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ADAPTIVE MODELLING AND MESHING FOR TIME DEPENDENT PROBLEMS BASED ON TIME AVERAGES

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Abstract. In this work we propose a dual weighted error estimator with respect to modelling and discretization error based on time-averages for evolutionary partial differential equations. This goal-oriented estimator measures the error of linear functionals averaged in time. It takes advantage of time averages and circumvents the solution of a nonstationary adjoint problem. We use the proposed estimator to solve convection-diffusion-reaction equations containing e.g. atmospheric chemistry models as reaction. This kind of equations are of major interest in meteorology.

1 Introduction

We present a goal-oriented duality based a posteriori error estimator and an adaptive strategy for the computation of functionals averaged in time for nonlinear time dependent problems. Error estimation with respect to a quantity of interest instead of the classical energy norm was presented in e.g. [8]. The concept of dual-weighted residual based (DWR) error estimation for the discretization error presented in [2] has entered to various fields, e.g. fluid dynamics [6] and optimization [1], [3]. Adaptvie modelling for free-surface flows was presented in [9], the concept of dual-weighted error estimation was extended to model error estimation e.g. in [5].

Functionals averaged in time are typically relevant for periodic or quasi-periodic solutions in time. Applications arise, e.g., in systems of convection-diffusion-reaction equations including a large amount of chemical reactions. In order to reduce the numerical complexity, we use simultaneously locally refined meshes and adaptive (chemical) models.

Such strategies come along with the question of how to control the discretization error and the model error.

These error parts are expressed in terms of output functionals. Hence, consideration of adjoint problems measuring the sensitivity of the functional output are needed. In contrast to the classical dual-weighted residual method we favor a fixed mesh and model strategy in time. Taking advantage of the (quasi-)periodic behaviour, only a stationary dual problem has to be solved. This implies that the computation of an evolutionary adjoint problem is circumvented. Storing the primal solution at every timestep is also not necessary. Only averaging in time is needed which is usually possible without serious problmes.

This a posteriori estimation technique is applied, e.g., to a system of convection-diffusion-reaction equations. The performance is checked by evaluating and comparing the estimated and exact errors for the mesh and the used model.

2 Variational problems and time-averages

Problem specification. We seek solutions $u \in W$ so that

$$(\partial_t u, \psi)_Q + \int_I B(u)(\psi)\, dt = (f, \psi)_Q \quad \forall \psi \in W, \tag{1}$$

for given data $f \in L^2(I, W')$ with

$$B(u)(\psi) := A(u)(\psi) + R(u)(\psi),$$

where A describes e.g. diffusion and convection and R describes a reaction model. $\Omega \subset \mathbb{R}^d$, $d \in \{2, 3\}$ is a Lipschitz domain and $I := [0, T]$ the time interval with $T > 0$. We consider the abstract variational problem in the Bochner space $W := H^1(I, V)$ with a Hilbert space V. Hence, functions in W are weakly differentiable with image in V.
By $(\cdot, \cdot)_Q$ we denote the L^2-scalar product in the time-space slab $Q := I \times \Omega$, $A : V \times V \to \mathbb{R}$ and $R : V \times V \to \mathbb{R}$ are semilinear forms supposed to be Frechét differentiable with respect to the first argument. The form R is the expensive part to solve, hence, a simplified model $R_m \approx R$ introducing less couplings is preferred.

Therefore, we seek an approximate solution $u_m \in W$ of the reduced system

$$(\partial_t u_m, \psi)_Q + \int_I B_m(u_m)(\psi)\, dt = (f, \psi)_Q \quad \forall \psi \in W, \tag{2}$$

with

$$B_m(u)(\psi) := A(u)(\psi) + R_m(u)(\psi). \tag{3}$$

By u_h and u_{hm} we denote the semidiscrete solutions corresponding to (1) and (2) in $H^1(I, V_h)$ with a conforming finite element space $V_h \subset V$, respectively.

Time-averages. We are interested in an accurate determination of a linear functional output

$$J : V \to \mathbb{R}$$

for a time averaged solution, e.g., in $J(\overline{u})$, where $\overline{u}$ denotes the time average

$$\overline{u} = \frac{1}{T}\int_0^T u\,dt.$$

The main goal of this work is the construction of an error estimator η in terms of this given functional:

$$\eta \approx J(\overline{u} - \overline{u}_{hm}).$$

Integration in time (by taking a test function constant in time) of equations (1) and (2) leads to the time averaged equations for $u, u_m \in H^1(I, W)$:

$$\sigma_T(u,\varphi) \quad + \overline{B}(u)(\varphi) \qquad = (\overline{f},\varphi) \quad \forall \varphi \in V, \tag{4}$$
$$\sigma_T(u_m,\varphi) + \overline{B}_m(u_m)(\varphi) = (\overline{f},\varphi) \quad \forall \varphi \in V, \tag{5}$$

where we use the linear forms $\sigma : W \times V \to \mathbb{R}$ and the semilinear form $\overline{B} : W \times V \to \mathbb{R}$ defined by

$$\sigma_T(u,\varphi) := \frac{1}{T}(u(T) - u(0),\varphi),$$
$$\overline{B}(u)(\varphi) := \frac{1}{T}\int_0^T B(u)(\varphi)\,dt.$$

The time average of B_m, denoted by $\overline{B}_m$, is defined analogous to $\overline{B}$. The (time averaged) residual of the reduced problem (5) is denoted by

$$\varrho_m(u,\varphi) := (\overline{f},\varphi) - \sigma_T(u,\varphi) - \overline{B}_m(u)(\varphi). \tag{6}$$

Using these prerequisites we can now formulate the estimator using stationary dual problems.

3 A posteriori estimation of discretization and model error

We will now present a dual-weighted error estimator. Using the time-averaged equations of the the primal problems (4) and (5) we formulate **stationary** dual problems as

$$z \in V : B'(\overline{\xi})(\varphi, z) \qquad = J(\varphi) \quad \forall \varphi \in V, \tag{7}$$
$$z_m \in V : B'_m(\overline{\xi}_m)(\varphi, z_m) = J(\varphi) \quad \forall \varphi \in V. \tag{8}$$

If $B(\cdot)(\cdot)$ or $B_m(\cdot)(\cdot)$ are nonlinear in the first argument, $z = z(\xi)$ and $z_m = z_m(\xi_m)$ depend on the choices $\xi, \xi_m \in V$. The resulting error estimator is based on fluctuations in time due to possible nonlinearities of B and B_m defined by

$$\begin{aligned} K(u)(\varphi) &:= \overline{B}(u)(\varphi) - B(\overline{u})(\varphi), \\ K_m(u)(\varphi) &:= \overline{B}_m(u)(\varphi) - B_m(\overline{u})(\varphi), \end{aligned}$$

These nonlinearities in t result from nonlinearities in the reaction parts R and R_m and nonlinearities of A in u, e.g. due to nonstationary coefficients in A

Using the definitions of these dual problems we can formulate a dual weighted error estimator with respect to a linear functional $J : V \to \mathbb{R}$.

Theorem 3.1. *If B and B_m are continuously Gâteaux differentiable, the discretization and model error with respect to the linear functional J can be represented by*

$$J(\overline{u} - \overline{u}_{hm}) = J(\overline{u} - \overline{u}_m) + J(\overline{u}_m - \overline{u}_{hm}), \tag{9}$$

where

$$\begin{aligned} J(\overline{u} - \overline{u}_m) &= -\sigma_T(u - u_m, z) - K(u)(z) + K(u_m)(z) - \overline{R}(u_m)(z) + \overline{R}_m(u_m)(z), \\ J(\overline{u}_m - \overline{u}_{hm}) &= \overline{\varrho}_m(u_{hm})(z_m - i_h z_m) - \sigma_T(u_m - u_{hm}, z_m) \\ &\quad + K_m(u_{hm})(z_m) - K_m(u_m)(z_m), \end{aligned}$$

and $z = z(\overline{\xi}) \in V$, $z_m = z_m(\overline{\xi}_m) \in V$ are the dual solutions of (7) and (8), respectively, to the linearizations at $\overline{\xi} = \lambda\overline{u} + (1-\lambda)\overline{u}_m$ and $\overline{\xi}_m = \lambda_m\overline{u}_m + (1-\lambda_m)\overline{u}_{hm}$ with appropriate $\lambda, \lambda_m \in [0, 1]$.

Proof. We split the proof into the derivation of the model error and the discretization error and start with the model error $J(\overline{u} - \overline{u}_m)$.

The mean value theorem ensures the existence of at least one $\lambda \in [0, 1]$ so that for $\overline{\xi} := \lambda\overline{u} - (1 - \lambda)\overline{u}_m \in V$ and $\overline{e}_m := \overline{u} - \overline{u}_m$ it holds

$$\begin{aligned} B'(\overline{\xi})(\overline{e}_m, \varphi) &= \int_0^1 B'(\overline{u}_m + s\overline{e}_m)(\overline{e}_m, \varphi)\, ds \\ &= B(\overline{u})(\varphi) - B(\overline{u}_m)(\varphi) \qquad \forall \varphi \in V. \end{aligned}$$

Let $z = z(\overline{\xi}) \in V$ be the associated dual solution of equation (7). Then it holds with (3), the time-averaged equations (4), (5) and the definition of $K(\cdot)(\cdot)$:

$$\begin{aligned} J(\overline{u} - \overline{u}_m) &= B'(\overline{\xi})(\overline{u} - \overline{u}_m, z) \\ &= B(\overline{u})(z) - B(\overline{u}_m)(z) \\ &= -\sigma_T(u - u_m, z) - K(u)(z) + K(u_m)(z) - \overline{R}(u_m)(z) + \overline{R}_m(u_m)(z). \end{aligned}$$

The discretization error $J(\overline{u}_m - \overline{u}_{hm})$ can be derived in a similar way: We use again the mean value theorem for $\overline{\xi}_m := \lambda\overline{u}_m - (1-\lambda)\overline{u}_{hm} \in V$ and denote by $z_m = z_m(\overline{\xi}_m) \in V$ the associated dual solution of equation (8). By $i_h : V \to V_h$ we denote an arbitrary interpolation operator. Using the time averaged residual (6) it holds

$$\begin{aligned} J(\overline{u}_m - \overline{u}_{hm}) =& B'_m(\overline{\xi}_m)(\overline{u}_m - \overline{u}_{hm}, z_m) \\ =& B_m(\overline{u}_m)(z_m) - B_m(\overline{u}_{hm})(z_m) \\ =& (\bar{f}, z_m) - \sigma_T(u_m, z_m) - \overline{B}_m(u_{hm})(z_m) + K_m(u_{hm})(z_m) - K_m(u_m)(z_m) \\ =& \overline{\varrho}_m(u_{hm})(z_m - i_h z_m) - \sigma_T(u_m - u_{hm}, z_m) + K_m(u_{hm})(z_m) - K_m(u_m)(z_m). \end{aligned}$$

□

4 Approximation of the estimator

Finite element approximation. We propose a discretization based on conforming finite elements for dimensions $d = 2$ or $d = 3$. According to this the mesh $\mathcal{T}_h$ of Ω consists of quadrilaterals or hexahedrals. By h_K we denote the diameter of a cell $K \in \mathcal{T}_h$ and by $Q_r(\mathcal{T}_h)$ the finite element space resulting from transformations $F_K : \hat{K} \to K$ of polynomials $\hat{\varphi}$ on a reference cell $\hat{K}$ of maximal degree $r \geq 0$ in each coordinate direction:

$$Q_r(T_h) := \left\{ \varphi \in H^1(\Omega) : \varphi|_K \circ F_K \in \mathbb{Q}_r(\hat{K}) \quad \forall K \in \mathcal{T}_h \right\}.$$

Hence, the finite element approximation of u_m is $u_{hm} \in V_h := Q_r(\mathcal{T}_h)^s$. The formulation for vector-valued problems is straight forward.

Assuming that $\mathcal{T}_h$ results from a globally coarser mesh $\mathcal{T}_{2h}$, we can define the higher order nodal interpolation operator to the coarser mesh $\mathcal{T}_{2h}$:

$$i_{2h}^{(2)} : Q_r(\mathcal{T}_h) \to Q_{2r}(\mathcal{T}_{2h}). \tag{10}$$

By $u_{2h}^{(2)}$ we denote the result of applying $i_{2h}^{(2)}$ to u_h.

In order to get an evaluable error estimator we have to approximate the exact formulation of theorem (3.1). More precisely we have to define approximations $\eta_h \approx J(\overline{u}_m - \overline{u}_{hm})$ and $\eta_m \approx J(\overline{u} - \overline{u}_m)$.
By z_h and z_{hm} we denote the solutions of the discrete problems corresponding to (7) and (8).

Definition of η_h. The numerically evaluable approximation η_h to $J(\overline{u}_m - \overline{u}_{hm})$ reads

$$\begin{aligned} \eta_h := \; & \overline{\varrho}_m(u_{hm})(z_{2hm}^{(2)} - z_{hm}) - \sigma_T(u_{2hm}^{(2)} - u_{hm}, z_{hm}) \\ & + K_m(u_{hm})(z_{hm}) - K_m(u_{2hm}^{(2)})(z_{hm}). \end{aligned}$$

We cannot expect that $\sigma_T(u^{(2)}_{2hm} - u_{hm}, z_{hm})$ is a good approximation to $\sigma_T(u_m - u_{hm}, z_{hm})$, because $u^{(2)}_{2hm}$ at one point of time contains errors of u_{hm} accumulated over time. Neglecting this part is justified for long time averaging ($T >> 1$) and/or periodic solutions.

To refine the mesh locally this global estimator has to be localized to get cell- or nodewise contributions to the error. Techniques to localize the different parts of the estimator can be found in [4].

Definition of η_m. Neglecting $\sigma_T(\cdot,\cdot)$ again and by the definition of $K_{R_m}(\cdot)(\cdot)$ we propose the following approximation to $J(\overline{u} - \overline{u}_m)$:

$$\eta_m := -\overline{R}(u_{hm})(z_h) + \overline{R}_m(u_{hm})(z_h). \tag{11}$$

Solving the primal discrete problem we get u_{hm} and z_h, z_{hm} solving the discrete dual problems. To evaluate the pure model error $-K(u)(z) + K(u_m)(z)$ a solution to a model better than R_m is needed. For that the primal problem has to be solved again which is too costly. However, neglecting this part leads to pretty good estimates as we show in the numerical results.

Remark 4.1. *Computing the solutions z of problem (7) and z_m of problem (8), respectively z_h and z_{hm}, is not costly because the adjoint problems are linear and stationary. Nevertheless one may replace z_m by z to reduce numerical costs. A comparison of the two approaches can be found in the numerical examples of [7].*

5 Numerical Examples

In this section we present two numerical examples. In the first example we only measure the model error using 3 different models for atmospheric chemistry. In the second example we apply the estimator of theorem 3.1 to a simple test case and refine the mesh and adapt the model simultaneously.

We solve a system of coupled convection-diffusion-reaction equations

$$\partial_t \mathbf{u} - \nu \Delta \mathbf{u} + \beta \cdot \nabla \mathbf{u} - \mathbf{R}_m(u) = \mathbf{f},$$

with the viscosity ν, the flow field β and the reaction model R_m.

In order to switch locally between these models, we introduce a non-overlapping partitioning of Ω into subdomains Ω_i, $i = 1 \dots M$,

$$\overline{\Omega} = \bigcup_{i=1}^{M} \overline{\Omega}_i.$$

Then in Ω_i the reduced model R^i is used and the reaction part R_m is defined by

$$R_m(u)(\varphi) := \sum_{i=1}^{M} R^i(u)(\varphi)_{|\Omega_i}.$$

To check the gentleness of the error estimator we introduce the efficiency index

$$I_{eff} = \frac{\eta}{J(\overline{u} - \overline{u}_{hm})},$$

which compares the estimated and the exact error. Hence, an efficiency index near to 1 implies that the error is estimated very well.

Model adaptivity for Atmospheric Chemistry Models. In this example we employ three different models. The used "exact" model R^1 is *RADM2*, a widely used model in atmospheric chemistry, see [11]. This atmospheric chemistry model contains 63 chemical species and 201 chemical reactions, where 5 species are *major gases*, whose concentrations are fixed. Therefore we have to solve a system of 58 coupled convection-diffusion-reaction equations. The *medium model* R^2 consists of 32 reactions (see [10]) and a traditional *low model* R^3 only of 3 reactions.

In this 3D example the computational domain in kilometres is $\Omega := (0, 20) \times (0, 20) \times (0, 1)$ and the computed time is one day. In order to keep the implementation as simple as possible temperature, pressure, turbulent viscosity and photolysis rates are fixed in space and time. The flow field is also fixed in space and time by $\beta := (-50, 100, 0)^T m/min$. The periodicity of the solution comes from a periodic source in the subdomain $\Omega_s := (13, 4) \times (16, 7) \times (0, 0.5)$ of NO (nitrogen oxide) and NO_2 (nitrogen dioxide). Starting with high emissions, they are reduced to zero at the middle of the day and increased again til the end of the day.

The goal functional is given by the mean value in time of O_3 (ozone) in the subdomain $\Omega_d := (13, 4) \times (16, 7) \times (0, 0.5)$:

$$J(\overline{u}) = \frac{1}{|\Omega_d|} \int_{\Omega_d} \overline{u}_{O_3}\, ds,$$

with the exact value

$$J(\overline{u}) \approx 3.144843e\text{-}02,$$

computed by using *RADM2* in the complete domain.

The adaption is chosen in a way, that the cells which sum up to 25% of the estimated error are adapted to R^1 and cells that sum up to the next 25% are adapted to the next better model; more precisely if the model of used at a cell is R^3 it is switched to R^2 otherwise from R^2 to R^1. Other adaption strategies can be found in [7].

The results can be found in table 1. We start with the cheap model R^3 in the complete domain, estimate the model error and adapt the model cellwise. As can be seen by the efficiency index I_{eff}, the error is estimated pretty good as I_{eff} is close to 1. The exact error decreases from step to step. Hence the localization of the estimated error works very well. The error of step 1 is reduced by a factor of nearly 100 by just using 20% of R^1 and 13% of R^2 at step 5. This shows that using the cheap model in the main part of the

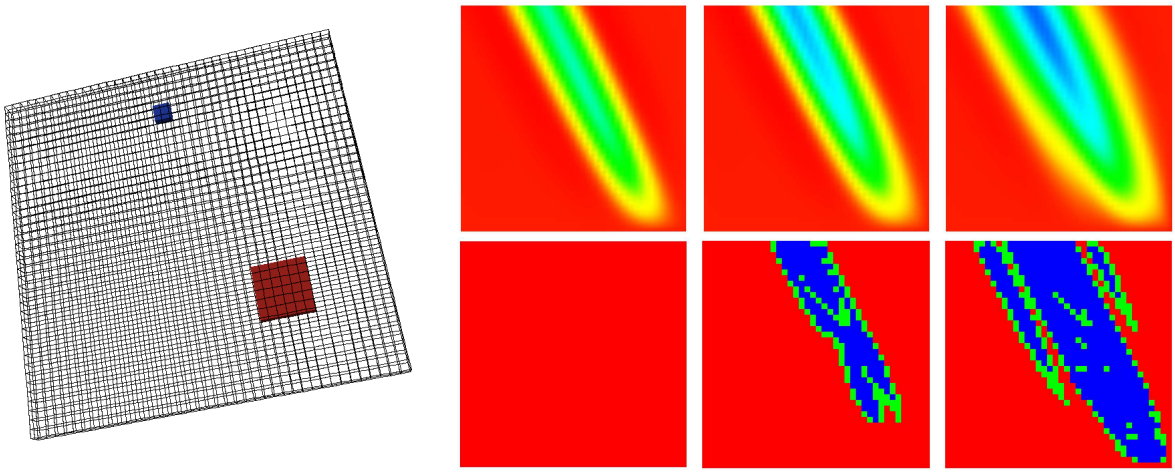

Figure 1: Left: Used mesh and area Ω_s of source term (red) and area Ω_d of goal functional (blue); Right: Mean solution O_3 at adaption steps 1,3 and 5 (above) and corresponding allocation of models R^1 (blue), R^2 (green) and R^3 (red) (below) of a cut at $250m$ height.

Table 1: Comparison of real and estimated model error

step	$\%R^1$	$\%R^2$	$\%R^3$	$J(\overline{u}_h - \overline{u}_{hm})$	η_m	I_{eff}
1	0	0	100	-5.68e-04	-6.04e-04	1.06
2	2	4	94	-1.65e-04	-1.79e-04	1.09
3	7	6	87	-9.29e-05	-1.02e-04	1.10
4	13	8	79	1.12e-05	8.61e-06	0.77
5	20	13	67	6.65e-06	5.86e-06	0.88

domain is absolutely sufficient. In figure 1 the allocation of the mean solution of ozone and the allocation of the models are pictured. As expected the model is adapted around Ω_s and Ω_d and along the route of transport according to the flow field β.

In figure 5 the development of the functional over time is shown. Although the estimator only measures time-averages, it can be seen that the functional output over time at step 5 is nearly the same as the output using *RADM2* in the complete domain.

Combined Mesh and Model Adaptivity In this paragraph we apply the complete estimator of theorem 3.1 to a test example and simultaneously refine the mesh locally and adapt the model cellwise. The estimated errors η_h and η_m are equilibrated, so that the mesh is not refined too much and/or the model is not adapted in too many cells.

We solve a system of three coupled convection-diffusion-reaction equations in the space-time slab $\Omega \times I := ((0,40) \times (0,10)) \times [0,50]$ with the viscosity $\nu = 10$, homogeneous Dirichlet condition on the lower boundary, homogeneous Neumann conditions on the

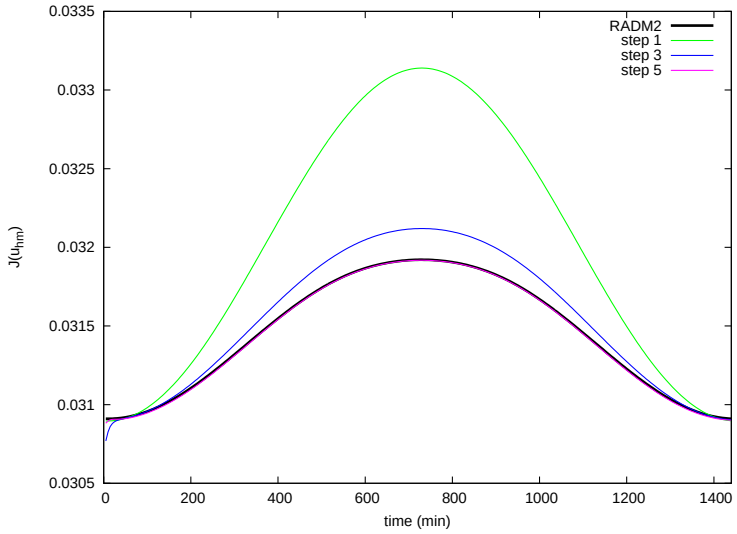

Figure 2: Comparison of computed ozone concentrations in *ppm* at adaption steps 1,3 and 5 to output of RADM2

remaining parts of $\partial\Omega$ and the periodic right-hand-side $\mathbf{f} = (f_1, f_2, 0)^T$

$$f_1(t,x) = \begin{cases} \psi(t) & \text{if } x \in \Omega_{s,1} \cup \Omega_{s,2}, \\ 0 & \text{else,} \end{cases}$$

$$f_2(t,x) = \begin{cases} \psi(t) & \text{if } x \in \Omega_{s,3}, \\ 0 & \text{else.} \end{cases}$$

with

$$\psi(t) := 1 + sin\left(\frac{3}{2}\pi + \frac{2\pi t}{10}\right),$$

and $\Omega_{s,1} := (25, 27.5) \times (0, 2.5)$, $\Omega_{s,2} := (32.5, 35) \times (5, 7.5)$, $\Omega_{s,3} := (30, 32.5) \times (2.5, 5)$. Thus the first component has sources in $\Omega_{s,1}$ and $\Omega_{s,2}$ and the second component a source in $\Omega_{s,3}$. We apply the reaction model $R^1(u) = (1, 1, -2)^T u_1 u_2$ and no reaction $R^2(u) = (0, 0, 0)^T$ and start with $R_m(u) = R^2(u)$.
The error of the mean solution of u_3 is measured with respect to the functional

$$J(\overline{u}) = \int_{\Omega_d} \overline{u}_3 \, ds,$$

with the subdomain $\Omega_d = (0, 10) \times (5, 10)$. We apply the time dependent flow field

$$\beta := (-10 - 30(1 + sin(3/2\pi + 4\pi t/10)), 10)^T,$$

so that the commutator terms $K(\cdot)(\cdot)$ do not vanish.
The exact value $J(\overline{u})$ was computed on a uniform mesh with approximately 4 million

step	#cells	$\%R_1$	$J(u-u_{hm})$	η_h	η_m	η	I_{eff}
1	4096	0	1.35e-02	0	2.01e-02	2.01e-02	1.49
2	4096	16	7.24e-03	-1.04e-05	9.87e-03	9.86e-03	1.36
3	9856	42	3.36e-03	-4.05e-06	4.88e-03	4.87e-03	1.45
4	9856	80	-6.65e-06	-6.98e-06	7.15e-07	-6.26e-06	0.94
5	28924	84	-1.68e-06	-2.11e-06	7.18e-07	-1.39e-06	0.83
6	77836	89	-7.86e-07	-9.47e-07	3.26e-07	-6.21e-07	0.79
7	186088	92	-3.31e-07	-4.11e-07	1.56e-07	-2.55e-07	0.77
8	461740	95	-1.56e-07	-1.76e-07	7.30e-08	-1.03e-07	0.66

Table 2: Development of estimated mesh and model error and comparison of estimated to real error

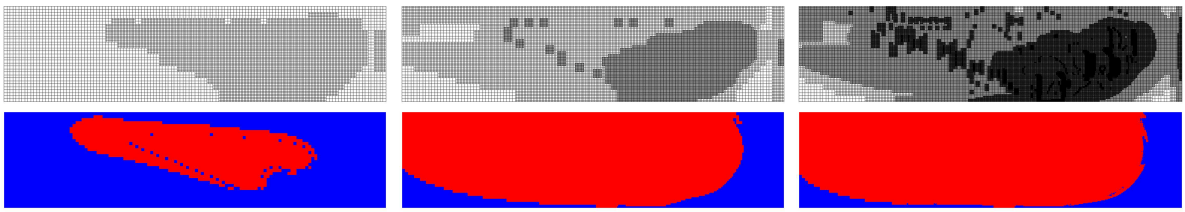

Figure 3: Local refined mesh and allocation of R_1 (red) and R_2 (blue) at steps 3, 5 and 7.

cells using Q_2 finite elements, the timestep $\Delta t = 0.0025$ and using the model $R^1(u)$ in the complete domain to

$$J(\overline{u}) \approx 1.350916847e\text{-}02.$$

In table 2 the results are presented. In the second column the number of cells of the local refined meshes are given. The mesh is not refined after the first step, because the discretization error is estimated to zero. The reason is that we start with $R_m = 0$ in the complete domain $\overline{u}_{hm,3}$ and $z_{h,1}$,$z_{h,2}$ are zero after the first step and from this η_h is zero. That the mesh is not refined after the third step is due to the equilibration of the error parts.

The overall estimation η gives a good approximation to the exact error as the efficiency index I_{eff} varies between 1.49 and 0.66, which shows pretty good behaviour of η. The estimated mesh and model errors decrease simultaneously. This shows that not only the estimation is reliable but rather the localization of the estimated terms lead to very good local estimates. A detailed inspection of the estimated parts compared to the estimation using higher order elements can be found in [7].

In figure 3 the local refined meshes and the model allocations are pictured. The mesh is mainly refined at the sources due to the righthandside f and the model is again adapted at the source, the area of the goal functional and the route of transport of the species. At step 5 the fine model is already used in nearly the complete domain. This is due to the problem setting, because the species are transported through large parts of the domain.

6 Conclusions

We presented a dual weighted a posteriori error estimator based on time-averages. The estimator circumvents the solution of a dual problem backward in time and uses a stationary dual problem instead. We can estimate the discretization and the model error separately and use these localized parts to equilibrate the errors. The numerical examples show a pretty good behaviour for the error estimation as well as for the used localizations.

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