MODELING OF ATMOSPHERIC TRANSPORT OF CHEMICAL SPECIES IN THE POLAR REGIONS

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ABSTRACT

This work is concerned with the reconstruction of unknown atmospheric distributions of species' concentrations and the simultaneous identification of unknown physical parameters. The physical and chemical processes are represented by a simplified chemical transport model. The second focus of the contribution lies on the development and the application of the adaptive techniques to the resulting inverse problem. The underlying theoretical framework is the Dual Weighted Residual (DWR) method for goal-oriented mesh optimization.

Index Terms— Atmospheric modeling, inverse problems, goal-oriented adaptivity, mesh optimization.

Introduction

In this contribution, we showcase the methods stemming from optimal control theory for modeling the transport of chemical species in the Earth's atmosphere by remote sensing techniques such as satellite imaging. The goal of the presented work is the reconstruction of three-dimensional time-dependent concentration fields of chemical constituents in the Earth's atmosphere using indirect measurements such as satellite-based observations. For the latter case, the observations are generally given in form of vertical column densities (VCD).

In the last years, significant effort has been spent on refining models to appropriately describe processes affecting the atmospheric constituent transport. The "general" chemical transport model is given by a system of weakly coupled parabolic equations. The coupling between the equations usually occur due to the chemical transformations, affecting the species' concentrations. The use of such models implies that the chemical mechanisms are precisely known. However, there are many situations in which these transformations cannot be modeled properly since the chemical mechanism is only poorly understood. Furthermore, depending on the form of the given measurements and the unknown parameters, the use of such a general model could be not appropriate. To address this issue, we propose a simplified model which allows to reconstruct the constituent concentrations together with unknown sources and sinks, including chemical transformations. However, other parameters can also be the goal of the computations. E.g. in the event that there are many candidates for modeling the chemical processes of a species, the reconstructed source/sink terms could also serve as a guideline for choosing the "right" mechanism.

The resulting problems are solved using the Galerkin finite element method. On uniformly refined meshes this method leads to the same algebraic systems as the discretization using finite differences. However, the Galerkin discretization offers the possibility for the systematic a priori and a posteriori error analysis. Moreover, the a posteriori error analysis gives the opportunity to optimize the meshes used in the solution process and in the error control.

To this end, we shortly describe the Dual Weighted Residual Method originally proposed in [1] and [2]. The method provides reliable a posteriori error estimators based on local residuals weighted by sensitivity factors computed with respect to a given quantity of interest. This leads to the concept of the goal-oriented adaptivity.

The outline of the contribution is as follows: Section 1 recalls the "general" chemical transport model. Then, we introduce a simplified model and the resulting inverse problem. Section 3 explains shortly the Galerkin discretization and the algorithmic aspects. In Section 4 we introduce the DWR method. We conclude the contribution by considering two numerical examples. The first example validates the proposed model whereas the second demonstrate the application of the presented adaptivity concept to a constructed example. We sum up by making some conclusions also concerning our further goals.

1. PROBLEM FORMULATION

In this section we consider a general model describing the transport of chemical constituents in the atmosphere. To this, end we consider a domain $\Omega \subset \mathbb{R}^3$ which covers a region of the atmosphere. The physical unknowns are the concentrations

of the n species denoted by $u_i, i = 1, \ldots, n$. We further denote by $\mathbf{v}(t,x)$ the wind field and by $D(t,x)$ the turbulent diffusivity tensor. Let $E_i(t,x)$ be the time rate of change of the species concentration due to any external process, $\bar{\beta}_i(t,x)$ the deposition velocity of species i and γ_i the surface sources. The rate of chemical transformations is denoted by f_i.

The evolution of the concentrations is described by the following weakly coupled system of the material balance equations

$$\begin{aligned} &\frac{\partial u_i}{\partial t} = \nabla \cdot (D\,\nabla u_i) - \mathbf{v} \cdot \nabla u_i + f_i + E_i \\ &u_i(t_0, x) = u_i^0(x), \\ &u_i(t,x) = u_i^{in}(t,x) \quad \text{on } \Gamma_I, \\ &D\,\frac{\partial u_i}{\partial \nu} = 0 \quad \text{on } \Gamma_O, \\ &D\,\frac{\partial u_i}{\nu} - \bar{\beta}_i\, u_i = \gamma_i \quad \text{on } \Gamma_G. \end{aligned} \tag{1}$$

The Eddy diffusivity tensor occurs due to the parameterizing the turbulent components of the wind. The parameterizing is done using the K-theory or the Monin-Obukhov length theory. A detailed description of atmospheric dispersion modeling is available e.g. in [3] and [4].

The couplings between the species occur due to the chemical reactions which lead to the nonlinearities in the system. This makes the mathematical analysis more complex. The most common model describing chemical kinetics is the so called Arrhenius model. The use of the Arrhenius model implies that each f_i is continuous and Lipschitz for c_i, $i = 1, \ldots, n$. Moreover, it holds $f_i \geq 0$ whenever $u_i = 0$. The physical meaning of this fact is that the concentration of a specie must be positive in order to be consumed in a reaction. An important property of the use of Arrhenius law is that we have the boundedness of the source term everywhere $|f_i| < \infty$. The boundedness of the concentrations u_i follows then from the continuity of f_i. Using these facts we can show the unique solvability of the chemical transport model. This allows for the definition of the so called solution operator which maps the unknown parameters in the system to the given measurements. The solution process then bases on this operator. The unknown parameters here could e.g. be source/sink terms, boundary conditions etc. For more details on the mathematical analysis of the equation (1) we refer to [5] and [6].

2. SIMPLIFIED INVERSE PROBLEM

In many instances the chemical and physical mechanisms are not precisely known. Thus the corresponding transformation terms f_i and E_i cannot be modeled. Moreover, the lack of the needed measurements poses a further problem which prohibits the use of the coupled systems such as (1). In order to circumvent these difficulties we consider a simplified model describing the evolution of a single species in the atmosphere

$$\begin{aligned} &\frac{\partial u}{\partial t} = \nabla \cdot (D\,\nabla u) - \mathbf{v} \cdot \nabla u + q, \\ &u(t_0, x) = u^0(x), \\ &u(t,x) = u^{in}(t,x) \quad \text{on } \Gamma_I, \\ &D\,\frac{\partial u}{\partial \nu} = 0 \quad \text{on } \Gamma_O, \\ &D\,\frac{\partial u}{\nu} - \bar{\beta}\, u = \gamma \quad \text{on } \Gamma_G. \end{aligned} \tag{2}$$

Here, for the sake of brevity we assume that the source/sink terms represented by q are unknown. In what follows we refer to this model as *state equation* and the variable u as *state*. The unknown source/sink term q will be referred as *control variable*. By introducing the simplified model we transform the system of nonlinear problems in a linear scalar equation which also simplifies the numerical treatment of the problem.

In order to reconstruct the chemical concentrations and unknown parameters we assume we are given some observations $C(u)$, where C stands for the projection operator which maps the state variable u to the space of measurements Z. We denote the corresponding norm by $\|\cdot\|_Z$. The related inverse problem reads: *Find the pair* $\{q, u\}$ *which satisfy the state equation* (2) *given the overspecification* $C(u)$.

Since the problem is ill-posed we regularize it by introducing the Tikhonov functional given by

$$J(q,u) = \|u - C(u)\|_Z + \frac{\alpha}{2}\|q\|_Q. \tag{3}$$

The first term corresponds to the data term and includes given observations. The second term is the regularization term with a small parameter $\alpha \geq 0$. Thus, we aim at the solution of the following optimal control problem:

$$\text{Minimize } J(q,u) \tag{4}$$

subject to the state equation (2).

3. ALGORITHMIC ASPECTS

The inverse problem is discretized using a so called $dG(0)cG(1)$ Galerkin discretization. Thus, for the temporal integration we employ the backward Euler method which corresponds to the discontinuous Galerkin method. A detailed description of the discretization schemes can be found, e.g. in [7]. For the discretization in space we use piecewise trilinear functions. This corresponds to the $\mathcal{Q}_1$ elements. It is possible to discretize the state and in this case we should only ensure that the discrete spaces used for the controls are subset of the space used for the state.

In order to solve the discrete system we first reformulate the optimization problem (4) as an unconstrained problem.

Employing the fact that the state equation admits a unique solution, we introduce the solution operator

$$S : Q \to V, \quad q \mapsto S(q),$$

where Q stands for the space of controls and V for the space of states. By these means we define the reduced cost functional

$$j : Q \to \mathbb{R}_0^+, \quad q \mapsto J(q, S(q)).$$

Thus, the unconstrained optimal control problem is given by

$$\min_{q \in Q} j(q) \tag{5}$$

The solution procedure bases on the first optimality condition

$$j'(q)(\delta q) = 0 \quad \text{for all } \delta q \in Q. \tag{6}$$

We solve the problem (6) by a Newton-type method using the conjugate gradient method in its inner iteration. Since the linear solver fulfills the requirement of matrix-freeness we avoid the assemble process for the Hessian matrix. For the assemble procedure of the product of Hessian with a vector tangent and additional adjoint problems must be solved in each Newton step. This can be accomplished using the so called adjoint approach. For the precise form of these auxiliary problems we refer to [8].

4. MESH OPTIMIZATION

Mesh adaptivity is well developed in the context of finite element discretizations (see, e.g., [9], and [2]). We consider here the goal-oriented adaptivity with the underlying theoretical framework given by the DWR method. Although it is possible to estimate the error with respect to a given quantity of interest (e.g. error in unknown parameters) we consider the cost functional $J(\cdot, \cdot)$ as the error measure. Then if we consider any solution $\{q, u\}$ of (4) and the corresponding finite element solution $\{q_{kh}, u_{kh}\}$ we have for the error the following representation

$$J(q, u) - J(q_{kh}, u_{kh}) \approx \sum_K \rho_K \omega_K + \sum_I \rho_I \omega_I \tag{7}$$

with local spatial and temporal cell residuals ρ_K and ρ_I, and weights ω_K and ω_I. Then, the spatial mesh adaptation is driven by the local error indicators $\eta_K := \rho_K \omega_K$ and the temporal mesh optimization by $\rho_I \omega_I$. Furthermore, the separation of different error contributions allows to define an adaptive algorithm based on a balancing principle. The derivation of the error estimator and its numerical implementation is given in [10] and [11].

5. NUMERICAL EXAMPLES

We discuss two numerical examples that both use the simplified model (2). The first example is concerned with the validation of the proposed model and comparing to the assimilated results done by ECHAM5, see [12]. In the second example we consider the concept of adaptivity as explained in the previous section.

5.1. Example 1

As first numerical example we verify the simplified inverse problem. The aim of the computations is the reconstruction of concentrations of bromine oxide in a region of the Arctics. Here we assume to be given integrated measurements at discrete time points together with distributed observations at a specific time point.

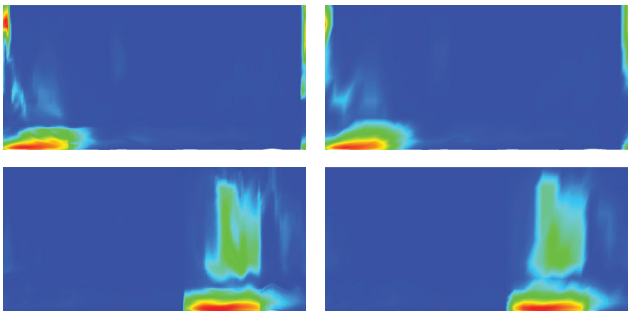

Fig. 1. Assimilated concentrations of bromine oxide at different time points (z-layer) (left column) and the calculated concentrations

For the vertical coordinate we use the terrain following σ vertical coordinate as described in [13]. The qualitative behavior of the solution can be studied in Figure 1. Here, we can see that the calculated concentrations of bromine oxide resemble the reference values very well.

5.2. Example 2

The second example is concerned with the application of the DWR method. In this test we prescribe an exact solution to be a gaussian plume moving in space and reconstruct the unknown concentrations. We use the same overspecification condition as in previous example. We compare the calculations done on the meshes with the finest resolution available and on the dynamically changing meshes which use the finest resolution only locally.

Figure 2 shows a sequence of reconstructed concentrations $u(t, x)$ at discrete time points and the corresponding locally refined meshes.

For the calculation the maximum number of nodes in the spatial grids is $N_{max} = 91\,155$ considered over all time points. For the temporal discretization $M = 66$ time nodes have been used. The achieved tolerance in the cost functional is $J(q, u) - J(q_{kh}, u_{kh}) \approx 10^{-6}$. If we repeat the calculations on the meshes with fine resolution everywhere then we need approximately $1\,000\,000$ nodes on spatial meshes and 240

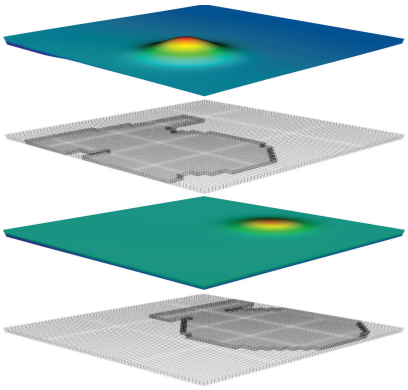

Fig. 2. Adaptive calculations with the corresponding optimized meshes

time nodes in order to achieve the same accuracy. Thus, the calculations show that we gain a significant reduction of the model.

Conclusions

In this work we propose a simplified model for the computations of concentrations of chemical species and unknown parameters entering the model in cases where the precise chemical mechanism is unknown or observations of some species involved in chemical mechanism are lacking. The resulting problem has been discretized using the Galerkin finite element method in time and space. To reduce computational costs, we presented a DWR error estimator which separates the different error sources. The numerical examples confirm the validity of the simplified model and show the automatic model reduction by using dynamically changing meshes in time.

The further steps are the application of the concepts of the goal-oriented adaptivity to the atmospheric transport using satellite based observations. A very important issue is the identification of largely perturbed observations, e.g. due to cloudiness. In order to cope with the problem, we want to apply image processing techniques, such as image segmentation (see e.g.[14].

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