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Predictor-Multicorrector Scheme for the Dynamic Diffusion Method

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Abstract. In this work we evaluate a predictor-multicorrector integration scheme for transient advection-diffusion-reaction problems using the Dynamic Diffusion method (DD). This multiscale finite element formulation results in a free parameter method in which the subgrid scale space is defined using bubble functions whose degrees of freedom are locally eliminated in favor of the degrees of freedom that live on the resolved scales. The time advancing scheme assumes that the subscales change in time. The formulation is compared with the Consistent Upwind Petrov-Galerkin (CAU) method using the same predictor-multicorrector scheme. Numerical experiments based on benchmark 2D problems were conducted to illustrate the behavior of this new algorithm applied to advection-diffusion-reaction equations.

Keywords. Multiscale Finite Element, Dynamic Diffusion Method, Predictor-Multicorrector Scheme, Advection-Diffusion-Reaction Problems

1 Introduction

For convection-dominated problems, the Galerkin solution exhibits a globally oscillating character and most of the time is meaningless. Using stabilized or multiscale methods more accurate and stable results can be obtained [2, 4]. Arruda et al. [1] proposed a discontinuous two-scale method where an artificial diffusion appears on all scales, named Dynamic Diffusion method (DD), and which stability and convergence properties do not rely on tune-up parameters. The additional diffusion is dynamically determined by imposing some restrictions on the resolved scale solution in the same spirit of the method presented in [6]. The methodology improves upon some discontinuous capturing methods and some subgrid diffusion approaches for transport applications. Here we extend the DD to transient problems using a continuous approximation setting.

In [8] three time advancing schemes for the DD method are presented, considering static

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and temporal variation of the subscales. All the methods are first-order time approximation schemes and they seem to be unconditionally stable, but further experiments need to be done to confirm this behavior. In this work we evaluate a second order predictor-multicorrector algorithm [7] for the time-marching scheme using temporal variation of the subscales. The remainder of this work is organized as follows. Section 2 briefly addresses the multiscale formulation and the time integration scheme. Numerical experiments are conducted in Section 3 to show the behavior of the proposed methodology for a variety of benchmark transport problems. Section 4 concludes this paper.

2 Governing Equations and Time Integration Scheme

Consider the time-dependent advection-diffusion-reaction equation: Find $u : \Omega \times (0, t_f] \to \mathbb{R}$ such that

$$\begin{aligned} \frac{\partial u}{\partial t} - \boldsymbol{\nabla} \cdot (\boldsymbol{\kappa} \boldsymbol{\nabla} u) + \boldsymbol{\beta} \cdot \boldsymbol{\nabla} u + \sigma u &= f \qquad \text{in } \Omega \times (0, t_f), \\ u &= g \qquad \text{on } \Gamma \times (0, t_f), \\ u(\mathbf{x}, 0) &= u_0(\mathbf{x}) \quad \text{in } \Omega. \end{aligned} \tag{1}$$

Here, $\Omega \subset \mathbb{R}^2$ is a polygonal domain with boundary Γ and t_f is the final time. Furthermore, $\boldsymbol{\kappa}$ is the diffusivity tensor, $\boldsymbol{\beta}$ is the flow velocity, σ is the reaction coefficient, f is a given outer source of the unknown scalar quantity u, and $u_0(\mathbf{x})$ represents the initial condition for the solution u. For simplicity, only Dirichlet boundary conditions are considered. It is assumed that $\boldsymbol{\beta} \in W^{1,\infty}(\Omega)$, $\sigma \in L^\infty(\Omega)$, $g \in H^{1/2}(\Gamma)$, $f \in L^2(\Omega)$, and that there exists a constant σ_0 such that $\sigma - \frac{1}{2}\boldsymbol{\nabla} \cdot \boldsymbol{\beta} \geq \sigma_0 > 0$.

For the finite element discretization, consider a triangular partition $\mathcal{T}_H$ of the domain Ω. The discrete settings are then defined by introducing the following two spaces: $V_h = \{u_h \in H_0^1(\Omega) \,|\, u|_{\Omega_e} \in \mathbb{P}_1(\Omega_e), \forall \Omega_e \in \mathcal{T}_H, u|_\Gamma = g\}$ and $V_B = \oplus|_{\Omega_e} V_B^{\Omega_e}$, where $\mathbb{P}_1(\Omega_e)$ represents the set of first order polynomials in Ω_e and $V_B^{\Omega_e} = span(\psi_B)$. The bubble function used is a cubic polynomial function defined by $\psi_B = 27 N_1^e(x,y) N_2^e(x,y) N_3^e(x,y)$, where N_j^e represents the local finite element function associated with the nodal point (coarse) j, $j = 1, 2, 3$ of element Ω_e. The DD method [1] for (1) can be given by: find $u_E = u_h + u_B \in V_E = V_h \oplus V_B$ with $u_h \in V_h$, $u_B \in V_B$ such that

$$\begin{aligned} &\int_\Omega \left(w_E \frac{\partial u_E}{\partial t} + w_E \boldsymbol{\beta} \cdot \boldsymbol{\nabla} u_E + \boldsymbol{\nabla} w_E \cdot \boldsymbol{\kappa} \boldsymbol{\nabla} u_E + \sigma w_E u_E \right) d\Omega \quad + \\ &\sum_{e=1}^{nel} \int_{\Omega_e} \boldsymbol{\nabla} w_E \cdot \xi(u_h) \boldsymbol{\nabla} u_E \, d\Omega = \int_\Omega w_E f \, d\Omega, \quad \forall w_E \in H_0^1 \oplus V_B. \end{aligned} \tag{2}$$

The coefficient $\xi(u_h)$ represents the amount of artificial diffusivity added by the numerical model. Applying the standard finite element approximation on each scale, we arrive at a local system of ordinary nonlinear differential equations to be solved

$$\begin{bmatrix} M_{hh}^e & M_{hB}^e \\ M_{Bh}^e & M_{BB}^e \end{bmatrix} \begin{bmatrix} \dot{U}_h^e \\ \dot{U}_B^e \end{bmatrix} + \begin{bmatrix} K_{hh}^e & K_{hB}^e \\ K_{Bh}^e & K_{BB}^e \end{bmatrix} \begin{bmatrix} U_h^e \\ U_B^e \end{bmatrix} = \begin{bmatrix} F_h^e \\ F_B^e \end{bmatrix}, \tag{3}$$

where U_h^e and U_B^e are, respectively, the nodal values of the unknowns u_h and u_B on each element Ω_e, whereas $\dot{U}_h^e$ and $\dot{U}_B^e$ are their time derivatives. More details of the local matrices and vectors in (3) can be found in [8]. Considering the assembly of the local system (3), a predictor-corrector algorithm [7] for typical benchmark problems is implemented as follows:

Step 1. Predictor Phase (i=0):

$U_h^{n+1,0} = U_h^n + (1-\alpha)\Delta t \dot{U}_h^n, \quad U_B^{n+1,0} = U_B^n + (1-\alpha)\Delta t \dot{U}_B^n,$

$\dot{U}_h^{n+1,0} = 0, \quad \dot{U}_B^{n+1,0} = 0$

Step 2. Corrector Phase (i=1,2,..):

2.1 Residual Force:

$R_1^{n+1,i} = F_h^{n+1} - (M_{hh}\dot{U}_h^{n+1,i} + M_{hB}\dot{U}_B^{n+1,i}) - (K_{hh}U_h^{n+1,i} + K_{hB}U_B^{n+1,i})$

$R_2^{n+1,i} = F_B^{n+1} - (M_{Bh}\dot{U}_h^{n+1,i} + M_{BB}\dot{U}_B^{n+1,i}) - (K_{Bh}U_h^{n+1,i} + K_{BB}U_B^{n+1,i})$

2.2 Solve $M^* \Delta\dot{U}_h^{n+1,i+1} = F^*$, with $M^* = M_1 - N_1 N_2^{-1} M_2$ and $F^* = R_1 - N_1 N_2^{-1} R_2$

$M_1 = M_{hh} + \alpha\Delta t K_{hh}, \quad N_1 = M_{hB} + \alpha\Delta t K_{hB}$

$M_2 = M_{Bh} + \alpha\Delta t K_{Bh}, \quad N_2 = M_{BB} + \alpha\Delta t K_{BB}$

2.3 Update Solution:

$U_h^{n+1,i+1} = U_h^{n+1,i} + \alpha\Delta t\Delta\dot{U}_h^{n+1,i+1}, \quad \dot{U}_h^{n+1,i+1} = \dot{U}_h^{n+1,i} + \Delta\dot{U}_h^{n+1,i+1}$

$U_B^{n+1,i+1} = U_B^{n+1,i} + \alpha\Delta t\Delta\dot{U}_B^{n+1,i+1}, \quad \dot{U}_B^{n+1,i+1} = \dot{U}_B^{n+1,i} + \Delta\dot{U}_B^{n+1,i+1}$

with $\Delta\dot{U}_B^{n+1,i+1} = N_2^{-1}(R_2^{n+1,i} - M_2\Delta\dot{U}_h^{n+1,i+1})$

where M_{hh} is the global matrix associated to M_{hh}^e and so forth for the other matrices. Here Δt is the timestep; subscripts $n+1$ and n mean, respectively, the solution on the timestep $n+1$ and n; α is a parameter, taken to be in the interval $[0,1]$; and the matrix $N_2 = (M_{BB} + \Delta t K_{BB}) \neq 0$ for $\xi(u_h) > 0$. In *2.2*, the small scale space of the unknowns $\Delta\dot{U}_B$ is condensed onto the resolved scale degrees of freedom, $\Delta\dot{U}_B = N_2^{-1}(R_2 - M_2\Delta\dot{U}_h)$, resulting in a system of ordinary differential equations involving only $\Delta\dot{U}_h$. The following average rule [6] is used to determine$\xi(u_h^k)$: $\xi(u_h^k) = c_b^{k+1}\varsigma(h)$, $c_b^{k+1} = \omega\tilde{c}_b^{k+1} + (1-\omega)c_b^k$ with $\omega \in [0,1]$ suitably chosen as $\omega = 0.5$ and $\tilde{c}_b^{k+1} = \frac{1}{2}\frac{|R(u_h^k)|}{||\nabla u_h^k||}$ if $||\nabla u_h^k|| > tol_\xi$ or zero otherwise. $R(u_h)$ is the residual, tol_ξ is a user given tolerance, and $\varsigma(h) = \sqrt{A_e}$ is the characteristic sub-grid parameter, where A^e is the area of finite element Ω_e, assumed constant. We fixed three steps in the Corrector Phase ($i = 1,2,3$) at each timestep for the first two applications in the next section. In the last numerical example we use a tolerance of 10^{-4} and a maximum number of 20 iterations at the Corrector Phase.

3 Numerical Studies

We compare the Dynamic Diffusion (DD) method with the Consistent Upwind Petrov-Galerkin (CAU) method [5] with the same time-marching predictor-multicorrector algorithm [7]. In the experiments, the domain Ω is discretized into N-by-N cells with two triangular elements in each cell, resulting in $(N+1)^2$ nodes and N^2 elements. The first experiment is a steady-state advection dominated problem presented in [3]. The flow is a rigid rotation about the center of a unit square domain, $\Omega = [-0.5, 0.5] \times [-0.5, 0.5]$, with velocity components given by $\beta_x = -y$ and $\beta_y = x$, $\sigma = f = 0$, the diffusivity tensor

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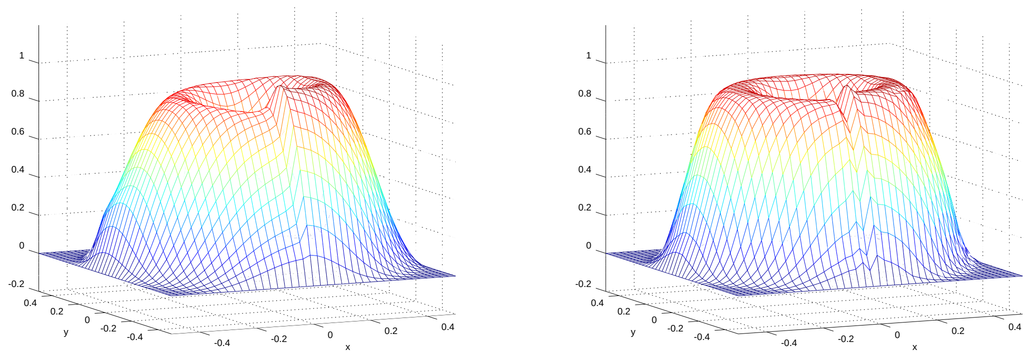
is $\boldsymbol{\kappa} = \epsilon \boldsymbol{I}$ with $\epsilon = 10^{-8}$ and $\boldsymbol{I}$ the 2-by-2 identity matrix. On the external boundary of the square u is set to zero, and on the internal 'boundary' $OA = \{x = 0; -0.5 \leq y \leq 0\}$, u is prescribed to be a sine hill. The initial conditions are $u_0 = -sin(2\pi\, y)$ on OA and $u_0 = 0$ on the rest of the domain. The steady-state solution is obtained when $\|\mathbf{u}^n - \mathbf{u}^{n-1}\| < 0.01\ \|\mathbf{u}^n\|$. We use a mesh with 40-by-40 cells, a fixed timestep size of $\Delta t = 0.1$, and $tol_\xi = 10^{-10}$. The exact solution is essentially a pure advection of the OA boundary condition along the circular streamlines. The elevation of u using CAU and DD schemes is shown in Figure 1. Observe that both nonlinear methods (CAU and DD) introduce a non-physical dissipation at the internal border, see Figure 1. However, the DD method performs better than the CAU scheme as shown in Figure 2.



(a) CAU method (b) DD method

Figure 1: Advection in a rotating flow field: elevation of u.

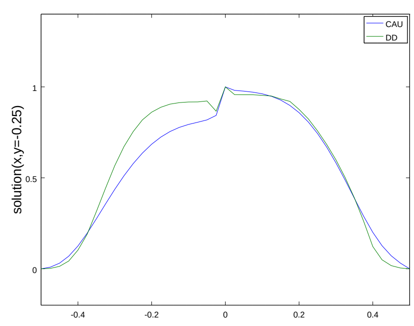


Figure 2: Advection in a rotating flow field: CAU and DD solutions for $y = -0.25$.

The second problem has as the exact solution a circular bubble with extremely sharp layers (see Figure 3(a)). The following parameters are chosen: $\boldsymbol{\kappa} = \epsilon \boldsymbol{I}$ with $\epsilon = 10^{-4}$ and $\boldsymbol{I}$ the identity matrix 2×2, $\sigma = 2$ and velocity field $\boldsymbol{\beta} = (\beta_x, \beta_y)^T$ with $\beta_x = -2(y-1)[r_0^2 - (x-x_0)^2 - (y-y_0)^2]$, $\beta_y = 2(x-1)[r_0^2 - (x-x_0)^2 - (y-y_0)^2]$ if $0 \leq (x-x_0)^2 - (y-y_0)^2 \leq r_0^2$, $\beta_x = \beta_y = 0$ otherwise, and $x_0 = y_0 = 0.5$, $r_0 = 0.25$. The source force and Dirichlet boundary conditions are chosen so that the exact solution is $u(x,y) = \frac{1}{2} + \frac{1}{\pi}\text{arctg}\left[a(r_0^2 - (x-x_0)^2 - (y-y_0)^2)\right]$, $a = 1000$. The initial solution is zero. We use a mesh with 40-by-40 cells, a fixed timestep size of $\Delta t = 0.5$ and steady-state

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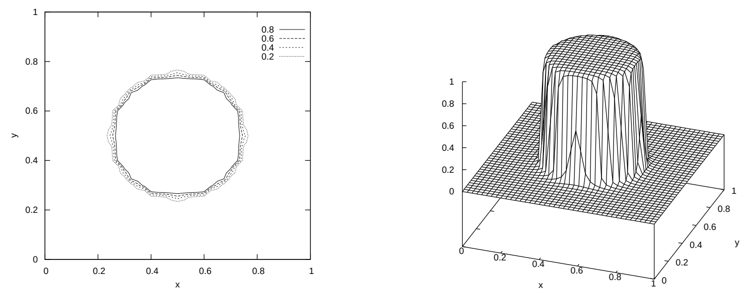
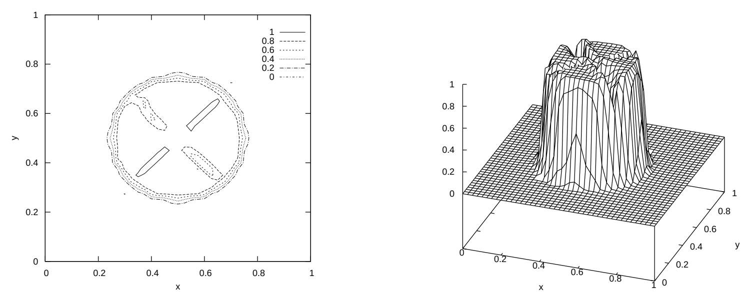
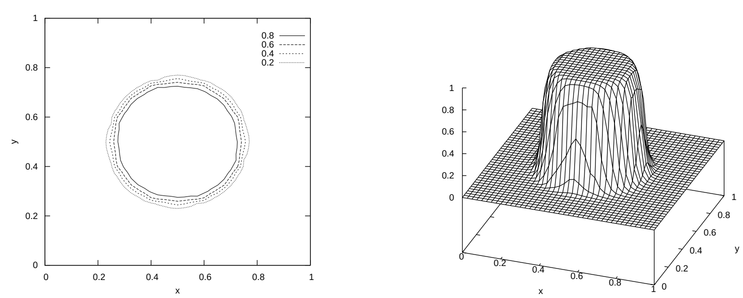
solution is obtained when $\|\mathbf{u}^n - \mathbf{u}^{n-1}\| < 10^{-4}\ \|\mathbf{u}^n\|$. The solution obtained by the DD scheme can represent the region of high gradient without oscillations, but with a relatively diffusive behavior, as can be best seen by comparing their level curves with the exact solution in Figure 3.



(a) Contours of Exact Solution. (b) Elevation of the Exact Solution.



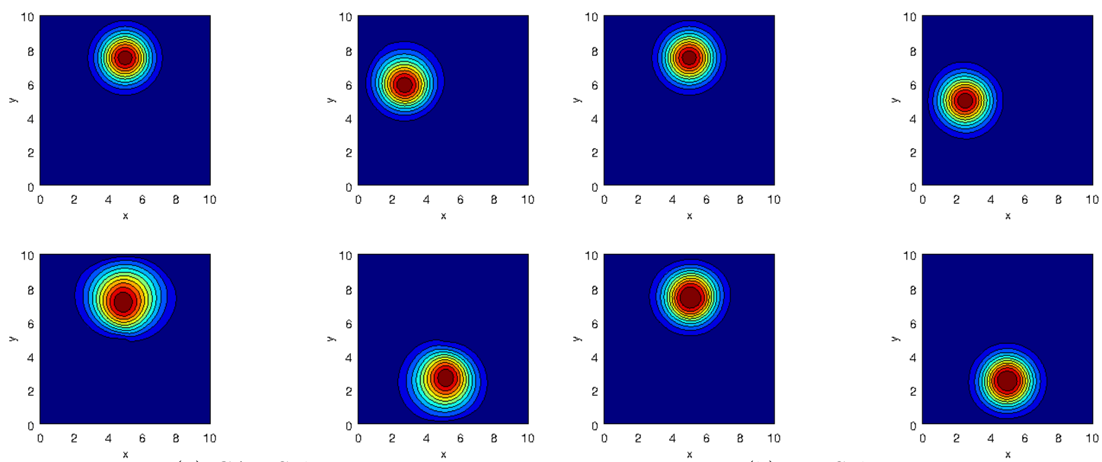
(c) Contours of CAU Solution. (d) Elevation of the CAU Solution.



(e) Contours of DD Solution. (f) Elevation of the DD Solution.

Figure 3: Solutions of the 2D advection-diffusion-reaction problem.

In this last numerical experiment, we solve a transient problem. A Gaussian "cone" is advected with zero diffusion ($\boldsymbol{\kappa} = \mathbf{0}$) along a circular path centered at the origin and interior to a square domain of size $[0, 10] \times [0, 10]$. The initial data is a smooth cone function centered at $(5.0, 7.5)$: $u_0(x,y) = e^{-0.5r}$, with $r = (x-5)^2 + (y-7.5)^2$. The boundary condition is $u(x,y) = 0$ on Γ, and the rotational flow field is: $\boldsymbol{\beta} = (\beta_x, \beta_y)^T$, where $\beta_x = -(y-5)$ and $\beta_y = (x-5)$. A 40-by-40 cells and a fixed timestep of 0.04 time units are chosen, and the simulation is carried out for a single rotation of period $(t = 6.28)$. Figure 4 shows the contours of the numerical solutions obtained using CAU and DD schemes at the initial position $(t = 0)$ and the subsequent steps $t = 1.6$, $t = 3.16$ and $t = 6.28$. The diffusive behavior of the DD schemes is also confirmed here, see Figure 5. Once more the DD method with the predictor-corrector scheme had a performance better than the CAU method.



(a) CAU Solution. (b) DD Solution.

Figure 4: Solutions of the rotating cone (clockwise from top left) at t=0, 1.6, 3.16, 6.28.

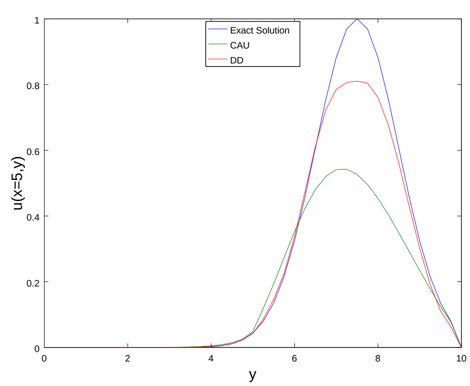


Figure 5: Solution $u(x=5,y)$ of the rotating cone at $t = 6.28$.

4 Conclusions

In this work we evaluated a predictor-multicorrector integration scheme for transient advection-diffusion-reaction problems using the Dynamic Diffusion method. In the numerical

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experiments we considered advection in a rotating flow field, a circular bubble with extremely sharp layers and a transient pure advection cone transport. The solutions obtained by the DD scheme can represent the region of high gradient without oscillations, but with a slightly diffusive behavior. However, the approximate solutions obtained with the DD method were less diffusive than the CAU method. Future works include convergence and stability of the transient scheme and new characteristic sub-grid parameters, such as the velocity field and the length scale at which the subgrid inertial effects take place.

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References

[1] N.C.B. Arruda, R.C. Almeida, and E.G.D. do Carmo, Dynamic diffusion formulation for advection dominated transport problems. Mecânica Computacional, vol 29, 2011–2025, (2010).

[2] F. Brezzi and L.D. Marini, Augmented spaces, two-level methods, and stabilizing subgrids. International Journal for Numerical Methods in Fluids, vol. 40, 31–46, (2002).

[3] A.N. Brooks and T.J.R. Hughes, Streamline upwind/Petrov-Galerkin formulations for convection dominated flows with particular emphasis on the incompressible Navier-Stokes equations. Computer Methods in Applied Mechanics and Engineering, vol. 32, 199–259, (1982).

[4] A. L. G. A. Coutinho, L.P. Franca, and F. Valentin, Numerical multiscale methods. International Journal for Numerical Methods in Fluids, 70:403–419, (2011).

[5] A.C.R.N. Galeão and E.G. Do Carmo, A consistent approximate speed-up upwind Petrov-Galerkin method for convection-dominated. Comp. Meth. Appl. Mech. Eng., vol. 10, 83–95, (1988).

[6] I. P. Santos and R. C. Almeida, A nonlinear subgrid method for advection-diffusion problems. Computer Methods in Applied Mechanics and Engineering, vol. 196, 4771–4778, (2007).

[7] T.E. Tezduyar and T.J.R. Hughes, Finite element formulations for convection dominated flows with particular emphasis on the compressible Euler equations. Proceedings of AIAA 21st Aerospace Sciences Meeting, AIAA Paper 83-0125, Reno, Nevada, (1983).

[8] A.M.P. Valli, L. Catabriga, I.P. Santos, R.C. Almeida, and A.L.G.A. Coutinho, Time integration schemes for a multiscale finite element formulation to solve transient advection-diffusion-reaction problems. Proceedings of the XXXV Iberian Latin American Congress on Computational Methods in Engineering, Fortaleza, CE, (2014).

