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APPROACHES IN WIND FIELD MODELING AND AIR QUALITY MONITORING SYSTEMS

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Abstract: There is an increasing interest in the research of methods for measuring, calculation, prediction and estimation of the level of pollutant in ambient air. Wind velocity is a major actor in atmospheric pollutant dispersion, so, together with experimental techniques, theoretical wind field models, combined with adequate interpolation methods, provide important tools for pollution assessment and air quality prediction. This paper firstly discusses some basic concepts of the variational analysis formalism, as a classic framework for wind field models over complex terrains. The discrete version of the variational wind field model in Cartesian coordinates can be used for interpolation of measured data and prediction of pollutant transport dynamics. The structure of an extended air quality monitoring system, integrating measurement stations, workstations and wind field model-based software applications, dedicated to construction of atmospheric parameters maps, is finally proposed.

INTRODUCTION AND MOTIVATION

Air quality assessment is nowadays a major objective of international community environmental politics [2], driving to an increased interest in investigation of theoretical approaches for modeling 3-D atmospheric velocity fields, on one side, and in developing efficient air quality monitoring systems [1], on the other side. Such complex informatics systems may integrate structured, periodically updated sampled data, resulted from air parameters measurements – for example pollutant concentrations or wind directions in Cartesian coordinates - with simulation wind field models, generating atmospheric maps as tools for pollution estimation and prediction, over given terrains and time intervals.

Accurate atmospheric wind fields' modeling is difficult from mathematical and computational perspective, as well as because of the random nature of atmospheric flow, requiring assurance of *mass consistency of models*. More precisely, the goal is to match the simulation values with the measured meteorological data, without perturbing the measured data. In consequence, the concept behind development of mass consistent wind field models is to minimize the distance among observed wind velocity values and computed values [7], thus driving to a *variational approach*.

There are several wind field computation modeling approaches presented in the literature [5], [6], [7], and all of them incorporate variational principles. At a first stage of the model calculation, the studied volume is discretized into a set of rectangular boxes, each one usually subdivided into rectangular grids. Then observed wind data are interpolated to all grid points of a reference level, and extrapolated to higher level surfaces, using a power law. At a second stage of computation, the interpolated data are adjusted using a variational method [4].

The paper is structured as follows. Firstly some basic concepts of variational analysis formalism, necessary to develop mass-consistent wind field models, are reviewed in brief and the equations of the basic wind field model are introduced. Then the computational version of the model is presented, together with the interpolation scheme for observed data. Finally, the structure of an air quality monitoring system is proposed and extensions for incorporating wind field models simulation software are discussed, for improvement of atmospheric maps generation.

PRELIMINARIES - VARIATIONAL ANALYSIS CONCEPTS

Given a real function $f : A \to \mathbf{R}$, with $A \subset \mathbf{R}^n$ an open set, $a \in A$ is a *local extremum* if $\exists r > 0$ such that $B(a,r) = \{x \in A : \|x - a\| < r\} \subset A$ and $f(x) - f(a)$ has a constant signum, $\forall x \in B(a,r)$. In brief, the *calculus of variations* states that integrals of the form $J(f(x)) = \int L(x, f(x), f_x(x))dx$, with $f_x = df / dx$ and L having continuous second partial derivatives have a stationary value (hence an extremum) only if the Euler-Lagrange differential equation

$$\frac{\partial L}{\partial f} - \frac{d}{dx}\frac{\partial L}{\partial f_x} = 0 \tag{1}$$

is satisfied.

In the case of *vector valued functions with multiple independent variables*, consider the hiperrectangular box $\Omega = \prod_{i=1}^{n}[a,b] \subset \mathbf{R}^n$, the space of functions with continuous first derivatives denoted $E = C_\Omega^1$ and let $f \in E$, such that $\boldsymbol{f} : \Omega \to \mathbf{R}^m$, $\boldsymbol{x} \mapsto \boldsymbol{f}(\boldsymbol{x}) = (f_1(\boldsymbol{x}), \ldots, f_m(\boldsymbol{x}))'$ with $\boldsymbol{x} = (x_1, \ldots, x_n)'$, $a \le x_i \le b$, $i = 1:n$, has continuous first partial derivatives $f_{kx_i} \overset{not}{=} \partial f_k / \partial x_i$, $i = 1:n$, $k = 1:m$; denote $f_{kx} = [f_{kx_1}, \ldots, f_{kx_n}]'$, $k = 1:m$. If the function $f \in E$ is an extremum for the integral map

$$J(\boldsymbol{f}) = \int_\Omega L(\boldsymbol{x}, \boldsymbol{f}(\boldsymbol{x}), \boldsymbol{f}_x(\boldsymbol{x}))d\Omega, \tag{2}$$

with L having continuous second partial derivatives, then f satisfies the set of m Euler - Lagrange equations [3]

$$\frac{\partial L}{\partial f_k} - \sum_{i=1}^{n}\frac{d}{dx_i}\cdot\frac{\partial L}{\partial f_{kx_i}} = 0,\ k = 1:m. \tag{3}$$

BASIC WIND FIELD MODEL

The theoretical background for the mass-consistent wind field model was early introduced in the works of Sasaki [4]. The idea is to define an integral function whose extremal solution minimizes the variance of the difference between the observed and the analyzed variable values, subject to given constraints. Consider *x*, *y* and *z* the three Cartesian coordinates and denote $\boldsymbol{V} = (u, v, w)'$, $\boldsymbol{V}^0 = (u^0, v^0, w^0)'$ the estimated and observed wind velocity, respectively. Using the Lagrange multipliers approach, the considered cost integral to be minimized is

$$J(\boldsymbol{V},\lambda)=\int_\Omega\left[\alpha_1^2(u-u^0)^2+\alpha_1^2(v-v^0)^2+\alpha_2^2(w-w^0)^2+\lambda\left(\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}+\frac{\partial w}{\partial z}\right)\right]dxdydz\,, \qquad (4)$$

where $\boldsymbol{V}(x,y,z)=(u,v,w)'$ is the wind field, α_i, with $\alpha_i^2=0.5\sigma_i^{-2}$, $i=1,2$, are Gauss precision moduli, σ_i are values of observation and/or deviations of the observed field from the desired adjusted field and $\lambda(x,y,z)$ is the Lagrange multiplier. Usually $w^0=0$ and $\lambda(x,y,z)$ signifies the velocity potential of the adjustment when $\alpha_1=\alpha_2=1$ [6]. The condition for stationary value of *J*, $\delta J=0$, for all four independent variables δx, δy, δz, $\delta\lambda$ drives to the Euler-Lagrange equations

$$2\alpha_1^2(u-u^0)=\frac{\partial\lambda}{\partial x},\ 2\alpha_1^2(v-v^0)=\frac{\partial\lambda}{\partial y},\ 2\alpha_2^2(w-w^0)=\frac{\partial\lambda}{\partial z},\ \frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}+\frac{\partial w}{\partial z}=0\,, \qquad (5)$$

subject to the boundary conditions $\lambda(u-u^0)=\lambda(v-v^0)=\lambda(w-w^0)$. The boundary condition $\lambda = 0$ is appropriate for open or "flow-through" boundaries, while for closed or "no-flow through" boundaries the normal derivatives of λ are set to zero, implying that no transport of mass across the boundary takes place. By differentiating the first three equations in (8) and substituting the results into the fourth, it results the Poisson equation for λ

$$\frac{\partial^2\lambda}{\partial x^2}+\frac{\partial^2\lambda}{\partial y^2}+\frac{\partial^2\lambda}{\partial z^2}=-2\alpha_1^2\left(\frac{\partial u^0}{\partial x}+\frac{\partial v^0}{\partial y}+\frac{\partial w^0}{\partial z}\right). \qquad (6)$$

Equation (6) is solved iteratively for λ with above mentioned boundary conditions and the adjusted velocity field is calculated using the first three equations in (5).

DISCRETE WINDFIELD MODEL AND INTERPOLATION SCHEME

The volume of interest Ω for the cost integral (4) is a rectangular box set on the earth's surface, with dimensions depending on the particular application. Within the box set, the volume is divided into a rectangular grid with intervals Δx, Δy, Δz, in the *x, y, z* directions, respectively (Fig.1). In the sequel, the indexes *i, j, k* denote grid positions in the *x, y, z* coordinates respectively.

Typically, the observed data consists of several horizontal wind speed and direction measurements near the earth's surface and since measurements of the vertical velocity component are rarely available, they are adjusted to a constant height Δz above the surface using a power law

$$u=u_0\left(z/z_0\right)^p. \qquad (7)$$

The exponent *p* is determined by atmospheric stability conditions or from a least-squares fit to multiple-level observed data [5].

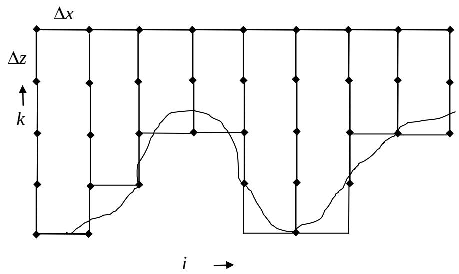

Figure 1

Grid structure for topography specification in two dimensions (adapted from [5]).

At every grid point *within the boundaries*, the Poisson equation (6) is approximated by a finite difference form

$$\frac{\lambda_{i+1jk}-2\lambda_{ijk}+\lambda_{i-1jk}}{(\Delta x)^2}+\frac{\lambda_{ij+1k}-2\lambda_{ijk}+\lambda_{ij-1k}}{(\Delta y)^2}+\left(\frac{\alpha_1}{\alpha_2}\right)^2\left[\frac{\lambda_{ijk+1}-2\lambda_{ijk}+\lambda_{ijk-1}}{(\Delta z)^2}\right]=-2\alpha_1^2\varepsilon_0 \quad (8)$$

where the divergence ε_0 of the interpolated wind field is given by

$$\varepsilon_0 \equiv \frac{u^0_{i+1jk}-u^0_{i-1jk}}{2\Delta x}+\frac{v^0_{ij+1k}-v^0_{ij-1k}}{2\Delta y}+\frac{w^0_{ijk+1}-w^0_{ijk-1}}{2\Delta z}. \quad (9)$$

In [5], an *irregular point* is defined as an interpolated grid point whose difference pattern has at least one boundary point and, in this case, the normal first derivative of λ at the boundary is approximated by a three-point forward or backward first difference, with *n* the normal direction,

$$\left.\frac{\partial\lambda}{\partial n}\right|_{l+1}=\frac{3\lambda_{l+1}-4\lambda_l+\lambda_{l+1}}{2\Delta n},\quad \left.\frac{\partial\lambda}{\partial n}\right|_{l-1}=\frac{-3\lambda_{l-1}+4\lambda_l-\lambda_{l+1}}{2\Delta n}, \quad (10)$$

respectively, depending on the index *l* of the boundary point. The normal derivative is set to zero on "no-flow-through" boundaries. If the difference pattern of the interpolated point does not include a boundary point, then it is called a *regular interior point*.

The entire system consisting of a difference equation (8) written for each interior grid point is solved iteratively and the solution is considered *convergent* when the relative change of every element λ_{ijk} is less than a prescribed value. Details concerning the numerical techniques are given in the literature.

Finally, with the resulted discrete values of λ, the *adjusted wind field values* are computed using the discrete version of the first three Euler-Lagrange equations in (5), respectively

$$u_{ijk}=\frac{1}{4}\left(u^0_{i+1jk}+2u^0_{ijk}+u^0_{i-1jk}\right)+\frac{1}{2\alpha_1^2}\left(\frac{\lambda_{i+1jk}-\lambda_{i-1jk}}{2\Delta x}\right), \quad (10)$$

$$v_{ijk}=\frac{1}{4}\left(v^0_{ij+1k}+2v^0_{ijk}+v^0_{ij-1k}\right)+\frac{1}{2\alpha_1^2}\left(\frac{\lambda_{ij+1k}-\lambda_{ij-1k}}{2\Delta y}\right), \quad (11)$$

$$w_{ijk}=\frac{1}{4}\left(w^0_{ijk+1}+2w^0_{ijk}+w^0_{ijk-1}\right)+\frac{1}{2\alpha_2^2}\left(\frac{\lambda_{ijk+1}-\lambda_{ijk-1}}{2\Delta z}\right). \quad (12)$$

The values of λ on the boundaries are computed with (10). The appropriateness of the final wind field depends on the specification of the parameters α_1 and α_2, in the integral form (4), which are chosen based on empirical considerations.

STRUCTURE OF AN AIR QUALITY MONITORING SYSTEM

The proposed air quality monitoring system (Fig. 2) comprises several fix or mobile stations, placed at the field level, destined to capture, with specific sensors and predefined frequency per hour, the values of air parameters of interest – such as concentrations of carbon monoxide, ozone, wind velocity, pressure, radiation, relative humidity, among others. Every hour, these stations also compute and transmit the average of the collected sampled data. So, for simplicity, the measurements are performed on line, but not in real time. The data are transmitted through wireless connection to a server, which has stored also the table of geographical coordinates for each measurement station. For each air parameter there are admissible values and the monitoring software application generates, according to a schedule or upon request and for desired time intervals, graphical representations of parameter evolutions, with eventual marked overflow limits.

The software system can be extended to incorporate also simulation programs based on discrete mass-consistent wind field models previously described and adjusted with the data collected by the measurements stations. The goal of such simulation programs is generation of atmospheric maps, thus providing an improved forecast of the evolution of specified air parameters and of their potential undesired limits overflow. For example, depending on the wind direction, one can predict if air pollutant agents – like carbon monoxide – may increase their concentrations, in next hours and in populated areas, above admitted limits.

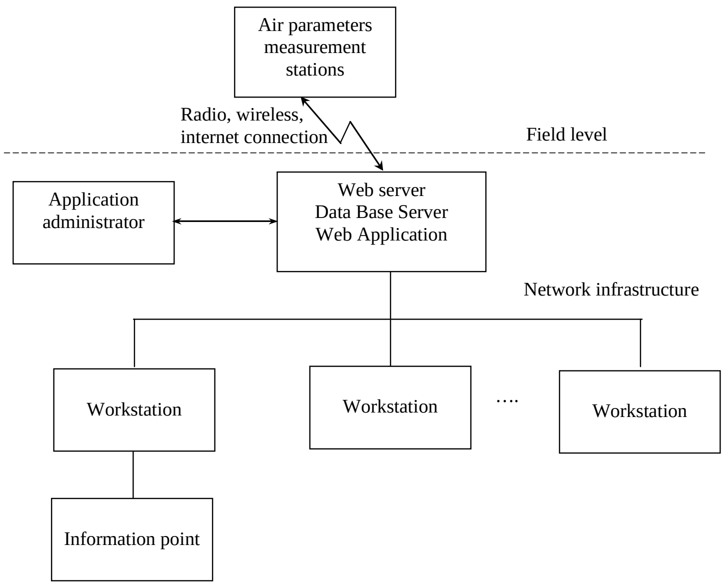

Figure 2
Air quality monitoring system with data base software, field level (measurement stations), wireless connection and network infrastructure.

CONCLUSIONS

The effort to monitor and predict air pollutant transport requires specific measuring infrastructure destined to collect sampled data over given time intervals, and to store the sampled data into data bases, on one side. Because the wind is a major actor in pollutant transport, wind field modeling is subject of intense research. The mass-consistency feature drives to variational modeling approaches, classic in the literature and which have as goal to minimize the variance of the difference between the observed and the analyzed variable values. Finally, a set of Euler-Lagrange equations is obtained for the wind velocity in Cartesian coordinates.

The finite difference version of these equations is the basis for complex simulation programs, in which measured sampled data in given grid points are extrapolated/interpolated with special numerical techniques. In experiments reported in the literature, the variational approach for mass-consistent wind field modeling provides nondivergent values of wind velocity; for example, for complex terrains in the USA, an experiment was performed taking approximately 30000 grid points (MATHEW, [5]), with simulation grid sizes $25 \times 33 \times 28$, $\Delta x = \Delta y = 4.3\text{km}$, $\Delta z = 50\text{m}$, σ_1 and σ_2 values equal to 1 and 0.01ms $^{-1}$ respectively, and a surface layer depth equal to about 100m.

An important future research direction is to adapt general discrete models to particular complex terrains of interest and to build corresponding simulation software which, in conjunction with air monitoring systems, makes possible generation of more accurate atmospheric maps for air pollutant transport forecast.

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