One-Dimensional Surrogate Models for Advection-Diffusion Problems

Matteo Aletti, Andrea Bortolossi, Simona Perotto, and Alessandro Veneziani

Abstract Numerical solution of partial differential equations can be made more tractable by model reduction techniques. For instance, when the problem at hand presents a main direction of the dynamics (such as blood flow in arteries), it may be conveniently reduced to a 1D model. Here we compare two strategies to obtain this model reduction, applied to classical advection-diffusion equations in domains where one dimension dominates the others.

1 Introduction

Many applications in scientific computing demand for surrogate models, i.e., simplified models which are expected to be computationally affordable and reliable from a modeling viewpoint. Problems presenting an evident main direction, such as blood flow in arteries, gas dynamics in internal combustion engines, etc., are naturally reduced to 1D equations along the coordinate of the main (or "axial" as opposed to "transverse") direction. Here we consider and compare two different strategies to get surrogate models for this kind of problems. The first procedure stems from an appropriate average of the equation along the transverse direction, combined with (plausible) problem-dependent simplifying assumptions. The second approach comes from a different representation of the axial and of the transverse dynamics, according to what has been called a Hierarchical Model (Hi-Mod) reduction [4].

M. Aletti • A. Bortolossi
Politecnico di Milano, Piazza Leonardo da Vinci 32, I-20133 Milano, Italy
e-mail: matteo.aletti@mail.polimi.it; andrea.bortolossi@mail.polimi.it

S. Perotto (✉)
MOX-Dipartimento di Matematica, Politecnico di Milano, Piazza Leonardo da Vinci 32, I-20133 Milano, Italy
e-mail: simona.perotto@polimi.it

A. Veneziani
Department of Mathematics and Computer Science, Emory University, 400 Dowman Dr., 30322, Atlanta, GA, USA
e-mail: ale@mathcs.emory.edu

A. Abdulle et al. (eds.), *Numerical Mathematics and Advanced Applications - ENUMATH 2013*, Lecture Notes in Computational Science and Engineering 103, DOI 10.1007/978-3-319-10705-9_44

In particular, transverse dynamics are represented by a modal expansion, that is supposed to require just a few modes for the nature of the problem. This leads to solve a system of 1D coupled equations. At the bottom line, when using just one transverse mode, this leads to a genuinely 1D model. For the sake of comparison, these two reduction procedures are applied to the following two-dimensional advection-diffusion problem

$$\begin{cases} -\mu \Delta u + \boldsymbol{b} \cdot \nabla u = f & in \ \ \Omega \equiv (0, L) \times (-R_0, R_0) \\ u = g & \text{on} \ \ \Gamma_{in} \equiv \{0\} \times (-R_0, R_0) \\ \mu \dfrac{\partial u}{\partial n} = 0 & \text{on} \ \ \Gamma_{out} \equiv \{L\} \times (-R_0, R_0) \\ \mu \dfrac{\partial u}{\partial n} + \chi u = u_{ext} & \text{on} \ \ \Gamma_{lat} \equiv \partial\Omega \backslash (\Gamma_{in} \cup \Gamma_{out}), \end{cases} \tag{1}$$

where x is the main direction, y is the transverse one, and with $\mu \in L^\infty(\Omega)$, $\boldsymbol{b} = (b_1, b_2)^T \in [W^{1,\infty}(\Omega)]^2$, $f \in L^2(\Omega)$, $g \in H^{1/2}(\Gamma_{in})$, $\chi \in L^\infty(\Omega)$, $u_{ext} \in L^2(\Gamma_{lat})$, $\mu \partial u/\partial n$ the conormal derivative of u. Standard notation are adopted for the Sobolev spaces. We distinguish in the domain Ω a supporting fiber Ω_{1D} aligned with the main stream and a set of transverse fibers γ_x, with $x \in \Omega_{1D}$, parallel to the secondary transverse dynamics. Since Ω coincides with a rectangle, $\gamma_x = \gamma$, for each x.

We assume suitable assumptions on the data to guarantee the well-posedness of the weak form of (1), i.e.,

$$\text{find} \quad u \in V \equiv H^1_{\Gamma_{in}}(\Omega) \quad \text{s.t.} \quad a(u, v) = F(v) \quad \forall v \in V, \tag{2}$$

with $a(u, v) = \int_\Omega [\mu \nabla u \cdot \nabla v + \boldsymbol{b} \cdot \nabla u v] \, d\Omega + \int_{\Gamma_{lat}} \chi u v \, d\Gamma$ and $F(v) = \int_\Omega f v \, d\Omega + \int_{\Gamma_{lat}} u_{ext} v \, d\Gamma - a(\rho_g, v)$, ρ_g denoting a lifting of g on Γ_{in}. Problem (1) models, for instance, the oxygen transport inside an artery. In this case, u represents the oxygen partial pressure, μ denotes the diffusivity of oxygen in blood, field $\mathbf{b}$ takes into account the blood dynamics, f is a generic sink or source term, g usually coincides with a concentration profile, the Robin boundary conditions model the absorption of the oxygen through the vessel walls, with χ depending on the absorption properties of the wall and u_{ext} measuring the oxygen partial pressure outside the vessel. For simplicity, we assume μ and χ constant.

When comparing the two approaches mentioned above, we address in particular the combination of models with different accuracy. For the first approach, this leads to what has been called a geometrical multiscale formulation [2]. For Hi-Mod reduction, this is obtained by selecting a different number of modes in different regions of the domain [4, 5].

2 A Transverse Average Model

We particularize the approach in [3] for modeling the transport of solutes in arteries with bifurcations to an elliptic setting. Let us introduce the transverse profile of the solution, given by

$$p(x,y) = \frac{u(x,y)}{U(x)} \quad \text{with} \quad U(x) = \frac{1}{|\gamma|}\int_\gamma u(x,y)\,dy,$$

$U(x)$ denoting the mean of the solution along the transverse (constant) section γ of Ω. As first modeling hypothesis, we assume that the profile p does not depend on x, i.e., only the mean of the solution may vary along the x-direction. Thus, after separation of variables, the solution u can be regarded as a certain profile varying in y tuned by a function varying along x, i.e., $u(x,y) = U(x)p(y)$. By exploiting this representation of u in the assignment of the boundary conditions on Γ_{lat}, i.e., on the boundary of γ, we get

$$\Big(\pm\mu\frac{\partial p(y)}{\partial y}\Big)\Big|_{y=\pm R_0} = \Big(-\chi p(y) + \frac{u_{ext}(x)}{U(x)}\Big)\Big|_{y=\pm R_0}.$$

Consistently with the previous assumption on p, we postulate that the ratio $u_{ext}(x)/U(x)$ is constant along the whole length of the domain. Finally, we constrain the advective field, by assuming $\nabla\cdot\boldsymbol{b} = 0$ and $\boldsymbol{b}|_{\Gamma_{lat}} = 0$. Since $\boldsymbol{b}$ is divergence-free, we can rewrite the full model (1) in a conservative form, as $-\mu\Delta u + \nabla\cdot(\boldsymbol{b}u) = f$. Now, integrating with respect to y along γ, we obtain

$$\begin{aligned}&-\mu\frac{\partial^2}{\partial x^2}\int_\gamma u(x,y)\,dy - \mu\frac{\partial u(x,y)}{\partial y}\Big|_{y=-R_0}^{y=R_0} + \frac{\partial}{\partial x}\int_\gamma \Big[b_1(x,y)u(x,y)\Big]\,dy\\ &+ \big(b_2(x,y)u(x,y)\big)\Big|_{y=-R_0}^{y=R_0} = \int_\gamma f(x,y)\,dy.\end{aligned}$$

By exploiting the Robin conditions and the hypothesis on $\boldsymbol{b}|_{\Gamma_{lat}}$, we have

$$\begin{aligned}&-\mu\frac{\partial^2}{\partial x^2}\int_\gamma u(x,y)\,dy + \chi\big(u(x,R_0) + u(x,-R_0)\big) + \frac{\partial}{\partial x}\int_\gamma \Big[b_1(x,y)u(x,y)\Big]\,dy\\ &= \int_\gamma f(x,y)\,dy + u_{ext}(x,R_0) + u_{ext}(x,-R_0).\end{aligned}$$

Now, we exploit the factorization $u(x,y) = U(x)p(y)$ assumed for the solution u together with the fact that, by definition, the mean of p along γ is equal to one, to get the desired averaged 1D model (the primes denoting x-differentiation)

$$-\mu U''(x) + (U(x)w_r(x))' + \sigma_r U(x) = f_r(x) \quad \text{for} \quad x\in(0,L), \tag{3}$$

with

$$
\begin{aligned}
w_r(x) &= \frac{1}{|\gamma|}\int_\gamma b_1(x,y)\,p(y)\,dy, \quad \sigma_r = \chi\frac{p(R_0)+p(-R_0)}{|\gamma|},\\
f_r(x) &= \frac{1}{|\gamma|}\int_\gamma f(x,y)\,dy + \frac{u_{ext}(x,R_0)+u_{ext}(x,-R_0)}{|\gamma|}.
\end{aligned}
\tag{4}
$$

The reduction procedure leads from a 2D advection-diffusion problem to a 1D advection-diffusion-reaction problem. To close the model we need to select a profile p in (4). For simplicity, it may be assumed constant or, more in general, it is suggested by physical considerations. It could be advantageous an automatic criterion to select p. A strategy in such a direction is proposed in the next section.

Remark 1 From a physical viewpoint, the most restrictive hypothesis for deriving model (3) is the independence of p on x. Nevertheless, the numerical validation shows that this surrogate model provides reliable results even when this hypothesis is not strictly guaranteed. The second assumption is reasonable, at least in haemodynamics, since the ratio $u_{ext}(x)/U(x)$ may be reliably considered constant. The two requirements on $\boldsymbol{b}$ are standard in a haemodynamic context. Hypothesis $\nabla\cdot\boldsymbol{b}=0$ ensures the incompressibility of the blood, while assumption $\boldsymbol{b}|_{\Gamma_{lat}}=0$ imposes a no-slip condition on Γ_{lat}.

2.1 A Geometrical Multiscale Approach

A geometrical multiscale formulation consists of coupling dimensionally heterogeneous models. The idea is to alternate a full-dimensional model with suitable downscaled models to be associated with the areas characterized by the most complex and by the simplest dynamics, respectively (see, e.g., [2, Chapter 11]). The identification of appropriate matching conditions and the location of the interface between the two models represent the main issues of this approach. We identify the full model with (1) and the downscaled model with (3). We choose $\Omega = (0,10)\times(0,1)$, $\mu=1$, $\boldsymbol{b}=(20,0)^T$, $f = 10\big((x-1.5)^2+0.4(y-0.5)^2<0.01\big)$, $\chi = 1$ and $u_{ext} = 0.02$. We assign a homogeneous Neumann condition on $\Gamma_{out}=\{10\}\times(0,1)$ and a profile compatible with the conditions along Γ_{lat} on Γ_{in}. In Fig. 1 (top-left), we provide the contour plots of the full solution approximated via linear finite elements on a uniform unstructured grid of 8,918 elements. The solution exhibits more significant transverse dynamics in the leftmost part of the domain, where the source term is localized. Conversely, the solution profile is less fluctuating in the rightmost part of Ω, as assumed in the derivation of model (3). This suggests to split Ω into two subdomains, Ω_1 and Ω_2, such that $\overline{\Omega}=\overline{\Omega}_1\cup\overline{\Omega}_2$. On Ω_1 we solve problem (1), while we resort to (3) in Ω_2. Both the problems are discretized via linear finite elements on uniform meshes. The coupling between the two models is performed via a relaxed Neumann/Dirichlet scheme. In more

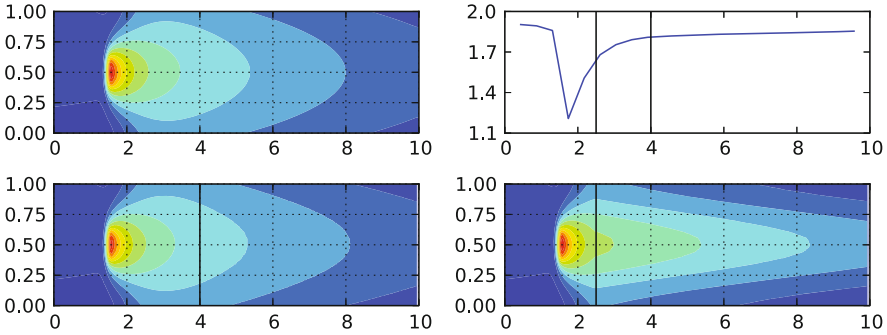

Fig. 1 Geometrical multiscale: full solution (*top-left*); graph of σ_r (*top-right*); coupled solution for Γ_4 (*bottom-left*) and $\Gamma_{2.5}$ (*bottom-right*)

detail, we exploit the derivative of the 1D surrogate solution u_2 to assign a constant Neumann condition on Ω_1 as $\mu \partial u_1/\partial n(x_i, y) = u_2'(x_i)$, where u_1 is the full solution defined on Ω_1 and $\Gamma_{x_i} = \{x_i\} \times (0, 1)$ identifies the interface $\overline{\Omega}_1 \cap \overline{\Omega}_2$. To correctly define the problem on Ω_2, we have to properly select the boundary condition at x_i and the solution profile. As Dirichlet data we assign $u_2(x_i) = |\gamma|^{-1} \int_\gamma u_1(x_i, y)\, dy$, while we follow a new approach to select $p(y)$ at x_i. The idea is to exploit the problem in Ω_1 instead of resorting to an a priori selection. Thus, we pick $p(y) = |\gamma| u_1(x_i, y) / \int_\gamma u_1(x_i, y)\, dy$. This definition justifies the prescription of a Neumann condition on the left hand side of Γ_{x_i} to allow the solution profile to develop freely. Indeed, the adoption of the surrogate model in Ω_2, implicitly assumes that p is completely developed at Γ_{x_i}. Figure 1 (bottom) compares two couplings associated with different interfaces, i.e., Γ_4 and $\Gamma_{2.5}$, respectively. The second choice introduces the interface where the transverse dynamics are still too significant, thus violating the hypothesis on a fully developed profile. We provide a bidimensional visualization also for the surrogate model simply by using relation $u(x, y) = U(x)p(y)$. In Fig. 1 (top-right) we show the reactive coefficient in (4), computed via the profile of the full solution. Since σ_r strongly depends on p, we argue that when the profile stabilizes, σ_r reaches a constant value. So a possible heuristic way to select Γ_{x_i} is to locate it in a region where σ_r is constant.

3 Hi-Mod Reduction

Hi-Mod reduction is an alternative approach to "compress" high dimensional problems. In this case, a full 2D (or even 3D) model is reduced to a system of 1D coupled differential problems associated with the dominant dynamics [4]. In the geometric setting of a Hi-Mod formulation, for any $x \in \Omega_{1D}$, we introduce a map ψ_x between the generic fiber γ_x and a reference fiber $\hat{\gamma}$, so that the computational domain Ω is mapped into the reference domain $\hat{\Omega} = \Omega_{1D} \times \hat{\gamma}$ via the map

Ψ, given by $\Psi(z) = \hat{z}$, where $z = (x, y) \in \Omega$, $\hat{z} = (\hat{x}, \hat{y}) \in \hat{\Omega}$, with $\hat{x} = x$ and $\hat{y} = \psi_x(y)$. In particular, for the domain Ω in (1) a unique map ψ can be used for each point $x \in \Omega_{1D}$. The Hi-Mod approach strongly relies upon the fiber structure postulated on Ω. The idea is to differently tackle the dependence of the full solution on the dominant and on the transverse directions. We perform a modal approximation of the transverse dynamics coupled with a Galerkin representation along the axial direction. The rationale driving this approach is that the transverse dynamics can be suitably described with a few degrees of (modal) freedom, resulting in a *hierarchy* of one-dimensional models which differ each other according to the number of included transverse modes. To state the Hi-Mod reduced formulation for problem (1), we move from the weak form (2). Now, let V_{1D} be a space spanned by functions defined on Ω_{1D} which properly includes the boundary conditions assigned along Γ_{in} and Γ_{out}, and let $\{\varphi_k\}_{k\in\mathbb{N}^+}$ be a modal basis of functions in $H^1(\hat{\gamma})$, orthonormal with respect to the $L^2(\hat{\gamma})$-scalar product and compatible with the boundary conditions along Γ_{lat}. As a consequence, we look for a reduced solution u_m which belongs to the Hi-Mod reduced space $V_m = \left\{v_m(x, y) = \sum_{k=1}^m \tilde{v}_k(x)\,\varphi_k(\psi(y)), \text{with } \tilde{v}_k \in V_{1D},\ x \in \Omega_{1D},\ y \in \gamma\right\}$. A conformity and a spectral approximability hypothesis are introduced on V_m to guarantee the well-posedness and the convergence of u_m to u [4]. We identify the Galerkin representation along Ω_{1D} with a finite element discretization, so that the modal coefficients belong to a finite element space $V_{1D}^h \subset V_{1D}$ associated with a partition $\mathcal{T}_h$ of Ω_{1D}. Thus, the Hi-Mod reduced form for (2) is: for a certain modal index $m \in \mathbb{N}^+$, find $\tilde{u}_k^h \in V_{1D}^h$, with $k = 1, \ldots, m$, such that $\sum_{k=1}^m a(\tilde{u}_k^h \varphi_k, \theta_i \varphi_j) = F(\theta_i \varphi_j)$, with $j = 1, \ldots, m$ and $i = 1, \ldots, N_h$, where θ_i denotes the generic finite element basis function in V_{1D}^h and with $N_h = \dim(V_{1D}^h) < +\infty$. From a computational viewpoint, the Hi-Mod formulation leads to solve a system of m coupled 1D advection-diffusion-reaction problems instead of problem (1). As in the derivation of the surrogate model (3), the Hi-Mod reduction procedure yields reactive terms, while no reactive contribution is included in the full model. The system is characterized by an $m \times m$ block matrix, where each block is an $N_h \times N_h$ matrix exhibiting the sparsity pattern typical of the selected finite element space.

The modal index m can be selected a priori moving from some preliminary knowledge of the phenomenon at hand [4] or automatically, driven by an *a posteriori* modeling error analysis [5]. Another important issue is the choice of the modal basis, in particular when Robin boundary conditions are assigned on Γ_{lat} as in (1). We build a specific modal basis able to automatically include these conditions. The idea proposed in [1] is to solve on $\hat{\gamma}$ an auxiliary Sturm-Liouville eigenvalue problem, with conditions on $\partial\hat{\gamma}$ coinciding with the conditions assigned on Γ_{lat}. We call this modal basis *educated basis*.

3.1 Piecewise Hi-Mod Reduction

Now, the idea is to properly exploit the hierarchy of models provided by the Hi-Mod reduced space to couple models with a different accuracy. A different choice for the modal index m identifies a reduced model with a certain level of detail in describing the phenomenon at hand. As a consequence, by properly tuning m over different regions of Ω, we are able to capture the local significant features of the solution with a relatively low number of degrees of freedom. Following [4], we denote this approach by *piecewise* Hi-Mod reduction. This leads to dimensionally homogeneous models (yet with a locally varying level of accuracy), as opposed to the geometrical multiscale approach. For instance, with reference to the test case in Fig. 1, we can preserve the two splittings of the domain identified by Γ_4 and $\Gamma_{2.5}$ and employ a number of modes in Ω_1 higher than in Ω_2, e.g., 5 and 2, respectively. This choice is motivated by the fact that the most complex dynamics are localized in Ω_1 and, consequently, more modes are demanded in this area. To glue the two models we employ a relaxed Neumann/Dirichlet scheme as in the geometrical multiscale formulation. At each iteration of this scheme, we apply a uniform Hi-Mod reduction on Ω_1 and Ω_2, separately, i.e., we solve two systems of coupled 1D problems with a block matrix of order $5N_h^1$ and $2N_h^2$, respectively N_h^i denoting the dimension of the one dimensional finite element space introduced on $\Omega_{1D} \cap \Omega_i$, for $i = 1, 2$. As detailed in [5], to rigorously formalize the piecewise Hi-Mod approach, we introduce a suitable broken Sobolev space, endowed with an integral condition which weakly enforces the continuity of the reduced solution in correspondence with the minimum number of modes common on the whole Ω. This does not necessarily guarantee the conformity of the piecewise reduced solution. This is evident in Fig. 2. The loss of conformity is particularly significant when the interface is located in an area involved by strong transverse dynamics. The reduced solution in Fig. 2 (left) is in good agreement with the full one in Fig. 1 (top-left) and it is very similar to the one in Fig. 1 (bottom-left).

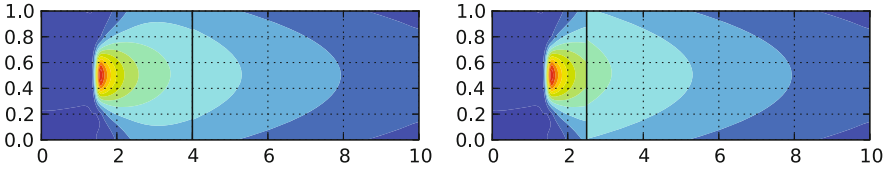

Fig. 2 Piecewise Hi-Mod reduction: reduced solutions associated with $\{5, 2\}$ modes, the interface is Γ_4 (on the *left*) and $\Gamma_{2.5}$ (on the *right*); $h = 0.05$ on Ω_{1D}

4 A Numerical Comparison

For a fair comparison between the two approaches, we consider here a test case where the "low-fidelity" model (the genuine 1D in the geometrical multiscale and a low-mode approximation in the Hi-Mod) are straightforwardly comparable. This means that we employ a single mode in the Hi-Mod approximation. In particular, we consider problem (1) with $\Omega = (0,6) \times (0,1)$, $\mu = 1$, $\mathbf{b} = (20,0)^T$, $f = 10\big([(x-1.5)^2+0.4(y-0.75)^2 < 0.01]+[(x-1.5)^2+0.4(y-0.25)^2 < 0.01]\big)$, $\chi = 3$ and $u_{ext} = 0.05$. The boundary conditions are as in Sect. 2.1 and the interface is located at $x = 3$. Numerical results are provided in Fig. 3. The top-left panel displays the full solution discretized via standard linear finite elements on a uniform unstructured grid of 5,084 triangles. The top-right panel shows the geometrical multiscale solution. This is fairly accurate even though it suffers from an underestimation of the reactive term induced by the 1D average. This is evident in the contour line associated with the value 0.09. The bottom panels display the Hi-Mod solution, having a "low-fidelity" model with $m = 1$ and two different models for the "high-fidelity" part. In particular, on the left we take $m = 3$ which is clearly not enough to capture reliably the solution in the leftmost domain. In the right-panel, with $m = 5$ we have a pretty accurate solution, where the inaccuracy present in the geometrical multiscale solution as well as the model non-conformity do not pollute significantly the results.

An extensive comparison between the two approaches cannot be clearly completed by these preliminary results. As a matter of fact, the computational advantages of the one approach over the other must be evaluated on 3D more realistic test cases, solved with compiled softwares. However, we may notice that, even though the Hi-Mod approach relies entirely on a "psychologically" 1D representation of the solution within a dimensionally heterogeneous framework, it may provide accurate solution also in presence of significant transverse components. For this reason, we do expect it may lead to easily implemented and manageable solvers, with

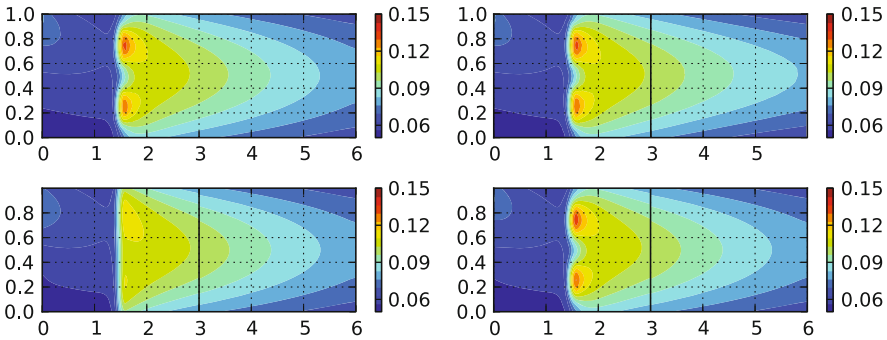

Fig. 3 Full solution (*top-left*); geometrical multiscale solution (*top-right*) and Hi-Mod solution with $\{3,1\}$ (*bottom-left*) and $\{5,1\}$ (*right*) modes

competitive performances in terms of both accuracy and efficiency. A framework of investigation of practical interest is the blood flow simulation in a network of arteries.

References

1. M. Aletti, S. Perotto, A. Veneziani, (2013 in preparation)
2. L. Formaggia, A. Quarteroni, A. Veneziani, *Cardiovascular Mathematics, Modeling, Simulation and Applications*, vol. 1 (Springer, Berlin/Heidelberg, 2009)
3. A. Krpo, Modélisation par des modèles 1D de l'écoulement du sang et du transport de masse dans des artères avec bifurcation, Master thesis, École Polytechnique Fédérale de Lausanne, 2005
4. S. Perotto, A. Ern, A. Veneziani, Hierarchical local model reduction for elliptic problems: a domain decomposition approach. Multiscale Model. Simul. **8**(4), 1102–1127 (2010)
5. S. Perotto, A. Veneziani, Coupled model and grid adaptivity in hierarchical reduction of elliptic problems. J. Sci. Comput. **60**(3), 505–536 (2014)