b_1\left(x,\psi_x^{-1}(\widehat{y})\right)\varphi_j(\widehat{y})\,\varphi_k(\widehat{y}),$$
$$r_{kj}^{0,0}(x,\widehat{y}) = \mu\left(x,\psi_x^{-1}(\widehat{y})\right)\varphi_j'(\widehat{y})\varphi_k'(\widehat{y})\Big\{\left[\mathscr{D}(\widehat{y})\right]^2 + \left[\mathscr{J}(\widehat{y})\right]^2\Big\} +$$
$$\sigma\left(x,\psi_x^{-1}(\widehat{y})\right)\varphi_j(\widehat{y})\varphi_k(\widehat{y}) + \varphi_j'(\widehat{y})\varphi_k(\widehat{y})\Big\{b_1\left(x,\psi_x^{-1}(\widehat{y})\right)\mathscr{D}(\widehat{y}) + b_2\left(x,\psi_x^{-1}(\widehat{y})\right)\mathscr{J}(\widehat{y})\Big\}.$$

Notice that in (11) the dependence of the reduced solution u_m on the main stream and on the transversal directions is split: coefficients $\widehat{r}_{kj}^{s,t}$ essentially collect the transversal contribution to the domain Ω_{1D}. We still recognize in (11) an ADR problem, the terms (I), (II) and (III) representing the diffusive, convective and reactive contribution, respectively.

From (8), (9) and (10) it is easy to see that the conversion from the full to the reduced framework is not one to one. Indeed a purely diffusive (advective) full term also yields reduced advective-reactive (reactive) contributions. The possible self-adjointness of the full problem is thus usually lost in the reduced framework. This property can be preserved in a few cases by a proper choice of the map ψ_x and of the reduced space V_m (see [3]).

From a computational viewpoint, solving (11) requires dealing with a small number of coupled 1D problems, provided that the modal index m is small enough. This is likely more convenient than solving the full problem (1).

Finally we point out that the computation of the $\widehat{r}_{kj}^{s,t}$'s in (12) simplifies considerably under particular assumptions on the data, e.g. for constant coefficients μ, $\mathbf{b}$, σ, or when the map ψ_x is affine (see [3] for the details).

4 Finite Element Approximation of the Reduced Problem

Formulation (11) can be understood as a *model semidiscretization* of the full problem (1), the transversal direction being discretized via the modal basis $\{\varphi_k\}$.

With a view to a full discretization of (1), we introduce a partition $\mathscr{T}_h$ of Ω_{1D} into sub-intervals $K_j = (x_{j-1}, x_j)$ of width $h_j = x_j - x_{j-1}$, and set $h = \max_j h_j$. We associate with $\mathscr{T}_h$ a finite element space $V_{1D}^h \subset V_{1D}$, with $\dim(V_{1D}^h) = N_h$, such that a standard density hypothesis of V_{1D}^h in V_{1D} is guaranteed.

The *discrete reduced formulation* is thus represented by system (11) solved on the subspace V_{1D}^h of V_{1D}, the test function ϑ coinciding now with the generic basis function ϑ_l of the finite element space, for $l = 1, \ldots, N_h$. Moreover, by expanding the unknown coefficients $\widetilde{u}_j^h$ in terms of the basis $\{\vartheta_i\}_{i=1}^{N_h}$ itself and by properly varying the indices k and l, we get a linear system with a $(m+1)N_h \times (m+1)N_h$ block matrix A. All the $N_h \times N_h$-blocks share the sparsity pattern proper of the adopted 1D finite element approximation, with the consequent benefits both in storing and solving the associated algebraic system.

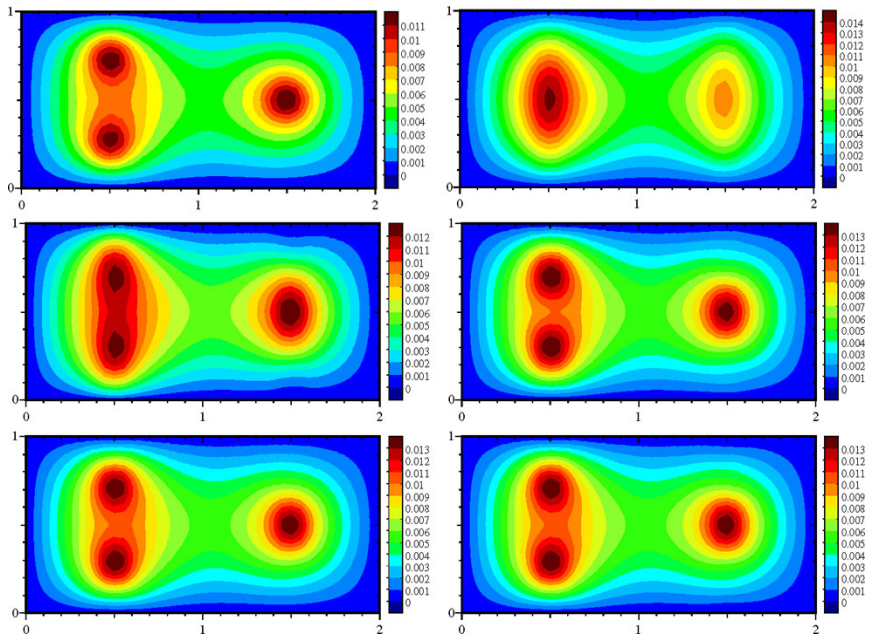

Fig. 2 Full solution u and reduced solutions u_2, u_4, u_6, u_8, u_9 (top-bottom, left-right)

5 Numerical Assessment

We look for a reliable and sufficiently accurate approximation of the full solution u to (1) by properly selecting the reduced space V_m in (3), namely the modal index m. The choice of m represents a crucial issue. It should be a trade-off between the needs to capture the main features of u and to contain the computational cost.

We adopt here a heuristic strategy where we first fix the index $m = 0$ and then we gradually increase such a value, while keeping it constant along the whole domain Ω_{1D}.

Let us focus on a purely diffusive differential problem exhibiting a heterogeneity in the corresponding source term. We solve the Poisson problem on the domain $\Omega = (0,2) \times (0,1)$, completed with homogeneous Dirichlet boundary conditions. The forcing term is localized in 3 circular regions of Ω, the function f in (1) coinciding with the characteristic function $\chi_{D_1 \cup D_2 \cup D_3}$, with $D_1 = \{(x,y) : (x-1.5)^2 + (y-0.5)^2 \leq 0.01\}$, $D_2 = \{(x,y) : (x-0.5)^2 + (y-0.25)^2 \leq 0.01\}$ and $D_3 = \{(x,y) : (x-0.5)^2 + (y-0.75)^2 \leq 0.01\}$. The associated full solution exhibits a peak in correspondence with each of the areas D_i, for $i = 1,2,3$ (see Fig. 2, top-left). Figure 2 gathers the reduced solutions corresponding to different choices for the modal index m. In particular it is evident the expected failure of the reduced solution u_2 (Fig. 2, top-right) to detect the two peaks of u along the straight line $x = 0.5$.

On the contrary u_2 already matches the exact value in correspondence with the peak in D_1 (notice the different scales). Nevertheless the reliability of u_m increases as m gets larger (Fig. 2, middle and bottom row).

These preliminary results confirm the convergence expected from classical Galerkin theory with the fulfillment of the assumptions *i)* and *ii)* in Sect. 3. It is worth pointing out that, even if a purely diffusive full model leads to an advective-diffusive-reactive reduced problem, the latter does not seem to suffer from convective or reactive numerical instabilities if $\mathscr{D}(\widehat{y})$ is small enough, since the convective-reactive terms are weighted by the diffusive coefficient μ itself (see [3]).

6 Conclusions and Future Developments

The preliminary numerical results in Sect. 5 suggest that the proposed dimensional reduction could be a reasonable approach for containing computational costs, in particular when both the domain and the problem at hand exhibit a "main stream direction". Many aspects deserve to be investigated. First of all the extension of the reduced approach to more complex problems (e.g., Oseen, Navier-Stokes equations). A second issue is the set-up of a mathematically sound procedure for selecting the proper modal index m. A possible approach could be based on the comparison between u_m and u_{m^+}, with $m^+ > m$. We investigate extensively this issue in [3]. An alternative solution is based on a domain decomposition approach, where different values of m are used in different parts of Ω ([3]): for instance, in the example of Fig. 2, a smaller value of m could suffice on the right half of the domain but not in the left half. In perspective this approach is suited to being coupled with a proper a posteriori modeling error analysis to get an automatic tool able to detect the most appropriate value m in the different parts of the domain in the spirit of a *model dimension adaptivity*.

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