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### MATHEMATICAL MODELLING OF SOCIO-ECONOMIC PROCESSES AND SYSTEMS

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Mixed Variational Properties for Some Fourth-Order Beam Problems

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Abstract: In this paper we study eigenvalue problems for fourth-order ordinary differential equations. These boundary problems usually describe the bending vibrations of a homogeneous beam. Our aim here is to present mixed variational forms depending on a wide class of boundary conditions. In particular, we show when the symmetry in variational formulations is available. This property ensures real spectrum of the corresponding problem. The effect of the theoretical results is illustrated by some realistic examples.

Keywords: EIGENVALUE, FOURTH-ORDER PROBLEM, MIXED FORMULATION, BILINEAR FORM

2010 Mathematical Subject Classification: 65N25, 65N30

1. Introduction

We consider the eigenvalue problem

\[ y''''(x) - (q(x)y'(x))^2 = \lambda r(x)y(x), \quad 0 < x < l, \quad (1) \]

subject to some boundary conditions. Here, \( \lambda \) is a spectral parameter; \( q(x) \) and \( r(x) \) are real-valued positive and continuous functions.

Problem (1) arises in the dynamical boundary-value problem describing free bending vibrations of a homogeneous beam (see, e.g. [1]).

In order to apply the various Galerkin type numerical methods, we have to present the two-point problem (1) in a weak form, when taking into account the boundary conditions. The problems of the type under consideration are appropriate to be presented in a mixed form [2,3] for purpose to be solved numerically by means of mixed numerical methods. An advantage of the mixed variational method is that, along with the unknown function (the displacement), one find an approximation also of its second derivative [2].

Let \( H^m(0,l) \) be the usual Sobolev space for a positive integer \( m \).

Let for \( z(x) \in H^2{[0,l]} \) from (1) we easily get the system:

\[
\begin{align*}
- y'' &= \xi \\
- z'' - (qy') &= \lambda r y.
\end{align*}
\]

(2)

2. Main Result

The principal purpose is to find from (2) a mixed variational formulation according to the boundary conditions and similarly to prove under which type of boundary conditions the resulting mixed mathematical model is symmetric.

Let us introduce the test functions \( y_j(x) \in H^1(0,l) \) and \( z_j(x) \in H^1(0,l) \). Multiplying the first equation from (2) by \( z_j \) and the second by \( y_j \) and integrating on the interval \( [0,l] \), we obtain:

\[ - \int_0^l y'' z_j \, dx = \int_0^l z_j \, dx \]

\[ - \int_0^l \left[ z'' - (qy') \right] y_j \, dx = \lambda \int_0^l r y y_j \, dx, \]

which yields

\[
- \int_0^l y' z_j' \, dx + \int_0^l z_j \, dx = \int_0^l z_j \, dx
\]

\[
- \left[ z'' - (qy') \right] y_j + \int_0^l \left[ z' y_j + qy' y_j' \right] \, dx = \lambda \int_0^l r y y_j \, dx.
\]

(3)

We denote by \( \xi \) any of the endpoints, i.e. \( \xi = 0;l \). Taking into account the boundary conditions, the products \( y' z_j \) and \( \left[ z'' - (qy') \right] y_j \) should be present at the endpoints as symmetric expressions with respect to the pairs of functions \( z_j; y \) and \( z_j; y_j \) and thus the problem under consideration would have symmetric mixed formulation.

(A) \( y' z_j \) is a symmetric expression at the endpoint \( \xi = 0;l \) when the boundary conditions at \( \xi = 0;l \) are of the type:

- \( (a_1) \quad y'(\xi) = 0; \)
- \( (a_2) \quad y''(\xi) = 0. \)

As \( - y'' = \xi \), the boundary condition of (2) is \( z(\xi) = 0 \). This would be an essential condition for the system (2), hence the function \( z_j \) would also satisfy this condition for (3);

- \( (a_3) \quad k_j y''(\xi) + y''(\xi) = 0, \) with \( k_j \neq 0. \)

This boundary condition is of type \( y'(\xi) - k_j z(\xi) = 0 \) for the system (2).

Thus at the point \( \xi = 0;l \) we have either \( y'(\xi)z_j(\xi) = 0 \) or \( y'(\xi)z_j(\xi) = k_j z(\xi)z_j(\xi) \), where \( k_j \neq 0. \) That means:
(B) \[ [z' - (q(y')^2)]y_{\xi} \] represents a symmetric expression at the endpoints, if the boundary conditions at \( \xi = 0; l \) are of the type:

- \((b_1)\) \( y(\xi) = 0 \).

This is an essential boundary condition, consequently the function \( y_{\xi} \) would satisfy it;

- \((b_2)\) \( y''(\xi) - q(\xi)y'(\xi) = 0 \), which for the problem (2) is transformed to:

\[
[z''(\xi) - q(\xi)y'(\xi)]y_{\xi}(\xi) = 0;
\]

- \((b_3)\) \( y'''(\xi) - q(\xi)y'(\xi) = k_2 y(\xi) + \lambda k_3 y(\xi) \), with \((k_2, k_3) \neq (0, 0)\).

For the problem (2) this equality takes the form:

\[
z''(\xi) - q(\xi)y'(\xi) = k_2 y(\xi) + \lambda k_3 y(\xi).
\]

Hence, it is clear that if at the endpoint \( \xi = 0; l \) there is a boundary condition of type \((b_1)\) - \((b_3)\), then either

\[
[z'(\xi) - q(\xi)y'(\xi)]y_{\xi}(\xi) = 0
\]

or

\[
[z'(\xi) - q(\xi)y'(\xi)]y_{\xi}(\xi) = -(k_2 + \lambda k_3)y(\xi)y_{\xi}(\xi),
\]

where \((k_2, k_3) \neq (0, 0)\).

That means:

\[
-y'z_{\xi}(0) = k_{1,0}z(0)z_{\xi}(0) - k_{1,1}z(l)z_{\xi}(l), \quad (4)
\]

where the constants \( k_{1,0} \) and \( k_{1,1} \) could be equal to zero.

Theorem 1. The mixed problem (2) has symmetric variational formulation if at any endpoint the boundary conditions are of the type \((a_i)(b_j), i, j = 1, 2, 3\).

Let us introduce the following symmetrical bilinear forms:

\[
a(u, v) = \int_0^l u'v'dx; \quad b(u, v) = \int_0^l uvdx;
\]

\[
a_l(u, v) = \int_0^l qu'v'dx; \quad b_l(u, v) = \int_0^l uvdx;
\]

\[
c(u, v) = k_{1,0}u(0)v(0) - k_{1,1}u(l)v(l);
\]

\[
c_l(u, v) = k_{2,0}u(0)v(0) - k_{2,1}u(l)v(l);
\]

\[
c_2(u, v) = k_{3,0}u(0)v(0) - k_{3,1}u(l)v(l).
\]

From (6), it is easy to present the variational formulation in symmetric equation

\[
y''(x) - q(x)y'(x) = \lambda x(x) + c_3(x, y, y')
\]

Obviously, the last presentation is symmetric with respect to the couples of functions \((z, y)\) and \((z_{\xi}, y_{\xi})\).

3 Application to Some Actual Problems

In this section we consider various tasks illustrating the result of Theorem 1. Some of them contain the spectral parameter in the boundary conditions (see, e.g. [4, 8-13]).

**Problem 1.** First we consider a mathematical model describing free bending vibrations of a homogeneous beam of constant rigidity. Both ends are fixed elastically and on these ends the servocontrol forces are in acting [6, 7, 8]:

\[
y'(x) - \gamma(x)y'(x) = \lambda r(x)y(x), \quad 0 < x < l,
\]

\[
y''(0) = y''(l) = 0,
\]

\[
y'''(0) - q(0)y'(0) = 0,
\]

\[
y'''(l) - q(l)y'(l) = 0.
\]

Here \( q(x) \) is a positive and absolutely continuous function on \([0, l]\), \( a \) and \( c \) are real constants such that \( a > 0, c < 0 \).

The first two boundary conditions are of type \((a_2)\).

Comparing with the adopted notations we have:

\[
l = l; \quad r(x) = l; \quad k_{1,2} = 0, i = 1, 2, \xi = 0; 1,
\]

\[
k_{3,0} = a, \quad k_{3,1} = c.
\]
Also \( c_f(u,v) = c_2(u,v) = 0 \) and on account of the sign of \( a \) and \( c \) the bilinear form \( c_f(u,v) = a(u(0)\psi(0) - c(u(1))\psi(1)) \) is positive.

It should be noted that the last two boundary conditions, containing the spectral parameter \( \lambda \), are related to the type \((b_3)\).

In this way, the Problem 1 assumes symmetric mixed variational formulation.

**Problem 2.** Let us consider the bending vibrations of a homogeneous rod, in cross-section of which the longitudinal force acts. The left end is fixed rigidly and the right one is fixed elastically and on the some endpoints the inertial mass is concentrated \([6, 9]\):

\[
y''(x) - (q(x) y'(x))^2 = \lambda r(x) y(x), \quad 0 < x < l,
\]

\[
y(0) = y'(0) = 0,
\]

\[
y''(1) - b_1 y'(1) - a_1 \lambda y(1) = 0, \quad y''(1) - a_2 \lambda y(1) = 0.
\]

Here \( q(x) \) is a positive and absolutely continuous function in \([0,1]\), \( a_1, a_2 \) and \( b_1 \) are real constants.

For this problem we have: \( l = 1; \ r(x) = 1 \).

The boundary conditions at the left endpoint are of type \((b_1)\) and \((a_1)\), respectively and furthermore

\[
k_{1,0} = k_{2,0} = k_{3,0} = 0.
\]

The last boundary condition is of type \((b_3)\) with

\[
k_{2,1} = 0, \ k_{3,1} = a_2.
\]

Such being the case, Problem 2 would have symmetric mixed variational formulation if the third boundary condition is of type \((a_1)\), \( i = 1,2,3 \). This is fulfilled in case when \( a_1 = 0 \) only, at that the condition is of type \((a_2)\) if \( b_1 = 0 \) and of type \((a_3)\) otherwise.

**Problem 3.** Consider the spectral problem \([10]\):

\[
y''(x) - (q(x) y'(x))^2 = \lambda r(x) y(x), \quad 0 < x < l, \quad 0 < x < 1,
\]

\[
y''(0) \sin \alpha - y'(0) \cos \alpha = 0,
\]

\[
(y''(0) - q(0) y'(0)) \sin \beta + y(0) \cos \beta = 0,
\]

\[
y''(1) \sin \gamma + y'(1) \cos \gamma = 0,
\]

\[
(y''(1) - q(1) y'(1))(c \lambda + d) - (a \lambda + b) y(1) = 0,
\]

where \( q(x) \) is a positive and absolutely continuous function on the interval \([0,1]\) and \( \alpha, \beta, \gamma, a, b, c, d \) are real constants such that \( \alpha, \beta, \gamma \in \left[0, \frac{\pi}{2}\right] \).

First, let us note that \( r(x) \) is assumed to be constant (equal to 1).

Evidently the first boundary condition is of type:

\[
(a_1) \text{ when } \alpha = 0, \text{ and thus } k_{1,0} = 0;
\]

\[
(a_2) \text{ when } \alpha = \frac{\pi}{2}, \text{ and again } k_{1,0} = 0;
\]

\[
(a_3) \text{ when } \alpha \in \left(0, \frac{\pi}{2}\right) \text{ and thus } k_{1,0} = \tan \alpha.
\]

Similarly, the third boundary condition is of type:

\[
(a_1) \text{ when } \gamma = 0 \text{ and thus } k_{1,1} = 0;
\]

\[
(a_2) \text{ when } \gamma = \frac{\pi}{2} \text{ and again } k_{1,1} = 0;
\]

\[
(a_3) \text{ when } \gamma \in \left(0, \frac{\pi}{2}\right) \text{ and thus } k_{1,1} = -\tan \gamma.
\]

For the second boundary condition we establish that it is of type:

\[
(b_1) \text{ when } \beta = 0, \text{ then } k_{2,0} = k_{3,0} = 0;
\]

\[
(b_2) \text{ when } \beta = \frac{\pi}{2} \text{ and again } k_{2,0} = k_{3,0} = 0;
\]

\[
(b_3) \text{ when } \beta \in \left(0, \frac{\pi}{2}\right), \text{ consequently } k_{2,0} = -\cot \beta, \ k_{3,0} = 0.
\]

According to Theorem 1, Problem 3 assumes symmetric mixed variational formulation if the last boundary condition is of type \((b_1), j = 1,2,3 \). The only way of this is \( c = 0 \), which yields that the last boundary condition is of type:

\[
(b_1) \text{ when } a \neq 0, b \neq 0, d \neq 0, \text{ at that } k_{2,1} = \frac{a}{d}, k_{3,1} = q_{\alpha} = \frac{a}{d};
\]

\[
(b_2) \text{ when } a = b = 0, d \neq 0, \text{ thus } k_{2,1} = k_{3,1} = 0;
\]

\[
(b_1) \text{ when } (a,b) \neq (0,0), d = 0 \text{ and } k_{2,1} = k_{3,1} = 0.
\]

As a conclusion, Problem 3 has got a symmetric mixed variational representation in case when \( c = 0 \) only.

**Problem 4.** This problem is derived from a wave equation which describes the vibration of a nonhomogeneous rod or beam clamped at one end (e.g., \([5, 7, 11]\)):

\[
y''(x) - (q(x) y'(x))^2 = \lambda r(x) y(x), \quad 0 < x < 1,
\]

\[
y(0) = y'(0) = 0,
\]

\[
y''(1) \sin \gamma + y'(1) \cos \gamma = 0,
\]

\[
(y''(1) - q(1) y'(1))(c \lambda + d) - (a \lambda + b) y(1) = 0,
\]

where the coefficients \( r(x) \) and \( q(x) \) are assumed to be real-valued and continuous functions, \( r(x) > 0, \gamma \in \left[0, \frac{\pi}{2}\right], \delta \in \left[0, \pi\right] \).

The boundary conditions at the left endpoint are of type \((b_1)\) and \((a_1)\), respectively, so that for Problem 4

\[
k_{1,0} = k_{2,0} = k_{3,0} = 0.
\]
Just like for Problem 3, the third boundary condition is of type: 

\((a_1)\) when \(\gamma = 0\) and thus \(k_{1j} = 0\); 
\(\quad (a_2)\) when \(\gamma = \frac{\pi}{2}\) and again \(k_{1j} = 0\); 
\(\quad (a_3)\) when \(\gamma \in \left(0, \frac{\pi}{2}\right)\) and thus \(k_{1j} = -\tan \gamma\).

In much the same manner, the fourth boundary condition is of type:

\((b_1)\) when \(\delta = 0\) or \(\delta = \pi\), then \(k_{2j} = k_{3j} = 0\); 
\(\quad (b_2)\) when \(\delta = \frac{\pi}{2}\) and again \(k_{2j} = k_{3j} = 0\); 
\(\quad (b_3)\) when \(\delta \in \left(0, \frac{\pi}{2}\right)\) \(\cup \left(\frac{\pi}{2}, \pi\right)\) and in this case \(k_{2j} = \cot \delta\); 
\(\quad k_{3j} = 0\).

Ultimately, in any case Problem 4 have symmetric mixed variational formulation.

**Problem 5.** At last we consider one more problem for which the spectral parameter appears in the boundary conditions [12, 13]:

\[ y^{IV}(x) - \left(q(x)y'(x)\right) = \lambda r(x)y(x), \quad 0 < x < \pi, \]
\[ y(0) = y'\left(0\right) = y''\left(\pi\right) = 0, \]
\[ y'''\left(\pi\right) - q(\pi)y'(\pi) + m\lambda y(\pi) = 0. \]

Here, \(q(x)\) and \(r(x)\) are real-valued functions from the space \(C[0, \pi]\), \(r(x) > 0\), and \(m \in R\) is a physical parameter [13] and \(l = \pi\).

The first three boundary conditions are of type \((b_1)\), \((a_1)\) and \((a_2)\), respectively, so that

\(k_{1j} = k_{2j} = k_{3j} = 0\) and \(k_{1j} = 0\).

The last boundary condition is of type \((b_3)\), and \(k_{2j} = 0\), \(k_{3j} = -m\).

Therefore, \(c_j(u,v) = 0\), \(c_j(u,v) = 0\), \(c_j(u,v) = m u(\pi)(v)\) and in any case Problem 5 have symmetric mixed variational formulation.

**3. Conclusions**

The paper contains a useful result related to the mixed formulation of fourth-order eigenvalue problems. Namely, requirements on the boundary conditions providing symmetrical presentation of the problem are proved. This result is demonstrated for various beam problems.

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MODELING OF THE 3D UNSTEADY MULTISCALE MULTIPHASE FLUID FLOW WITH SHOCKS: NUMERICAL METHODS AND IMPLEMENTATION ALGORITHMS

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Abstract: Numerical simulation is widely applied in the fluid dynamic research. Unsteady multiphase flow with high Mach and Reynolds numbers has high physical and mathematical fidelity and a special approach of its correct modeling is required. In this paper the appropriate numerical methods and special algorithms of implementation are developed for high-performance numerical modeling using the modern computational systems. The results of validation tasks and problems of practical importance are presented.

Keywords: COMPUTATIONAL FLUID DYNAMICS, GPU COMPUTING, LRnLA ALGORITHMS, SHOCK WAVES, DROPLET BREAKUP

Introduction

Since the second half of the twentieth century, high-performance computer technologies have been widely used to solve problems in computational fluid dynamics [1]. At the moment, computational fluid dynamics (CFD) is one of the main methods for solving engineering problems of designing parts, devices and other objects with the required fluid dynamic properties.

For high-precision modeling “from the first principles,” meaning without specifying and narrowing the mathematical formulation of the problem, it may be necessary (but not sufficient) to use detailed grids and a large number of iterations in the calculation. Let some estimates be given. The numerical region is characterized by some size range, which is usually determined by the characteristic spatial scale for the simulated process. The number of discrete elements along one axis is usually has to be taken in the range of 10^5 - 10^6 or more. Consequently, the number of iterations in time is determined by the characteristic time scale for the considered process, taking into account the restrictions on the time step, for example, the Courant condition. The number of time steps can be up to 10^6 or more for actual tasks. Thus, the number of operations for calculating a single cell of a numerical scheme is 10^7-10^8 for one numerical experiment. The operation of calculation of a single cell of a numerical scheme may require dozens of elementary operations of addition-multiplication for the simplest explicit schemes up to tens of thousands, depending on the complexity of the numerical scheme.

To solve problems of this scale [2], it is necessary to use modern computer hardware with a complex hierarchical structure of computing units and memory system. From set of modern computing systems the ones equipped with graphic accelerators are outstanding due to their high performance at a relatively low cost [3; 4]. For the effective use of such computing systems it is necessary to develop and use suitable calculation algorithms that take into account their features. So, effective implementation must be adapted to the hierarchical structure from the CPU memory to the registers CPU/GPU without creating bottlenecks that slow down the speed of calculation [5]. In addition, the problem of efficient parallelization of the algorithm, taking into account the massive parallelism of the GPU, remains relevant. A separate issue remains the requirement of saving memory when building an implementation algorithm, with the help of which it is possible to simulate a domain with as large as possible number of cells within the available memory of the given computer. Due to the fact that the video card’s memory is less than the RAM of the CPU, the video card’s memory is often not enough to store the entire computing area, which makes the problem to exchange between the GPU memory and the CPU one. To build an effective implementation, it is advisable to take into account these issues.

The content of the paper is the following. In the next section the mathematical and numerical model is set. Then the proper implementation algorithm is described. Third section is devoted to the validation of the program based upon the algorithm and numerical scheme. In the following section the simulation results of some real tasks of practical importance are considered. In the conclusion we summarize the research.

I. Governing equations and numerical scheme

1.1 Equations of gas dynamics

The system of Navier-Stokes equations describing the dynamics of a viscous compressible fluid or gas in three-dimensional space [6], is represented as

\[
\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x_i} = 0,
\]

where \( U = (\rho, \rho u_i, E) \) are the gas variables, \( F(U) = \left[ \rho u_i, \rho u_i u_j + P, u_i E + P, u_i \right] \) are fluxes, pressure tensor \( P_{ij} = \rho \delta_{ij} - \mu \frac{\partial u_i}{\partial x_j} + \frac{\partial u_i}{\partial x_j} (\zeta - \frac{2}{3} \mu) \delta_{ij} \) taking the viscous forces into the account. The system is extended by the equation of state \( p(\rho, \epsilon) \). More complex equations of state are considered for the fluid mixtures [7].

We rewrite the fluxes to separate pure convective (Euler) and viscous (Navier-Stokes) parts as follows:

\[
\frac{\partial U}{\partial t} + \frac{\partial F^E}{\partial x_i} + \frac{\partial F^{NS}}{\partial x_i} = 0,
\]

where \( F^E = [\rho \ u_i, \rho u_i u_j + p \delta_{ij}, u_i (E + p)] \) and

\[
F^{NS} = [0, -\mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) (\zeta - \frac{2}{3} \mu) \delta_{ij}] - \mu \left( \frac{\partial u_i}{\partial x_j} \right) \delta_{ij} \left( \frac{\partial u_j}{\partial x_i} \right) + \frac{\partial u_i}{\partial x_j} (\zeta - \frac{2}{3} \mu) u_i - \kappa \frac{\partial E}{\partial x_i}.
\]

1.2 Runge-Kutta discontinuous Galerkin method

Suppose we construct a numerical solution of the fluid dynamics system in the domain \( G \subset \mathbb{R}^3 \), \( t > 0 \) with boundary \( \partial G \) with some given initial conditions for \( t = 0 \) and boundary conditions. We introduce the discretization of the space \( G \) using a grid of finite volumes.

In each cell \( L \), we introduce a set of basis functions \( (\phi^p) \), and the solution will be sought as an expansion in this basis for each
component of the desired vector \( U = u_i(t) \phi^i(x) \), while the basis coefficients are functions of time.

In this paper, we use a generalization of this method to approximate dissipative terms in the Navier-Stokes equation, known as the LDG method (local discontinuous Galerkin method [8]). We introduce a set of new variables for spatial derivatives in the flux \( F_i^{NS} \)

\[
W = \frac{\partial u_i}{\partial x_j}, \quad S = \frac{\partial T}{\partial x_i};
\]

and for them we apply the same expansion in the basis.

Obtained expressions are inserted into the main equations and the condition of the orthogonality of the residual to all basis functions is accepted to obtain the system of ODE on the basis coefficients:

\[
\frac{d u_m(t)}{dt} + \int_{\Omega} (F^{EU} + F^{NS}_m) \varphi_m n^i d\Sigma - \iiint_{\Omega} F_i \frac{\partial \varphi_m}{\partial x_i} dV = 0;
\]

\[
w_m(t) = \int_{\Omega} u_i n^i \varphi_m d\Sigma - \iiint_{\Omega} u_i \frac{\partial \varphi_m}{\partial x_i} dV;
\]

\[
s_m(t) = \int_{\Omega} T n^i \varphi_m d\Sigma - \iiint_{\Omega} T \frac{\partial \varphi_m}{\partial x_i} dV;
\]

Calculation of \( \int_{\Omega} F_i^{EU} \varphi_m n^i d\Sigma \) is made using the specified Riemann solver [9].

Numerical solution of the given ODE is performed using the explicit Runge-Kutta method with the limiter [10, 11].

### 2. DiamondTorre implementation algorithm

In the introduction of the paper the necessity of the proper algorithm of implementation for the constructed numerical scheme has been noticed. This paper is considered the DiamondTorre algorithm. Originally developed as an optimal locally-recursive non-locally asynchronous algorithm [12] for explicit numerical schemes with the stencil “cross”, in this paper DiamondTorre algorithm is being developed the RKDG scheme of the method for solving gas dynamics problems. Despite the fact that the stencil of the RKDG method itself is not a “cross”, each of its substage has a substencil “cross” [13].

The calculation of the problem using this algorithm is conveniently thought of as filling the computational area with towers. The essence of each brick of the tower with coordinates \((x_i, y_i, t_k)\) is performing part of the calculation according to a numerical scheme over the entire segment \((x_i, y_i, N_{z}, t_k)\), it can be execution stages of calculation of dissipative members, Runge-Kutta or limiters. We will assume that the coordinates of the tower are the coordinates of its lower left brick in the \(xt\) plane. The parameter \(N_T \geq 1\) determines how many time steps are calculated during the first iteration of the algorithm. In the \(xt\) plane each tower is built bottom up on the \(t\) axis, and for \(x\) in the direction of its slope. At each iteration of the algorithm filling the area in the \(xy\) plane goes from right to left, starting from the right border at \(x\), and on each \(x_i, i \in 0, ..., N_{x} - 1\) towers are built through one along the \(y\) axis, while if \(x = x_i\) the towers were built only on even \(y\), then at \(x = x_{i-1}\) towers are built only on odd \(y\). We use the fact that the substage calculation algorithms have all the pattern of type “cross”, with dependencies on the adjacent six cells.

The development of the fluid solver is made using the CUDA C++ technology. The DiamondTorre algorithm is friendly to CUDA programming tools as the Torres are evaluated by CUDA blocks and each \(z\) component inside the Torre is associated to each CUDA thread. Data copying between GPU and CPU is diminished.

### 3. Validation

Several validation problems are considered: 1D, 2D and 3D.

**Fig. 1.** The performance test of the developed software based on the DiamondTorre algorithm for different GPUs.

The performance tests show very good results. Gained speed is more than \(10^8\) cells per second on top-tier GPU. Full Navier-Stokes solver is considered in the examination. The results of testing on wide range of processors are shown in figure 1.

**Fig. 2.** (a) – the convergence of the solver for the 1D advection test; (b) – the results of density profile for 1D Sod problem.

In figure 2 the results of 1D testing are shown. Fig. 2a describes the convergence order of the RKDG scheme based upon linear basis and 2-stage Runge-Kutta method investigated using the pure advection setting. In the 2b one can see the results of solving the Riemann problem of Sod [9], showing good shock capturing and low dissipation of the scheme.

**Fig. 3.** (a) – 2D supersonic \(M=10\) flow past a wedge, density levels drawn; (b) – density field for the 2D flow past a step obstacle, \(M=3\).

In fig. 3 the widely used two-dimensional test problems of the flow past the wedge (fig. 3a) and the flow past the forward-facing step (fig. 3b). The good agreement with the known data is obtained.

Finally, the test of spherical Sod problem is considered [9]. The initial setting at the 3D Cartesian grid and the simulated density profile is shown in fig. 4.
Validation results show good quality of obtained solutions, allowing the application of the software for the practical problems.

4. Modeling results and discussion

The actual problems that researchers are usually faced with are complex flows of many components/phases and/or complex geometry. Due to the high performance of considered CFD solver, the “brute force” method of using extra-high grid resolution is possible to apply for these types of problems.

The first considered problem is the process of interaction between the shock wave and the heterogeneity. In fig. 5 the result of simulation of M=2 shock interacting with the high-density heterogeneity of complex initial shape (particularly inspired by letters K and L) is shown.

Fig 5. Interaction of a M = 2 shock with a high dense heterogeneity At = 0.9 of complex shape; density gradient field

From the knowledge of bubble-shock interaction problem, one can get that for the case of At > 0 the flow has unstable turbulent pattern [14], as proven by the current simulation.

The second problem concerns the secondary breakup of liquid droplets in the gas flow [15]. The following setup is used: M = 0.3 flow is given at initial time, the spherical droplet of incompressible fluid having surface tension force is put in the flow. The ratio between the kinetic energy of the flow and the Laplace energy of droplet (Atwood number At) describes the behavior of the droplet consistency. Experimental and numerical data shows that there are different regimes of the droplet breakup depending on the At number.

For this numerical experiment the current RKDG code for the gas is combined with the special GPU LBM solver for simulating non-compressible liquid. Gas simulation is much more computationally difficult, so the liquid solution is treated as the boundary condition for the gas at every time step. Simulation is performed using GeForce GTX 1080 GPU during several hours. Grid size is 256×128×128 for each simulation.

We obtain the qualitative agreement with the known pattern of the droplet breakup [15, 16, 17].

5. Conclusion

The main results of the paper are following. In the framework of the work, a numerical scheme for solving Navier-Stokes equations for a three-dimensional Cartesian grid is created. For the scheme, the GPU algorithm implementation of DiamondTorre is developed. A software package using CUDA C++ is developed. Positive results of the program validation for the series 1D, 2D and 3D tests are obtained. Application of solver for solving complex engineering research problems of the interaction of the gas inhomogeneity with a shock and the disintegration of droplets in a gas stream is shown.

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References


APPLICATION OF LAPLACE TRANSFORM IN FINANCE

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Abstract: Laplace’s transformation is an important chapter of Mathematical Analysis. At present it is widely used in various problems of signal theory, physics, mechanics, electro – techniques and economics. Laplace’s transformation is the simplest and most economical method that leads directly to the required resolution of many of the various technical problems that arise when solving them. In this paper we will become acquainted with the basic concepts of operational mathematics and its application in economy. Not many analytic solutions exist for present discounted value problems but by using Laplace transform we can deduce some of the closed form solutions quite easily. There will be shown the connection between the current discounted value in finance and Laplace transformation.

Keywords: LAPLACE TRANSFORM, FINANCE, PRESENT VALUE, CASH FLOW, RATE, PERIOD.

1. Introduction

Before we consider the transformation of Laplace, we analyze the meaning of the integral of a complex function of the real argument.

Let it be \( f(t) \) a complex function of the real \( t \) argument given in the segment \([a, b]\). As it is known, such a function may appear in the form: \( f(t) = u(t) + iv(t) \)

The integral of the function \( f(t) \) in the segment \([a, b]\) with the definition is determined by the equation

\[
\int_{a}^{b} f(t) \, dt = \int_{a}^{b} u(t) \, dt + i \int_{a}^{b} v(t) \, dt
\] (1)

Similarly, the infinite integral of that function is defined in \((0, \infty)\):

\[
\int_{0}^{\infty} f(t) \, dt = \int_{0}^{\infty} u(t) \, dt + i \int_{0}^{\infty} v(t) \, dt
\] (2)

provided that both right-side integrals are convergent.

Since the integral of a complex function of the real variable is defined by the equations (1) or (2) by two common integrals, then all the properties and the integration methods of the latter are true also for the integrals of the complex functions of the real argument.

Below we will be dealing with the integral of the forms (1) and (2). Considering the fact that the purpose of introducing the operational method is mainly the implementation direction of this method, we are not dwelling on the necessary conditions of convergence of such integrals but will be limited to the integral of the functions \( f(t) \) that meets these conditions: [1], [2], [3], [4]

1. The function \( f(t) \) is continuous in \((0, +\infty)\) combined with its derivatives up to any necessary order, with the exception of possibly a finite number of first type of critical points in each finite segment.
2. \( f(t) = 0 \) for \( t < 0 \).
3. The function \( f(t) \) increases in absolute value no sooner than an exponential function. So there are numbers \( M > 0 \) and \( S_{0} > 0 \) such that for each term \( t \) we have: \(|f(t)| < Me^{S_{0}t}\).

The number \( S_{0} \) that enjoys the above quality is called the growth indicator of the function \( f(t) \). In particular when the function \( f(t) \) is limited then it can be consider \( S_{0} = 0 \). The fulfillment of the above conditions ensures the existence of many integrals of the form (2) that we will consider below. We are now going to determine the transformation of Laplace.

Consider the product of the function \( f(t) \) with the real argument \( I \) with the exponential function \( e^{-pt} \) where \( p \) is a complex number \( p = s + i\alpha \)

\[
e^{-pt} \cdot f(t)
\] (3)

Function (3) is again a complex function of the real argument:

\[
e^{-pt} \cdot f(t) = e^{-(s+i\alpha)t} \cdot f(t) = e^{-st} \cdot f(t) \cdot e^{-i\alpha t} = e^{-st} f(t) \cos \alpha t - i e^{-st} f(t) \sin \alpha t
\]

We will now show that when a function \( f(t) \) meets the above conditions, then the integral

\[
\int_{0}^{\infty} e^{-pt} f(t) \, dt = \int_{0}^{\infty} e^{-st} f(t) \cos \alpha t \, dt - i \int_{0}^{\infty} e^{-st} f(t) \sin \alpha t \, dt
\] (4)

converges, even absolutely provided that: \( \text{Re} \ p = s > S_{0} \).

According to the definition for the convergence of the integral (4), the existence of each of the right-side integrals is necessary and sufficient. Let’s analyze the convergence of the first.

\[
\int_{0}^{\infty} e^{-st} f(t) \cos \alpha t \, dt < \int_{0}^{\infty} e^{-st} f(t) \cos \alpha t \, dt < M\int_{0}^{\infty} e^{(s-S_{0})t} \, dt = \frac{M}{s-S_{0}}
\]

Similarly, the second integral on the right side of (4) is evaluated.

The integral (4) converges to the entire complex plot area \( p \) extending to the right of the line \( \text{Re} \ p = S_{0} \). The proving method also follows that only the real part of the number \( p \) determines the convergence of the integral (4).

Integral (4) defines a function of the parameter we mark \( F(p) \), namely:

\[
F(p) = \int_{0}^{\infty} f(t)e^{-pt} \, dt.
\]

The function \( F(p) \), is called the Laplace image of function \( f(t) \). The function \( f(t) \) is called the original function.
As has been stated above, it follows that the fulfillment of the above three conditions is sufficient for the function \( f(t) \) to be original. Below we will call original only the functions that meet those three conditions. This tightening of the class of originals is not very sensible from the practical point of view.

If \( F(p) \), is a reflection of the function \( f(t) \), then it says:

\[
L \{ f(t) \} = F(p) \quad \text{or} \quad F(p) \to f(t)
\]

**Theorem.** If the function \( F(p) \), is an image, then:

\[
F(p) \to 0 \quad \text{when} \quad \text{Re } p = s \to +\infty
\]

Truly, it is known that \(|a + ib| = \sqrt{a^2 + b^2} \leq |a| + |b|

So:

\[
|F(p)| \leq \int_0^\infty e^{-at} f(t) \cos{\omega t} \, dt + \int_0^\infty e^{-at} f(t) \sin{\omega t} \, dt
\]

or

\[
|F(p)| \leq \frac{M}{s - s_0} + \frac{M}{s - s_0} \to 0 \quad \text{for} \quad s \to +\infty
\]

Based on this theorem it can be said that the necessary condition for a given function \( F(p) \), to be an image of a function \( f(t) \), is to complete the reconciliation:

\[
\lim_{\text{Re } p \to +\infty} F(p) = 0
\]

**2. Finding the original when the image is rational**

In the practice of the usage of the operational calculus, we often find it when the function \( F(p) \), is rational. By the end of this paragraph we will deal precisely with the problem of finding the original when the image is rational:

\[
F(p) = \frac{b_0 p^m + b_1 p^{m-1} + \ldots + b_{m-1} p + b_m}{a_0 p^n + a_1 p^{n-1} + \ldots + a_{n-1} p + a_n} = \frac{\phi(p)}{\psi(p)}
\] (5)

We note, first, that the rational fraction \( F(p) \) should be regular because otherwise the condition is not met:

\[
F(p) \to 0 \quad \text{as} \quad |p| \to \infty
\]

which is necessary for the function \( F(p) \), to be an image. So we will have \( m < n \).

In relation to the denominator \( \psi(p) \) of the fraction \( 5 \) we distinguish these cases:

**I. The function \( \psi(p) \) has only simple roots (not repeated).**

We mark the roots of the polynomial \( \psi(p) \) with \( \alpha_1, \alpha_2, \ldots, \alpha_n \). Then it can be written in the form:

\[
\psi(p) = (p - \alpha_1)(p - \alpha_2) \ldots (p - \alpha_n)
\]

while the function \( F(p) \), can be expanded:

\[
\frac{\phi(p)}{\psi(p)} = \frac{A_1}{p - \alpha_1} + \frac{A_2}{p - \alpha_2} + \ldots + \frac{A_n}{p - \alpha_n}
\] (6)

Since for the function \( \frac{A_1}{p - \alpha_1} \), the original is \( A_1 e^{\alpha_1 t} \), then based on the property of linearity and equation \( 6 \) we will have:

\[
\frac{\phi(p)}{\psi(p)} \to A_1 e^{\alpha_1 t} + A_2 e^{\alpha_2 t} + \ldots + A_n e^{\alpha_n t}
\] (7)

To find the coefficients we: multiply the two sides of \( 6 \) with \( p - \alpha_1 \) and using the fact that \( \alpha_1 \) is the root of \( \psi(p) \), i.e., the draw \( 6 \) takes the form:

\[
(p - \alpha_1) \left( \frac{\phi(p)}{\psi(p)} \right) = A_1 + (p - \alpha_1) \left( \frac{A_2}{p - \alpha_2} + \ldots + \frac{A_n}{p - \alpha_n} \right)
\]

Now we get the limit on both sides of this draw for \( p \to \alpha_1 \). It is clear that the right-side borders will be \( A_1 \). So we will have:

\[
A_1 = \lim_{p \to \alpha_1} (p - \alpha_1) \frac{\phi(p)}{\psi(p)} = \lim_{p \to \alpha_1} \frac{\phi(p)}{\psi(p) - \psi(\alpha_1)}
\]

from where \( A_1 = \frac{\phi(\alpha_1)}{\psi'(\alpha_1)} \) (8)

In the role of \( \alpha_1 \) it could be each of the roots \( \alpha_2, \ldots, \alpha_i, \ldots, \alpha_n \), therefore in the general form we will have:

\[
A_i = \frac{\phi(\alpha_i)}{\psi'(\alpha_i)}
\]

II. Among the roots of the denominator \( \psi(p) \) there are such that are repeated.

Let \( \alpha, \beta, \ldots, \lambda \) be the roots of the polynomial \( \psi(p) \), while the numbers \( a, b, \ldots, l \) indicate how many times each of them is rooted. In this case, the polynomial \( \psi(p) \) may appear in the form:

\[
\psi(p) = (p - \alpha)^a (p - \beta)^b \ldots (p - \lambda)^l
\]

As it is known from the expansion of regular rational fractions into elemental fractions, each factor of the form \( (p - \delta)^d \) corresponds to the elemental fraction with denominator

\[
(p - \delta)^d (p - \delta)^{d-1} \ldots (p - \delta)
\]

So the function \( F(p) = \frac{\phi(p)}{\psi(p)} \) in this case will be presented in the form:
\[
\frac{\phi(p)}{\psi(p)} = \frac{A_1}{(p-\alpha)^n} + \frac{A_2}{(p-\alpha)^{n-1}} + \ldots + \frac{A_b}{p-\alpha}
\]
\[
\frac{B_1}{(p-\beta)^a} + \frac{B_2}{(p-\beta)^{a-1}} + \ldots + \frac{B_b}{p-\beta}
\]
\[
\frac{L_1}{(p-\lambda)^c} + \frac{L_2}{(p-\lambda)^{c-1}} + \ldots + \frac{L_c}{p-\lambda}
\]

Let us now see how the decomposition coefficients that are marked with the same letter are counted, e.g. coefficients \(B\). Similarly, coefficients that are written in other letters are calculated. Multiply both sides of the equation (10) with \((p-\beta)^b\):

\[
(p-\beta)^b \frac{\phi(p)}{\psi(p)} = B_1 + B_2 (p-\beta) + \ldots + B_b (p-\beta)^{b-1} + (p-\beta)^b \cdot \sigma(p)
\]

(11)

\(\sigma(p)\) denotes the sum of all elementary expansions (10) that does not belong to coefficients \(B\). There is no factor of the form \((p-\beta)^k\) in the denominator \(\sigma(p)\), so the denominator is not canceled for \(p = \beta\). Taking the limits of both sides of the equation (11) for \(p \to \beta\) to find:

\[
B_1 = \lim_{p \to \beta} \left[ (p-\beta)^b \frac{\phi(p)}{\psi(p)} \right] = \lim_{p \to \beta} \left[ B_1 + B_2 (p-\beta) + \ldots + B_b (p-\beta)^{b-1} + (p-\beta)^b \cdot \sigma(p) \right]
\]

(12)

We now derive both sides of (11) in relation to \(p\), then we have:

\[
\frac{d}{dp} \left[ (p-\beta)^b \frac{\phi(p)}{\psi(p)} \right] = B_2 + 2B_2 (p-\beta) + \ldots + b(p-\beta)^{b-1} \cdot \sigma(p) + (p-\beta)^b \cdot \sigma(p)
\]

Considering again the limits of both sides for \(p \to \beta\) we find:

\[
B_2 = \lim_{p \to \beta} \frac{d}{dp} \left[ (p-\beta)^b \frac{\phi(p)}{\psi(p)} \right]
\]

Let \(k\) be any number from \(1\) to \(b\). We derive both sides of (11) in relation to \(p\), \(k-1\) times and find:

\[
\frac{d^{k-1}}{dp^{k-1}} \left[ (p-\beta)^b \frac{\phi(p)}{\psi(p)} \right] = (k-1)!B_k + \ldots + (b-(k-1)) (b-k) B_k (p-\beta)^{b-k} + \ldots + (p-\beta)^b \cdot \sigma(p)
\]

\[
+ \frac{d^{k-1}}{dp^{k-1}} \left[ (p-\beta)^b \cdot \sigma(p) \right]
\]

We move to the limit for \(p \to \beta\) on both sides of the above equation. It is clear that on the right side it will remain \((k-1)!B_k\) alone and if we divide it with the \((k-1)\) we find:

\[
B_k = \frac{1}{(k-1)!} \lim_{p \to \beta} \frac{d^{k-1}}{dp^{k-1}} \left[ (p-\beta)^b \frac{\phi(p)}{\psi(p)} \right]
\]

(13)

If instead of \(\beta\) we take another root of the polynomial \(\psi(p)\), then according to the formula (13) we find coefficients that belong to that root. After finding the coefficients there is no difficulty in finding the original. As it is well known, each term of expansion (10) of the form:

\[
\frac{B_k}{(p-\beta)^{b-k+1}}
\]

corresponds to the original:

\[
\frac{B_k}{(b-k)!} e^{\beta k}
\]

Then the original corresponding to the function \(\phi(p)/\psi(p)\) deduced in form (10) is:

\[
A_1 \frac{t^{\alpha-1}}{\alpha!} e^{\alpha t} + A_2 \frac{t^{\alpha-2}}{(\alpha-2)!} e^{\alpha t} + \ldots + A_b e^{\alpha t} + B_1 \frac{t^{b-1}}{(b-1)!} e^{\beta t} + B_2 \frac{t^{b-2}}{(\beta-2)!} e^{\beta t} + \ldots + B_b e^{\beta t} +
\]

(14)

\[
+ L_1 \frac{l^{b-1}}{(l-1)!} e^{\phi t} + L_2 \frac{l^{b-2}}{(l-2)!} e^{\phi t} + \ldots + L_c e^{\phi t}
\]

Remarks: If in formula (13) we get \(b = 1\), then we will certainly have \(k = 1\) and this formula results in the same formula (8). For this reason, if in the expansion of the polynomial \(\psi(p)\) some roots are simple, then for finding the respective coefficients use the formula (9).

3. The Accumulated Value

If matured interest is added to the principal at the end of each period for which the interest is calculated and then this interest earns interest, it is said that the interest is compounded. The amount of initial principal and total interest is called the compound sum or accumulated value. [5]

Let’s note:

- \(P\) = the initial principal or the discounted value of \(S\)
- \(S\) = the sum of \(P\’s\) or accumulated value of \(P\)
- \(t\) = total number of interest periods
- \(r\) = interest rate

Let \(P\) be the principal at the beginning of the first period and \(r\) the interest rate for the conversion period. We will calculate accumulated values at the end of consecutive periods of conversion for \(t\) periods.

At the end of the first period:

- Interest matured \(P \cdot r\)
- The accumulated value \(P + P \cdot r = P(1 + r)\)
At the end of the second period:

Interest matured: \( P \cdot (1 + r) \cdot r \)

The accumulated value:

\[ P(1 + r) + P \cdot (1 + r) \cdot r = P(1 + r)^2 \]

At the end of the third period:

Interest matured: \( P \cdot (1 + r)^2 \cdot r \)

The accumulated value:

\[ P(1 + r)^2 + P \cdot (1 + r)^2 \cdot r = P(1 + r)^3 \]

Continuing this way we would get the accumulated values:

\[ P(1 + r), P(1 + r)^2, P(1 + r)^3, \ldots \]

They form a geometric progression \( t \) whose term is:

\[ S = P(1 + r)^t \quad \text{(15)} \]

4. Relation Between Present Value and Laplace Transform

In business transactions it is usually necessary to determine the level of principal \( P \) today, that will be accumulated at a compound interest rate \( r \) in a given sum \( S \) on a given date (interest period from that moment). By formula (15) we have:

\[ P = \sum_{n=0}^{T} \frac{S(t)}{(1 + r)^n} \quad \text{(16)} \]

In other words, it is the amount that we would be willing to pay today in order to receive a cash flow or a series of them in the future. [6] Now by using an exponential series we can write equation (16) as,

\[ P = e^{-rt} \sum_{n=1}^{T} S(t) \quad \text{(17)} \]

In the limiting case replacing summation to an integral, equation (17) can be written as

\[ P = \int_0^T e^{-rt} S(t) \, dt \quad \text{(18)} \]

Again here \( T \) is some finite quantity. So if we consider as \( T \rightarrow +\infty \), equation (18) will becomes

\[ P = \int_0^{\infty} e^{-rt} S(t) \, dt \quad \text{(19)} \]

Equation (19) is nothing other than the definition of Laplace’s transformation, hence: [6]

\[ P(r) = L\{S(t)\} \quad \text{(20)} \]

Suppose successive \( t \) payments are to be made, \( k_1, k_2, k_3, \ldots, k_t \), where: \( k_1 \) to be settled after a year, \( k_2 \) after two years and so on. How much is the amount to be deposited today in one bank account in order to get enough savings to afford all future payments when the annual interest rate is \( r \)?

So what is the present value of all payments?

We start from formula (15) and apply it for the foregoing. To have the quantity \( k_1 \) after one year we have: \( k_1 = P(1 + r) \), from where, the amount we need to deposit today is \( P = \frac{k_1}{1 + r} \). To have the quantity \( k_2 \) after two years: \( k_2 = P(1 + r)^2 \Rightarrow P = \frac{k_2}{(1 + r)^2} \), and so on. The full amount that needs to be deposited today, so that all payments are covered is:

\[ P = \frac{k_1}{1 + r} + \frac{k_2}{(1 + r)^2} + \frac{k_3}{(1 + r)^3} + \cdots + \frac{k_t}{(1 + r)^t} \quad \text{(21)} \]

If the payments are the same, \( k_1 = k_2 = k_3 = \ldots = k_t = k \) then

\[ P = \frac{k}{1 + r} + \frac{k}{(1 + r)^2} + \frac{k}{(1 + r)^3} + \cdots + \frac{k}{(1 + r)^t} \quad \text{(22)} \]

This is nothing but a series of geometric progression at a time \( \frac{1}{1 + r} \) that:

\[ P = \frac{k}{1 + r} \cdot \frac{1 - \frac{1}{(1 + r)^t}}{1 - \frac{1}{1 + r}} = \frac{k}{r} \left[ 1 - \frac{1}{(1 + r)^t} \right] \quad \text{(23)} \]

If we use Laplace transformation

\[ L\{k\} = \frac{k}{r} \int_0^T e^{-rt} \, dt = \frac{k}{r} \quad \text{(24)} \]

Example. Estimate the current value of a $1000 instant spill series at the end of each year when the annual interest rate is 10%.

Solution: \( P = \frac{1000}{10} = 10000\) $.

4. Conclusions

1) Laplace transformation is the simplest and most economical method that leads directly to the required resolution of many of the various technical problems that arise when solving them.

2) Using the Laplace transformation we easily obtain a definitive analytical solution to the problems of the present discounted value where was shown the close relationship existing between the actual discounted value in finance and the transformation of Laplace. [6]

3) The result in this paper increases the practical benefits of Laplace transformation particularly in finance.

4) Laplace transformation is the major resource for discounted value functions to illustrate complex problems.

5. References

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INVESTIGATION OF CONVERGENCE OF $\xi$ APPROXIMATIONS ON COMPLEX NUMBER PLANE

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Abstract: In this study, the convergence behaviour of the $\xi$ approximants for the exponential operaor is investigated on the entire complex plain. The purpose of this study is to develop an algorithm to observe how to transform a initial region on the complex plane defined by $\xi$ approximants.

Keywords: LIE OPERATORS, COMPLEX RECURSIVE FUNCTIONS, EVALUATION OPERATORS

1. Introduction

In this study, the convergence behaviour of the $\xi$ approximants for the exponential operators is investigated on the entire complex plain.

Exponential operators play important roles in many branches of science and engineering. They can be constructed to characterize the solutions of various mathematically formulated problems. Exponential operators give quite accurate results for the short-term evolution but causes error accumulation for long-term evolution when they are employed through a numerical approximation scheme based on time discretization. Hence we need to evaluate exponential operators in a global and rapidly converging manner.

System with n degrees of freedom will be characterized by $x_1, x_2, ..., x_n$ complex variables, which are considered as the coordinates of a point or components of a vector in an n-dimensional complex vector space.

\[(x_1(t), x_2(t), ..., x_n(t)) : \text{System}\]

\[x_1, x_2, ..., x_n : \text{Phase space vector components in this system.}\]

Hence $Q(t_f, t_i)$ global evolution operator is defined as

\[Q(t_f, t_i) = Q(t_f) \cdot x(t_i)\]

where $t_i$ and $t_f$ denote the initial and final states respectively. If factorization of evolution operators is considered as a sequence of rather simple global evolution operators then the evolution operator can be written as follows

\[Q(t_f, t_i) = e^{(t_f-t_i)S}\]

where $S$ is defined through

\[S = \sum_{j=1}^{n} \sigma_j(t) \cdot x_j \cdot \Delta t_j\]

so Q evolution operator can be assumed to be written as

\[Q = e^{f(x)} = \prod_{j=1}^{n} e^{\sigma_j(t) \cdot x_j} \cdot \sigma_j(t) = t \cdot f_j\]

where $L = f(x)$ and

\[f(x) = \sum_{j=1}^{n} f_j \cdot x_j \]

This equation is factorization formula for the one-dimensional case.

The definition of the evolution operators and their relations with the solutions of a differential equations are presented. Also the effects of the evolution operators on the functions is obtained as follows:

for $j = 0$

\[Q^{(0)} f(x) = e^{\sigma_0(t) x} = f(x + \sigma_0(t))\]

for $j = 1$

\[Q^{(1)} f(x) = e^{\sigma_1(t) x} = f(e^{\sigma_1(t)} x)\]

for $j = n$ by $x \rightarrow \frac{1}{\sqrt{n}}$ transformation

\[Q^{(n)} f(x) = e^{\sigma_n(t) x} = f\left(\frac{x}{\sqrt{n}}\right) \]

The essential approximation is to truncate

\[\xi = \lim_{n \to \infty} e^{\sigma_n(t) x} = f\left(\frac{x}{\sqrt{n}}\right)\]

to a finite order. By this way it produces the following approximation.

\[\xi_n(x, t) = \prod_{j=1}^{n} Q^{(j)}(x)\]

If the infinite product representation of Q converges then the following result can be obtained:

\[\xi(x, t) = Qx = e^{f(x)} x = \lim_{n \to \infty} \xi_n(x, t)\]

A recursion relation for these approximants can be shown as follows:

\[\xi_{n+1} = \prod_{j=1}^{n} Q^{(j)}(x) e^{\sigma_{n+1}(t) x} = \prod_{j=1}^{n} x \cdot \left(1 - \sigma_{n+1}(t) x\right)\]

As a result we can easily obtain that

\[\xi_{n+1} = \xi_n(x, t) \cdot \left(1 - \sigma_{n+1}(t) x\right)\]

And this is a recursion relation with an initial member evaluated as follows:

\[\xi_1(x, t) = x e^{\sigma_1(t)} = x e^{f_1(t)}\]

Although this is a simple recursion relation, the existence of $f_1$ may not be suitable for numerical purpose depending on the value of $f_1$. So we can normalize $\xi$ approximants as follows:

\[\xi_{n+1} = \xi_n \cdot \sigma_{n+1}(t)\]

Then the final recursion relation becomes as follows:

\[\xi_{n+1}(x, t) = \frac{\xi_n(x, t)}{1 - \sigma_{n+1}(t) \xi_n(x, t)}\]

The relation between the final and the previous approximants can be given as

\[\xi_n(x, t) = \xi_n(x, t) \cdot \sigma_1(t)\]

In this study the convergence of the $\xi$-approximant sequences in the complex plane is main issue. The above transformation of $\xi_n$ to $\xi_{n+1}$ can be interpreted as applying some basic elementary transformations consecutively. For this reason the following transformations are presented

\[w_1 = f_1(x) = x^n, 0 \leq r < \infty, 0 \leq \phi \leq \frac{2\pi}{n}\]

\[w_2 = f_2(x) = -\sigma_1 w_1, 0 \leq r < \infty, 0 \leq \phi \leq 2\pi\]

\[w_3 = f_3(x) = 1 + w_2, 0 \leq r < \infty, 0 \leq \phi \leq 2\pi\]

\[w_4 = f_4(x) = \frac{1}{w_3}, 0 \leq r < \infty, -\phi \leq \phi \leq 0\]

\[w_5 = f_5(x) = w_4 - 1, 0 \leq r < \infty, 0 \leq \phi \leq 2\pi\]
\[ w_6 = f_6(z) = \frac{1}{\sigma_{n+1}} w_5 \quad 0 \leq r < \infty \quad 0 \leq \varphi \leq 2\pi \]

\[ w_7 = f_7(z) = \frac{1}{\sigma_{n+1}} w_6 \quad 0 \leq r < R \quad 0 \leq \varphi \leq 2\pi \]

As can be easily seen we get the main transformation function when we apply these consecutive transformations.

\[ w_7 = w_6 = \left( \frac{1}{\sigma_{n+1}} \right)^\frac{1}{n+1} \left( \frac{1}{\sigma_{n+1}} (w_4 - 1) \right)^\frac{1}{n+1} \left( \frac{1}{\sigma_{n+1}} (w_2 - 1) \right)^\frac{1}{n+1} \]

\[ = \left( \frac{1}{\sigma_{n+1}} \right)^\frac{1}{n+1} \left( 1 + w_2 - 1 \right)^\frac{1}{n+1} = \left( \frac{1}{\sigma_{n+1}} \right)^\frac{1}{n+1} \left( 1 - \sigma_{n+1} w_2 - 1 \right)^\frac{1}{n+1} \]

\[ = \left( \frac{1}{\sigma_{n+1}} \right)^\frac{1}{n+1} \left( 1 - \sigma_{n+1} (\xi_n^2) - 1 \right)^\frac{1}{n+1} \]

\[ z \to \xi_n \]

\[ = \left( \frac{1}{\sigma_{n+1}} \right)^\frac{1}{n+1} \left( 1 - \sigma_{n+1} (\xi_n^2) \right)^\frac{1}{n+1} \]

Therefore one can obtain a singularity free initial region on the \[ \xi_n \]–plane by determining the locations of these singularities and discarding them from the domain.

Here \( \sigma_n(t) \) functions are assumed to be given and the \( \xi \)-approximants’ nature are determined by these \( \sigma_n(t) \) functions. The main purpose of the examination of this convergence is to give important information about the convergence of finite product sequences that appears during the factorization of these sequences.

The purpose of this study is to develop an algorithm to find out or observe how the above recursion relation defined via \( \xi \)-approximants transform a given initial region on the complex plane defined by \( \xi \)-approximants and a develop a computer program based on this algorithm. By this computer program we can expect to be able to examine the regional changes during the consecutive recursion transformations ant to put forward some theorems by investigating this program outputs.

A singular point taken in the domain can carry us to infinity on the \[ \xi_{n+1} \]–plane as can be noticed through

\[ \xi_{n+1} = \frac{\xi_n}{(1 - \sigma_{n+1} \xi_n^2)^\frac{1}{n+1}} \]

Therefore one can obtain a singularity free initial region on \( \xi_n \)–plane by determining the locations of these singularities and discarding them from the domain.

In this study, the original contribution is the separation of the recursion relation between two consecutive \( \xi \)-approximants into basic simple consecutive transformations.

The other contributions are the construction of an algorithm that evaluates the region variations through the consecutive transformations and to develop a computer program to execute this algorithm. The computer program is written in C++ language and Mathematica is used for graphics.

### 2. Conclusion

In this study has shown for the \( \sigma_n(t) \) sequences that shrink fast enough that the equivalent in the \( \xi_n \)-plane of a circular region without a singularity for the \( \xi_1 \)-plane will remain without singularity in the \( \xi_n \) series, regardless of \( n \) and time.

### 3. References

1. Introduction

It is known that air pollutants (e.g. carbon monoxide, sulfur oxides, nitrogen oxides, particulate matters) have harmful effects on the environmental and human health. Most air pollutants emitted from human-made sources: mobile sources such as transportation or stationary sources such as factories, power plants. Some air pollutants emitted from natural sources such as volcanic eruptions, forest fires (https://www.epa.gov/). Many researchers have been studying on the estimation of air pollutants and their effects by different methods. Some studies are about the different area of the world. For examples, emissions amounts for Tokyo Bay Area; NE Atlantic region; Tyrrhenian Sea; Turkish Straits; sea of Marmara; Danish Ports were estimated by Onagawa [1]; Carlton [2]; Trozzi and Vaccaro [3,4]; Keskin and Vardar [5], Kanbay and Vardar[6]; Kılıç [7] and Deniz [8]; and Saxea and Larsena [9] respectively. On the other hand, Corbett and Fischbeck [10], Corbett and Koehler Kılıç [7] and Endresen [12] were estimated globally annual emissions.

In this study, as an example of the emission estimation; the amounts NOx emitted from transit vessels passing through the Bosphorus are calculated by using fuzzy inference system in MATLAB. Bosphorus (see Fig.1 it was taken from http://www.bosphorusstrait.com/the-bosporus-strait/map-of-bosphorus/) connects Marmara sea and Black sea with the length 29.9 km. and the width ranges between 700 and 1500 meters.

Fig. 1 Bosphorus

2. Objectives and Method

The amounts NOx emitted from transit vessels were calculated by using the methodologies explained in studies of Trozzi and Voccaro (see [3, 4]) and Kılıç (see [7]). Amounts of emissions were calculated by the following equation;

\[ E_i = t \cdot P \cdot (EF)_i \cdot \text{[Engine Load]} \]

where \( i \) is the pollutant type, \( t \) is time, \( P \) is engine power in kilowatts (kW), \( (EF)_i \) is emission factors of pollutant \( i \), \( \text{[Engine load]} \) is the percentage of full power of the engine. It is assumed that the engine runs 80 % load of the power of engine (Engine load is 0.8) and 4 generators work during the cruising time and run 75% load of the power of auxiliary engine. Due to the traffic and weather conditions, the cruising times are between \( t_1 =1.54 \) hours and \( t_2 =2.42 \) hours. The gross tonnages and engine powers are given according to the ship types on Tab.1 (see [7]). \((EF)_{NOx}\) according to the ship and working types is presented on Tab. 2.

**Table 1: The Ship Types and Engine Power**

<table>
<thead>
<tr>
<th>Ship Types</th>
<th>Engine Power (kW)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gross Tonnage</td>
<td>&lt;500</td>
</tr>
<tr>
<td>Bulk Carrier</td>
<td>500</td>
</tr>
<tr>
<td>Cargo Ship</td>
<td>850</td>
</tr>
<tr>
<td>Tanker</td>
<td>751</td>
</tr>
</tbody>
</table>

**Table 2: \((EF)_{NOx}\) according to the ship and working types**

<table>
<thead>
<tr>
<th>SHIP TYPES</th>
<th>WORKING TYPE</th>
<th>((EF)_{NOx})</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bulk Carrier</td>
<td>CRUISING</td>
<td>17.7</td>
</tr>
<tr>
<td></td>
<td>HARBOUR</td>
<td>13.5</td>
</tr>
<tr>
<td></td>
<td>MANOEUVRE</td>
<td>14.0</td>
</tr>
<tr>
<td>Cargo Ship</td>
<td>CRUISING</td>
<td>14.9</td>
</tr>
<tr>
<td></td>
<td>HARBOUR</td>
<td>13.3</td>
</tr>
<tr>
<td></td>
<td>MANOEUVRE</td>
<td>12.6</td>
</tr>
<tr>
<td>Tanker</td>
<td>CRUISING</td>
<td>14.0</td>
</tr>
<tr>
<td></td>
<td>HARBOUR</td>
<td>12.3</td>
</tr>
<tr>
<td></td>
<td>MANOEUVRE</td>
<td>12.2</td>
</tr>
</tbody>
</table>

By using the equation (1), the amounts of \( E_{NOx} \) according to ship types and their gross tonnage for one ship are calculated. The results are presented on Tab. 3.
The number of ships (Tanker, general cargo and bulk carrier) passing through the Istanbul strait was recorded as 42553 in 2016 and the number of ships according to ship types are given on Tab. 4, (it was taken from the web-site of DTGM (2016): https://atlantis.udhb.gov.tr/istatistik/gemigecis.aspx of DTGM).

**Table 4: Number of Ships Passed Bosphorus**

<table>
<thead>
<tr>
<th>Ship Types</th>
<th>&lt;999 grt (Group 1)</th>
<th>1000-9999 grt (Group 2)</th>
<th>&gt;99999 grt (Group 3)</th>
<th>Total Number of Vessel</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tanker</td>
<td>110</td>
<td>7964</td>
<td>807</td>
<td>8881</td>
</tr>
<tr>
<td>Cargo Ships</td>
<td>320</td>
<td>23177</td>
<td>2354</td>
<td>25851</td>
</tr>
<tr>
<td>Bulk Carrier</td>
<td>92</td>
<td>7017</td>
<td>712</td>
<td>7821</td>
</tr>
</tbody>
</table>

Despite six groups of vessels on Tab.3, the total number of ships are only three groups. On Tab. 3 all three groups are divided separately two sub-groups. The numbers of the ships of the subgroups are unknown. Hence the fuzzy inference system (FIS) could be appropriate solution method. The mandani type FIS with various shaped fuzzy membership functions was created. The membership functions were experienced by taking into account the cruising time and the different gross tonnages possibilities (see Fig. 2, Fig. 3 and Fig. 4).

3. Results

By using Fuzzy Inference System in Mathlab, the variation of $E_{NOx}$ values for different ship types according to the gross tonnage of the ships can be seen and the results are also illustrated by the surfaces (see Fig. 5).
4. Conclusion

The amount of NOx emission from transit ships passing through the Bosphorus is estimated by using fuzzy inference system. Estimations were calculated for three different ship types. The effect of gross tonnage and cruising speed changes of vessels were taken into consideration in the fuzzy model. It seems that the maximum amount of NOx occurs from the cargo ships. The results is given as surface too.

5. References


AIR SPACE ROUTING AND FLIGHTS PLANNING: A PROBLEM STATEMENT AND DISCUSSION OF APPROACHES TO SOLUTION

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Abstract: Air routing has become an important problem of recent years. Wide implementation of idea to use a free routing airspace (FRA) over the Europe and idea of exploiting FRA as a main airspace management resource to reduce air traffic problems revealed a necessity of a new look to a routing problem. Many previous solutions relied on predefined topology of airways and ability to exploit well-developed methods known in graph theory. Meanwhile the problem was current due to many factors needed to be involved in the airspace as a 3D-space: air management restrictions and different air spaces regulation rules, weather conditions, danger areas, aircraft’s characteristics, pilots’ preferences, etc. Moreover, the appearance of FRA has made it inappropriate to use previous algorithms. Most of these algorithms required a definite topology with known routing points connected with predefined edges, while the FRA may have only border points to fly into or fly out of the area and no definite edges inside. The task of constructing the route became the same difficult as obvious: any pilot can fly directly through the FRA, but the route should be built and confirmed prior to a take-off. Problem comes even more evident if considered for the unmanned flying vehicles (UFV) and the need for robots or AI systems to solve the routing problem by itselfs. As a topping of the complexity of the problem, one may consider the upcoming difficulties of airspace congestion in FRA. Despite the problem is known for areas close to airports, it is still current to plan routes avoiding flights conflicts in the air and to avoid FRA high congestion. There are different researches on some particular problems and some approaches to solve these problems. Nevertheless, there is no complete problem statement yet. This research was focused on need of understanding the full scope of problems for air routing to understand the ability to build an efficient solution for the problem as a whole.

Keywords: ROUTING PROBLEM, AIR ROUTING, FLIGHTS MANAGEMENT, FLIGHTS OPTIMISATION, ALGORITHM ANALYSIS

1. Introduction

The problem of air routing nowadays comes with a few starting points:

- The main goal is to find route between departure and destination airports.
- The second goal typically is to have some reduce of fuel burn. Nevertheless, one should mention that there are estimates that optimal routes are able to give typically only 1–3% of fuel burn reduce.
- It is also assumed that all routes exist within the air space that can be predefined typically both by lateral dimension boundaries and altitude limits.
- It is assumed that there are many possible routes in airspace should exist and there are some routes that can be considered optimal (or at least one). Nevertheless, one can consider situation of reaching conditions that any of these routes are inappropriate for the particular type of aircraft (i.e. with respect to its fuel capacity and/or possible altitude limit).
- A longer route is expected to be closer to “straight” route (a great circle route).

Most researches on air routing problem are made with some of following assumptions:

- the most valuable optimization could be made within cruise stage (due to it is the main part of any flight with the most fuel burned, and climb/descend stages are much shorter or can not be optimized because of predefined fuel burn rates etc.);
- the problem of 3D routing is often reduced to 2D routing considering only cruise flight stage to be able to make notable influence;
- the problem of finding the shortest path is considered solvable with some graph algorithm like Dijkstra or A* (same as in on ground routing) without respect to vertical trajectories optimization and/or wind optimization (nevertheless these algorithms are less useful in FRA – Free Routing Area).

One recent research [1] showed the great decrease of algorithm running time with a wind optimized approach algorithm compared to classical shortest path search on graph (like Dijkstra and A* algorithms). Nevertheless, the algorithm does not consider so named 3D-routing. There are also some other researches dedicated to routing in FRA [2].

Some other researchers [3-4] offer considering both weather conditions (winds, temperature) and flight altitudes and they showed that it is more efficient to consider all conditions while building the path compared to step by step consideration of each type of conditions after initial shortest path search. There are also some similar direction researches [5-8].

However, most of approaches offered do not consider possible RADs (Route Availability Document) influence. This means there should be used a combined approach to be able to find a complex air route through both a FRA and a standard airspace (with a regular net of airways). One of possible solutions with respect to PRDs (Prohibited, Restricted and Dangerous areas) was offered in [9] based on China airspace experience.

2. Prerequisites and means for solving the problem

Now, the current airspace routing problem understanding includes a set of the following problems:

- Path construction – a problem to find a path between airports of departure and destination with respect to RAD constraints: avoid, mandatory, etc.
- Path optimization – a problem to have best path according to:
  - Length (shortest flight distance)
  - Time (fastest flight)
  - Fuel consumption (cheapest flight)
  - Weather conditions: wind, temperature, etc. (both fastest and cheapest flight)
- Path compliance – a problem to have an appropriate path including:
  - Vertical path profile (heights or flight levels distribution over the path)
  - Smoothness (pilot preferences compliant flight and smooth path) – pilot requested path options (waypoints, segments, areas, avoid areas etc.), ability to fly (matching aircraft technical abilities, avoiding sharp turns and impossible maneuvers, pilots and passengers convenient maneuvers).

Solving the problem requires a set of goals to be defined. It is obvious that a software should be developed also. The following goals in problem solution are ordered according to its importance decrease.
1) 100% success in route construction between departure and destination points. Success rate must involve as a successful result a completely correct answer whether the path exists or not (this mean that if the route search failed then the customer should be completely convinced that there is no any possible route in given circumstances to fly).

2) Build a set of fully optimized routes. The set of resulting routes must include three offered routes (in some ideal circumstances this would be the same single route):
   a. the shortest route – distance optimized only,
   b. the fastest route – time & fuel optimized (evidently, with respect to weather conditions and fuel consumption),
   c. the cheapest route – cost optimized (evidently, with respect to weather conditions, fuel consumption and FIR costs).

3) Quickest delivery time for the first found route. Possibly this time should not exceed 30 seconds. Next, the customer must see the progress in optimization, so each next optimized route (better than initial and each previous route) should be delivered in less than each next 30 seconds. Route delivery delay for more than 2 or 3 minutes should be considered as a long search and customer should be offered to decide whether to keep searching or to use the latest found route.

4) Separate processing of route inexistence. This should be a response to customer’s request to perform totally route availability search, which may take a longer time. The decision whether to wait a longer time should be passed to customer.

Many researches still consider routing problem in air space as a plain problem. Nevertheless, it remains a 3D problem and according to restrictions and peculiarities of an air space, there is a set of task to be solved separately:

- Take-off / Climb and Landing / Descend. According to SID/STAR configuration there should be found a set of initial points to start routing. These points are evidently different to a departure and destination points of airports. This yields the path search between two sets of points (ADEP_SET and ADES_SET) instead of search between only two points (ADEP and ADES). Vertical profile for take-off (including direct climb and/or step-climb) and landing (descend) should be considered in current step. Regarding a set of flight levels one may expect up to 64 points on both ADEP_SET and ADES_SET ends for the routing (i.e. 3–8 FL × 4–8 take-off/landing edges = 12–64 initial routing points).
- Determined flight (flight via airways). According to known and predefined air routes, there should be a known solution to find route on a graph (a topology). The difficulty of the problem is due to restrictions set (like RADs) and combinatorial explosion (regarding a huge or fast growing number of involved waypoints and edges).
- “Free” flight (flight via FRA). Peculiarity of the problem for the general routing problem approach is that there are no predefined edges between waypoints and it requires a topology to be generated “artificially” to be able to solve the problem with the same algorithm like in case of flight via airways. This problem actually is a problem of connecting two sets of points: area fly-in and area fly-out. Despite of seeming simplicity of a free flight, the problem looks quite different and requires some kind of particular solution to be used.
- Short flight route. This could be considered as a special case of routing problem concerning only to build the shortest route, while the problem of optimization can be abandoned. The actual result of optimization can be less useful in most circumstances of a short flight. This can be yielded with a higher cost of optimization efforts compared to implementation of a simple direct flight (shortest path flight) or insignificant benefit of optimization.

One should remember to define, at least formally, a set of metrics to be able to understand finally if the route fits all the needs. These metrics may help to make both a better route during route construction procedure and allow a pilot to decide whether he is satisfied with a route offered. Among others, a set of metrics to understand the quality of routes should include following estimates:

- Successfulness – existence of a route
- Smoothness – calculation of route direction changes
- Duration – overall required time
- Cost – overall fuel consumption + FIR costs

3. Solution of the examined problem

There is set of a very interesting and promising approaches based on a so named “nature inspired approaches”. Those considered are mostly the optimization algorithms, like ant algorithm, artificial bee colony algorithm (used in [3]), blind naked mole rat algorithm [10], rolling swarm of locust model [11], and grasshopper optimization algorithm [12–13]. Nevertheless, some of these algorithms have not been applied to solve of an air space routing problem. Here in this paper I offer to exploit the idea of a locust swarm move due to its behavior similarity to aircrafts flights.

First, a locust swarm acts as a space oriented unit – it moves in particular direction like having some target. Second, a locust swarm flies actually and it is vulnerable to winds – this is very similar to aircraft flights wind vulnerability. Third, the algorithm can be used both to construct and to optimize routes.

Let’s consider an artificial locust swarm behavior as a model for multi-routing solution approach. Each single locust could be considered as a solution for routing problem. Each locust in a swarm of N species can act in a definite way: “jump & fly” or “land on & eat”.

“Jump & fly” should be made between waypoints p_i \in P with number of waypoints |P|. These waypoints are considered to be a food source for locust. The initial food quantity at each waypoint can be eaten by a single locust or a group of locusts, the number q_i=[q(p_i)\in\mathbb{N} (0..|N|)] of locust species able to eat at particular waypoint could be measured also as a quantity of food at the waypoint. The number q_i=[q(p_i)] may also define a maximum number of locust species able to stay at waypoint p_i. The set of q_i=[q(p_i)] \in \mathbb{N} \cup \{0\} can be included in set of parameters for the model. Each waypoint can be considered to have the same quantity of food \forall i \in \mathbb{N}, i \leq |P|, j \in \mathbb{N}, j \leq |P|: q_i=p_i=Q(p_i) or different quantity of food \exists i \in \mathbb{N}, i \leq |P|, j \in \mathbb{N}, j \leq |P|: q_i\neq q(p_i). This should depend on problem specifics – the simplest approach to routing can be considered with \forall i \in \mathbb{N} \cup \{0\}: q_i=1.

After locust eat it have to move forward. The direction for the swarm can be generally defined by a vector \vec{D} from initial point to destination point. This vector also gives a line of attraction for the swarm (and each locust in a swarm, respectively). So, the swarm would have two attraction forces: swarm self-atraction force to keep swarm together and swarm direction vector attraction force.

According to eat action each locust will choose the next waypoint filled with a food. The hunger will force the locust and a swarm to move forward and not to return back to “empty” waypoints.

The jump is an act of movement from one waypoint to next waypoint. When a locust jumps to next waypoint with a food it may be considered mandatory to eat a portion of food – the quantity of food at the point to be decreased. Each locust can “decide” to stay and eat if there is still a food at the waypoint and the swarm attraction not forces it to move again. This “decision” can be implemented via act of zero-length jump (means to stay at a waypoint). All jumps should be made over the predefined topology edges (if there are airways topology) or to some neighboring waypoint (if there are no topology edges, like in FRA).
The fly action is a situation, when there are no vacant and non-empty neighboring waypoints. In case of predefined topology, some next to neighbor waypoint can be used with respect to swarm attraction force and swarm direction vector. In case of absence of predefined topology edges (FRA) the next waypoint can be selected only with respect to presence of food and attraction forces (swarm and direction). The fly distance should be regulated with a gravity force (the distance is shorter if the force is greater).

The swarm attraction force can be used also to find a way between and around obstacles. It is expected that there could be some waypoints on the border of each obstacle, and a part of a swarm should stick around an obstacle at each of such waypoints. This means the waypoints on the border of the obstacle is being saturated to prevent other locusts to stay at the waypoint. And when the swarm moves forward behind the obstacle the swarm attraction should force the locusts from behind to move and follow the swarm.

It may happen that the swarm can divide into two swarms, if the swarm attraction force for some part of locusts becomes low. But we leave this case for further consideration.

Swarm attraction force can be calculated as a vector from a single locust position to a middle point of all species locations:

\[ \mathbf{F}_n = \sum_{i \neq n} \frac{q_n}{d_{ni}^2} \mathbf{r}_{ni} \]

Alternatively, swarm attraction force can be understood as a swarm noise. Once a single locust finds a food it may be considered to keep quiet. Contrary, there can be a sound of locust flight, attracting all locust species left at the back to follow the swarm. This may affect the locusts from the back to choose direction to the swarm forward position and not to repeat some curved ways. So, the swarm attraction force should be calculated for each locust as a vector from its current position to the swarm “sound”, produced with those species in-flight. If we have a subset of locusts performed a fly, then there is a flight vector for each flying/jumping locust defined with its initial and destination position and a sum vector of the swarm noise can be found. Nevertheless, this alternate approach requires more calculations instead of having only predefined waypoints position, and this may yield inappropriate computational difficulty of the algorithm.

4. Results and discussion

A custom software solution for the algorithm was developed using Microsoft Visual Studio 2015 in C++ programming language. Currently, an initial test of a locust swarm algorithm for solving routing problem was made as a plain routing with randomly generated topologies. Simulations were performed on a Dell Inspirion notebook (model no. 3737-5683) with Intel Core i7 processor. The results of simulations are presented in Table below.

Simulations were made for different topology sizes, described with number of waypoints and number of edges in a graph. Different sizes of the locust swarms were used to find out which swarm size could be enough to find best route. The number of steps is the number of waypoints between starting and finishing points. The time of each simulation is given in milliseconds. The route length is expected to be a dimensionless value according to random generated waypoints’ coordinates.

As one can mention, swarm size was selected as a value compared to number of waypoints. Nevertheless, a test of a single locust ability to find a route was made. It was found, that in case of a large topology (250 and 1000 waypoints) a single locust was unable to find a route between starting and finishing point within a predefined limit of iterations. Other swarm sizes were calculated as a 1/10, 1/5, 1/4, 1/3, 1/2, 2/3, 3/4, 4/5 and 1/1 of number of waypoints.

For small topologies (30, 50 and 100 waypoints), the shortest route was found by the swarm with number of locusts in it not less than a half of number of waypoints (size of swarm ≥15, ≥25 and ≥50 respectively). However, for bigger topologies (250 and 1000 waypoints) the size of the swarm needed to find the shortest route decreased (size of swarm ≥62 and ≥100) revealing that 1/4 or even 1/10 could be enough. This is a particularly interesting result with the algorithm implementation.

Among the cases considered, with the growth of a swarm size the number of steps in the algorithm can decreased faster compared to route length. For example, when the number of waypoints was 50 and the swarm size was 25, a route with 4 steps was found, but it was not the shortest one yet.

<table>
<thead>
<tr>
<th>Table: Simulations results.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Waypoints</td>
</tr>
<tr>
<td>30</td>
</tr>
<tr>
<td>50</td>
</tr>
<tr>
<td>100</td>
</tr>
<tr>
<td>250</td>
</tr>
<tr>
<td>1000</td>
</tr>
</tbody>
</table>

5. Conclusion

The problem of air space routing was discussed and some key features differing the problem from a known on-ground routing problem were defined. A set of nature inspired optimization approaches was analyzed and an approach of an artificial locust swarm was chosen as an appropriate one. The algorithm of an artificial locust swarm routing (ALSR) was offered and partly developed. First results of the simulations are very promising and expected to be enhanced and improved in further researches. Some fine tuning features for the algorithm would be implemented to fit all the requirements, including routing in FRA and giving an appropriate route smoothness. In addition, a weather forecasts and
avoidance areas should be involved in an algorithm to satisfy real flights requirements.

6. Acknowledgement

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7. Literature

APPLYING QUEUE THEORY AT STUDY OF REFUSALS OF REQUESTS RECEIVED IN UNIVERSAL AUTOMOTIVE SERVICE

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Abstract: The refusal of requests received in a universal automotive service workshop in the city of Rousse was investigated. The present work analyses the average monthly requests from the workshop customers. The number of the actual repairs was also determined. The work in the service have been seen as a mass service system with a non-stationary mid-month incoming stream with queries. The basic values of the system parameters were calculated under non-stationary conditions and Mat Lab application was created. After the model has been validated, a service conversion option was proposed to reduce the refusals. The proposed approach can serve as a methodology for analysing and optimizing of the activity of other universal automotive service.

Keywords: queue theory, refusals of requests, modelling, universal automotive service, correction, operating mode, work organization

1. Introduction

In the maintenance of transport equipment the main objective is the technical condition of the fleet to be always correct, using minimal resources. This can be achieved with different strategies and methodologies. The most modern trends used in the maintenance of vehicles is the development of different methods and methodologies for predicting the technical condition change [13].

Outsourcing the maintenance of vehicles is the most widely used method. The most common reasons for using this are:
- freeing resources for core business activities;
- improving productivity and quality;
- saving of funds;
- use of external competencies;
- transfer of the risks [10].

Using outsourcing has a number of drawbacks. The first is related to the employment of the service itself, which is the time for repair of the damaged vehicle (the time for order / order processing). The second disadvantage is related to the quality of the performed repairs / service.

The full query processing time includes the queue time and the time for processing the query itself. Queue is directly dependent on the time required for the query to be processed, i.e., the shorter the processing time for the query is, the queue is the smaller as well.

According to the online business catalog “bussines.bg” there are 30 vehicle workshops in the town of Rousse [3]. The average number of working posts in these workshops is 7, which means that the working posts for servicing and repairing cars in Rousse are 210. In 2009, 90 871 cars were registered in city of Rousse [4]. From what has been written here follows that there will be a chronic shortage of working posts in the city. A queue of damaged cars will be produced in the workshops. For many workshops, getting big queues leads to denial of potential customers and financial losses. The purpose of this report is to provide a practical solution to this problem by researching a specific workshop.

The goal will be achieved by setting and solving the following tasks:
- collecting and processing statistical information from the services of a universal automotive workshop based on previous periods;
- defining the type of mass-service system;
- input modelling;
- solving the system of differential equations;
- defining the main features of the system;
- preparing proposals for adjusting the regime or organization of work in the workshop.

2. Exposition

In order to describe the operation mode of the car service, considered as a mass service, it is necessary to know the characteristics of the incoming flow of cars considered as a stochastic process, the service intensity, the maximum length of the tail and the number of service units [6, 11].

For the inbound flow of freight we can make the following assumptions:
- ordinary flow - The probability of two or more cars occurring for an elementary time interval is infinitely small compared to the probability of occurrence of only one car. The normality feature means that the cars come as single, not in group of two,three and so on at the same time.
- flow without consequences - the number of cars arriving in the system for time interval Δt does not depend on how many vehicles have already arrived, i.e. does not depend on the history of the studied phenomenon (the flow without action afterwards (Poisson flow).
- stationarity / non-stationarity of the flow [8, 13] - for sufficiently long periods of time - 1 month, 6 months, 1 year, etc. it is possible to assume the steady-state of the incoming stream, that is to say, with certain conventions, the probability of occurrence of a certain number of cars in a given, sufficiently long interval depends only on the length of that interval. Generally, in arbitrary periods, the λ stream is non-stationary λ = λ (t). This non-stationarity is clearly distinguishable over a period of one business year (about 300 working days).

For service intensity data by the service owner, it is known that the service time of a vehicle is a relatively constant quantity and is about half a working day (4 hours) based on a plan, μ = const. Regarding the number of service channels (servers), if necessary it can reach up to 3 (1≤n≤3). Two installers are needed to ensure continuous work for 8 hours on one channel. Again, according to the owner's data with more than m = 12 waiting in the queue, he refuses the order of the day, or the client renounces himself. To test the system's operation, it is necessary to find the probability that the system will have a number of cars at the time t when operating the n server [7, 2]

\[ P_k(t) = \frac{m^k}{k!} \cdot \frac{\mu^t}{t!} \cdot \left( \frac{\mu}{\lambda} \right)^t, \quad k = 0, n + m, t \in [1, T], 1 \leq n \leq 3, \quad (1) \]

where for one period T is taken one full working month T = 1 of 12 months. The beginning of the first working month t = 1 coincides with the astronomical beginning of the year, and the end of the last working month t = T = 12, with the end of the astronomical year.

For the queue theory model, the following can be summarized: a non-stationary stream of requests with density λ (t), supplied to a mass service system with s serving channels. Request service time is a random variable with an indicative distribution and parameter μ = const. A car arriving at a busy time stands in the waiting line and "patiently" waits for service, unless there is more than m = 12 in the service queue, a limited waiting system and a limited number of cars in the queue. The main indicator will be the intensity of returned requests, and at what time of year these peaks are the highest, as well as the average number of underserved queries in those peaks.
From everything told above so far, it can be said that the system is of type (M / M / s) in non-stationary mode. To describe a system of this type, the following system of differential equations of Kolmogorov (Erlang-Kolmogorov) [mitrofanova] is in effect [1, 7]:

\[ \frac{dP_n}{dt} = -\lambda P_n(t) + \mu P_{n+1}(t) + \mu(n+1)P_{n-1}(t) \]

\[ \frac{dP_n}{dt} = \lambda P_{n-1}(t) - (\lambda + n\mu)P_n(t) + \mu(k + 1)P_{n+1}(t) \]

\[ \frac{dP_n}{dt} = \lambda P_{n+1}(t) - (\lambda + (n+1)\mu)P_{n+1}(t) + n\mu P_{n+1}(t) \]

\[ \frac{dP_n}{dt} = \lambda P_{n-1}(t) - (\lambda + (n-1)\mu)P_n(t) + n\mu P_{n+1}(t) \]

\[ \frac{dP_n}{dt} = \lambda P_{n+1}(t) - (\lambda + n\mu)P_{n+1}(t) - n\mu P_{n-1}(t) \]

\[ n \text{ is the number of channels and the maximum queue length} \]

When entering difficulties. A Matlab program was developed to solve a system (2), the following trigonometric line is selected, non-linear to the quoted ratios:

\[ \lambda(t) = a_0 + a_1 \cos(wt) + b_1 \sin(wt) \]

the coefficients \(a_0, a_1, b_1, w, \) calculated by the least squares method are:

\[ a_0 = 154.734331, \quad a_1 = -2.134153, \quad b_1 = -31.383019, \quad w = 0.66038 \]

(4)

The coefficient of determination is \(R^2=0.8132\) (statistically significant).

The coefficients \(a_0, a_1, b_1, w, \) estimated by the minimax method are:

\[ a_0 = 154.760396, \quad a_1 = -12.684669, \quad b_1 = -30.630357, \quad w = 0.647557 \]

(5)

Figures 1 and 2 show the graphs of \(\lambda(t)\) with coefficients calculated by least squares method and minimax method.

For the service intensity of one channel - \(\mu, \) taking into account the service time of one car from one channel (we consider the working month for 25 days), we receive a \(\mu = 50\) cars a month from a single channel for a month.

The starting state of the system \(P_k(0)\) is unknown. It is known that these types of processes are persistent and after a long period of time they enter into regular mode of operation. Therefore, an initial state may be taken arbitrarily. The integration of the system needs to be done not for a period of time but for a sufficient number of periods. In this way, probability functions \(P_k(t)\) begin to bend to their regular values. After repeated integration with different end times it was found that only after 5-6 periods the \(P_k(t)\) functions enter the regular mode (for two adjacent periods, remain the same). Accuracy is also increased here, with integration being done over 20 periods, with the difference of all \(P_k(t)\) in the last and penultimate periods being less than \(10^{-5}\) for each \(t.\) Taking into account the proximity of \(\lambda(t)\) calculated by the coefficients of (4) and (5), all calculations are further made at \(\lambda(t)\) by coefficients of (5) (minimax method).

The following graphs reflect the results of the system decision (2) at the following values:

\[ \lambda(t) \text{ calculated with coefficients of (5) } \mu = 50, \ n = 3 \ (3 \text{ running servers)}, \ m = 12 \ (up \ to \ 12 \ in \ the \ queue). \]

Figure 3 illustrates the probability of having exactly \(k\epsilon[0;3]\) cars in the system. It is noteworthy that the most likely values for a
small or zero number of cars are between 5 and 9 months (May-September).

$$V_r = \int_{t_1}^{t_2} \lambda(t)P_{n+m}(t)dt = \int_{t_1}^{t_2} P_1(t)dt$$  \hspace{1cm} (7)$$

Fig. 3 Graph of the probability of having exactly the \(k\in[0;3]\) vehicle in the system

Fig. 4 Graph of the likelihood of having an exact \(k\in[4;7]\) vehicle in the system

Fig. 5 Graph of the likelihood of having an exact \(k\in[8;11]\) vehicle in the system

Fig. 6 A graph of the probability of having an exact \(k\in[12;15]\) vehicle in the system with \(\lambda(t)\), calculated by the coefficients of (5)

Fig. 7 Graph of the density of failures

In Fig. 6 shows that shortly after the fourth to the middle of the ninth month the probabilities of a big queue grow at high speed, with a peak coming just before the seventh month.

The probability of rejection is given by $$P_{n+m}(t)$$, i.e. all channels and places in the queue are busy and the arrived request will be denied (in Figure 6 the curve with purple color). It is also essential to know the density of declined queries. They are given with:

$$P_1(t) = \lambda(t)P_{n+m}(t)$$  \hspace{1cm} (6)$$

Fig. 7 reflects the density of failures. Again, it is noticeable that in Fig. 7 the density of failures strongly starts to increase after the fourth month. The highest value is about 7 months after it starts to decrease. The volumes of returned requests $$V_r$$ calculated between arbitrary times $$t_1$$ and $$t_2$$ are given by:

Table 2 Results of the calculations

<table>
<thead>
<tr>
<th>Months</th>
<th>Average number of returns</th>
<th>% from all returns</th>
</tr>
</thead>
<tbody>
<tr>
<td>4-6</td>
<td>44.26</td>
<td>27.11</td>
</tr>
<tr>
<td>6-8</td>
<td>74.83</td>
<td>45.84</td>
</tr>
<tr>
<td>8-10</td>
<td>30.92</td>
<td>18.94</td>
</tr>
<tr>
<td>5-9</td>
<td>125.51</td>
<td>76.89</td>
</tr>
</tbody>
</table>

Table 2 shows that almost 77% of the returned applications are for a period of 4 months - from the beginning of May to the beginning of September.

Research shows that with constant work of 3 channels (6 people) there is a marked unevenness in the main indicators of the system. The ineffective mode of operation of the system leads to the need to take adequate measures to optimize it. According to the data from the owner of the garage, the hire of an additional third worker on each channel i.e. a 50% increase in the workforce would not lead to a linear decrease in service time by 50%, and a working day (4 hours) for repair, the time would fall to about 3 hours. Hiring more people from three people per channel does not lead to a decrease in service time.

There is a variant in which three additional people are appointed for a period of 4 months from the beginning of May until the beginning of September. The service speed of $$\mu = 50$$ will increase for this period at $$\mu = 66,667$$, with the other indicators not changing.
In Fig. 8 is a graph of the density of failures when hiring a supplementary labour for a period of 4 months. It appears that in the troubled period, returns have substantially decreased. There are also two large peaks, around the beginning of the year and after the beginning of the fourth month. They can be neutralized in a similar way, but it is not always possible to hire a workforce for a short time.

![Graph of the density of failures in μ different during the season with high intensity of orders](image)

**Fig. 8** Graph of the density of failures in μ different during the season with high intensity of orders

In the proposed option to improve system performance the returned orders are 57.32, which is 2.85 times less than the original volume.

The study described in this report is also applicable to other repairers because of the similarity of organization of work in them, which is similar to the inputs of the system.

3. **Conclusion**

1. The theoretical results obtained are intended to clarify the behavior of the system at any time of the day for periods of approximately equal non-stationary intensity (accuracy to constant) of arrival and service.

2. A way is proposed to approximate the input flow density by the most general average statistics.

3. A methodology has been proposed for modeling and testing of the characteristics of a universal car service with similar non-stationary behavior as well as universal car service with a number of service units.

4. When system characteristics are unsatisfactory, the theoretical results will determine what adjustments in service intensity and/or number of channels are to be made for better performance. This would save time and problems of the “trial and error” type.

5. For the study, given the average behavior of intensity, the “average tail length” characteristic is sufficiently synchronized with the theoretical predictions (Table 1 and Figure 8). With sufficient statistics and measurements (a fairly accurate approximate intensity) for other universal car repair shops, it will provide theoretical characteristics that are close enough to the real ones.

6. Improvements can be made at no extra cost (for example opening new positions). This can be done by organizing a job involving more workers. This organization of working time will have the necessary effect in minimizing and adjusting the waiting time and the number of failures. This would result in a much more efficient way of working for the system itself. The waiting time will be approximately the same regardless of the arrival of the cars. The total average waiting time will also be reduced.

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Evaluation of robustness in ASR for different ‘Front-End’ methods
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Abstract: Some feature extraction methods suffer performance degradation in different environments. So it has become a necessity to search for new methods that perform better in different types of conditions. Therefore we can make a comparison of the new found methods to evaluate their performance and to determine which is best in multi-condition tests in order to have a more robust ASR system.

Keywords: FEATURE EXTRACTION, DEGRADATION, PERFORMANCE, ASR.

1. Introduction
Speech recognition, is commonly known as automatic speech recognition (ASR), is the process of converting an acoustic signal, captured by a microphone or a telephone, to a text. The main goal of speech recognition is to get effective ways for mankind to communicate with computers, for example, voice-controlled personal computers. A speech recognizer can be divided mostly in two parts: ‘front-end’ and ‘back-end’. The general structure of a speech recognizer is shown as below.

The purpose of the ‘Front-End’ is to extract feature vectors from a speech signal. The feature vectors can capture the important characteristics of an utterance. When an unknown utterance is presented a feature vector is obtained. In this paper we study three major feature extractions ‘Front-End’ in order to get an overview of the situation in which we are studying.

These methods consist in: Gammatone Filter Cepstral Coefficients (GFCC) [1], Mel Frequency Cepstral Coefficient (MFCC) [2], and Perceptual Linear Prediction Coefficients (PLPC) [3]

2. Data Description
One of the major factor that leads to degradations in the performance of ASR systems is the presence of noise in the environment. Such degradations in performance can be due to the mismatch between the conditions in which the systems are trained and the ones in which they are operated.

Some speech enhancement approaches are found really well to deal with unknown noise and filtering such as, Spectral Subtraction, Spectral Normalization. We will see and deal with the parameters that affect the ASR like: pitch, intensity, duration, voice quality, voice strength and the signal to noise ratio [4].

Based on it, data descriptions are shown below:
Type of recognition system: Speaker-independent continuous speech recognition
Front-ends: PLPCC, MFCC, GFCC,
Back-end: Hidden Markov Modelling (HMM) with context-dependent 4-mixture triphone HMMS
Number of coefficients in a vector: 39 (13 static + 13 delta + 13 delta-delta coefficients; Static coefficients include 12 coefficients + log energy coefficient)
Window size (sec): 20 ms
Step size (sec): 10 ms
Sampling rate: 16kHz
Speech Database: IEEE, Aurora-4
Training set: 4578 utterances spoken by 546 speakers
Test set: 1258 utterances spoken by 134 speakers
Noise Type: White Gaussian noise
SNR range: 0dB, 5dB, 10dB, 15dB, 20dB, clean

3. Experimental Results
To evaluate the performance of the ASR System we will use the WER (Word Error Rate) algorithm. Below we will show the results of our experiment in Table 1 and Fig.2:
### Table 1. The results in percentage of correctly recognized phonemes in various SNR environments

<table>
<thead>
<tr>
<th>Phonemes</th>
<th>SNR (dB)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0 dB</td>
</tr>
<tr>
<td>PLPC</td>
<td>10.72</td>
</tr>
<tr>
<td>MFCC</td>
<td>12.12</td>
</tr>
<tr>
<td>GFCC</td>
<td>7.71</td>
</tr>
</tbody>
</table>

**Fig. 2** Graphical presentation of the results in the various SNR environments

### 4. Conclusions

Amongst the three conventional feature extraction front-ends (MFCC, PLPC and GFCC), it is obvious that PLPC is the worst performing front-end. All of them have up to 62% accuracy in clean environment. Also, the recognition rate of PLPCC in adverse environment is lower than GFCC and MFCC. In noisy conditions (0-20dB SNR), LPCC performs approximately 2-5% worse than PLPCC and MFCC.

Between PLPC and MFCC, MFCC performs slightly better than PLP in general. In all of the above three plots, MFCC performs approximately up to 2% better than PLP, except for the static feature at 5dB SNR, where MFCC is 2% worse than PLP.

GFCC is either performing equally to or better than the three conventional front-ends. In clean, 20dB and 0dB conditions, GFCC has approximately the same recognition rate as MFCC. In all other conditions, GFCC outperforms MFCC by 4-5%.

This method can also be applied in improvement of the measurement uncertainty at reference [5]

### 5. References

OPTIMAL HYDRO-THERMAL COORDINATION WITH A MAXIMUM RES POWER UTILIZATION STRATEGY CONSTRAINTS MODEL

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Abstract: This paper presents a formal and practical approach onto the short-term evaluation of the impact of the different RES power generation technologies. All these are considered stochastic and basically unreliable in the active power balance but they also seem to be an irreplaceable part of the electric power generation in the future. Here a generalized hydro-thermal coordination optimization model is presented aiming to help a day-ahead power balance impacts analysis and some further risk assessment to the EPS security and resilience.

Keywords: OPTIMIZATION MODELING, HYDRO-THERMAL COORDINATION, RES POWER GENERATION

1. Introduction

The contemporary environmental requirements for the operation of the EPS lead to an increase in the installed nature-friendly renewable power resources (RES) production [1-5]. The model presented in this paper aims to assesses and evaluate the impact of increased RES generation in the EPS in a short-term power production planning when a certain strategy for max RES power production is aimed as well as evaluating on one side the different RES producers and on the other the implicit financial impact they introduce in the production power planning. A major feature of these plants is that the peaks of renewable production are often in periods of low system load, which in turn affects the overall management of the EPS. In such periods it might be necessary to reject part of the renewable production. Another purpose of the planning optimization model is to reduce the amount of unused renewable energy [3] by optimizing the combined operation of the thermal power plants and the PHPS storage capacities and to achieve minimum values for the costs of the production activity. The model is constructed for the general case of an EPS with generally nonlinear thermal, HPS and PHPS.

The production of HPPs is determined by the available inlet water quantities. If there is a possibility of accumulation (sufficient useful volume of the tank), the HPP can produce energy when needed (under the circumstances of energy shortages). In many countries worldwide, at a peak load periods, HPPs are mainly used as peak, regulating and preserving capacities. Pumped storage power plants (PSPP) posses the potential to accumulate the processed water quantities (presence of a lower reservoir) and are used for balancing loads, being practically the most flexible and multifunctional elements of the EPS. In the peak load periods PHPSs operate in generator (turbine) mode, and in low load periods and in the inability to reduce the power output of other generating units, they operate in pumping mode by pumping water from the bottom into the upper tank as controllable loads. In addition to importing the requested extra load into the system, they accumulate part of the surplus electricity, which is later attributed to the peak periods at a higher price. This reversible cycle (turbine-pump, load-generator) helps to prevent frequent and multiple stops and starts of thermal units or prevents changes in the output levels of the nuclear and thermal generators [6-11].

The criterion for the efficient operation of PHPP is the financial income from the plant’s operation that is generally determined by the difference between the sold electricity production and the purchased electricity consumed in the operation of the pumps [5,12]. From an economic point of view the accumulation process is a "cost with recovery in the future". If the accumulated energy is not sold in the future periods at better prices (this condition guarantees a positive revenue), these costs will also include the cost of the lost economic benefits as the unit was idle and waited for the corresponding economically advantageous period. Thus the energy accumulation may prove itself technically necessary from the point of view of the EPS but economically unprofitable for the PHPS owner. Sometimes it may be necessary to release water from the above reservoir (primal energy resource waste) to turn on the load in future periods according the major EPS balance requirements, and in this case there must be a mechanism to stimulate the PHPS owner. Energy storage is economically justified when the cost of the electricity used by the pumps is less than the electricity generated and sold, taking into account the accumulation-production cycle losses.

The system load changes with daily, weekly and seasonal patterns and these changes lead to the respective changes of the generating plants power outputs. When PHPPs are available system operators accumulate cheaper energy produced during low load periods and inject it into the grid during peak periods when the process is cost-effective. Where there is an opportunity to accumulate energy (large dams are built), the power injections may be postponed, having in mind that this is not a "surplus" energy storage but it can later participate in energy production or balance market. Power plant using RES (exception of HPPs of stored water) generally are considered as incapable of storing their primal energy source [13] (water, solar radiation, etc.) and when aiming to use the whole availability of these stochastic RES power plants they usually increase the EPS balance problems [5,12,14].

With the increase of the share of renewable wind and solar generally uncontrollable stochastic power plants, PHPPs become an indispensable element in the EPS operation that assures the balance as a buffer to reconcile the specifics of the renewable generation and consumer load schedules[15-18]. This is extremely important most of the contemporary EPS as optimization of the coordinated work of the three different generating types are involved in order to minimize the total operation costs in the EPS and preserve the active power balance. The model presented in this paper aims to optimally model the functioning and operation of HPPs and PHPPs as an active power balance tool in order to minimize the total EPS costs with different origin of the RES power production and also with the respective attention to the specifics of the different hydro-power plants under consideration, generally at limited water availability circumstances.

Hydro-power generation is known for many ears and the HPPs have a considerably long exploitation period, some of them more than 50 years. So hydro-power plants are build in different moments and in different terrain thus leading to different efficiency of each plant. Many power plants also struggle from limited water quantities or tank volumes that further limit their operation. In some terrains the processed primal water resource of a HPS may be used again by another HPS that is below the first one, making a hydro-power cascade and thus optimizing the utilization of the limited water resource. Cascades lead to other problems in the optimization modeling.

The importance of energy storage increases with the increased RES power generation penetration [16,17,19]. Energy storage is applied for smoothing short-term fluctuations in the power generation of wind and solar plants due to wind gusts or clouds, for electric power source for longer periods of RES generation intersections (at night or when it is windless), as a back-up power
source, for example a in case of a main network failure, or as a main or auxiliary energy source of for vehicles, etc. So depending on their purpose, the energy storages are considered system-general, in the distribution network or local [17]. The former are a tool of the Electricity System Operator for tertiary frequency control and cross-border exchanges. They are powerful facilities, predominantly connected to the power transmission network of hydro-power stations, with the possibility of storing water in an upper tank. The second is a device whose capacity is proportional to the load of a distribution line. These are installed in distribution substations or transformer stations. The third ones are in scale with the load of an individual consumer who needs to be fed when the primary source drops out. They are installed in the user’s property.

When combining conventional thermal power generation and water a separate class of EPS optimization problems emerge - those of optimal hydro-thermal coordination. [5,7,9,19-21].

The hydro-thermal optimal coordination model presented here is a high-dimensional non-linear mixed-integer model because of the presence of reversible accumulation-generation power plants. HPPs with their responsiveness to meet load changes and speed are the top balance and peak sources for most EPS. Taking into account the fact that the costs of the water as a primary energy resource is practically inconsistent with those of conventional thermal power plants, HPPs have a significant impact on the total EPS operating and production costs, usually in the direction of their reduction [1,20-22].

2. Model Formulation

The presentation here models the formation of an optimal strategy for combined thermal and hydro power generation when a significant power is injected in inappropriate moments from renewable power generators. Active power balance should be satisfied at any moment and the possible alternative for renewable power generation rejection has to be properly presented and evaluated. No start or stop of a thermal unit is allowed in the optimization horizon so if the max RES power utilization strategy is adopted optimal operation plan for systems controllable loads (pumps) has to be elaborated thus leading total costs reduction, peak shaving and steady thermal power operation. In the model formulation a certain nomenclature is used and it is given below.

FORECASTED VALUES USED IN THE MODEL:

\[ D_j \] - load forecast
\[ P_{Wi} \] and \[ P_{Si} \] - forecasts for the wind and solar production
\[ P_{Resj} = P_{Wi} + P_{Si} \] - expected summary renewable production
\[ \sum_{j} \Delta L_{Res,j} \] - resulting load in a time interval \( j \)

NOMENCLATURE FOR THE THERMAL GENERATION UNITS

\( i \) - thermal unit,
\( c_i \) - price for fuel for 1 MWh for a thermal unit \( i \)
\( P_{ic}, P_{imin} \) and \( P_{imax} \) - power output level, minimal and maximal admissible values of the thermal unit’s \( i \) operational range in MWh \( i \) in a unit interval \( j \)

The work of a thermal unit \( i,j \) is the function \( f(P_{ic}) \) and the total costs for its operation for the whole planning horizon is \( \Sigma c_i f(P_{ic}) \)

NOMENCLATURE FOR THE HPS AND PHPS:

\( r \) - reservoirs
\( k \) - power stations (HPS and PHPS)
\( m_k \) - available number of pumps in a \( k \)-th PHPS with similar operation values, that in the fixed level of the pump \( P_{p,k} \)

\[ V_{min}^{rs}, V_{max}^{rs}, V_{min}^{r,usable}, V_{max}^{r,usable} \] - minimal and maximal usable water reservoir \( r \)
\[ V_{r,j} \] - water reservoir \( r \) volume at the end of the time interval \( j \)
\[ F_{r,j} \] - water flow in \( r \) during a unit interval \( j \)
\[ R_{r,j} \] - unprocessed water from \( r \) in a unit interval \( j \). Unprocessed water quantity includes controllable water release as well as uncontrollable losses such as evaporation.

\[ P_{PkJ} \] - power used by the pumps of \( k \) in a unit interval \( j \)
\[ P_{Pmk,j} \] - power used by the pump \( m_k \) in a unit interval \( j \)
\[ P_{Hk,j} \] - power produced by the turbines of \( k \) in \( j \)
\[ P_{Pmj} \] - minimal and maximal pump capacity of \( k \)
\[ P_{PHk,j} \] - available (fixed) pump level of a pump \( m_k \)
\[ 0 \leq n_{ij} \leq m_k \] and integer is the number of pumps working in \( j \)

\[ \psi_{PH} \] and \( \phi_{PH} \] - water consumption \((m^3/MWh)\) for plant \( k \) in both generation and accumulation mode

\( \eta_k \) - efficiency coefficient for a PHPS plant \( k \)
\( v_{kj} \) - artificial binary variable for the operation mode of a PHPS \( k, v_{kj} = 1 \) if the mode is pumping in \( j \)

\( w_{mk,j} \) - artificial binary variable for the operation mode of a pump \( m_k \), \( w_{mk,j} = 1 \) if pump \( m_k \) is working at a fixed level \( P_{Pmj} \) in \( j \)

The operational curve of a HPS with neglecting the water head may be expressed via the following linear functions:

\[ Q_{Hk,j} = \psi_{PH} P_{Hk,j} \] - processed water quantity by the turbines of plant \( k \) in a unit interval \( j \)

\[ Q_{PHk,j} = \phi_{PH} P_{PK,j} \] - processed water quantity by the pumps of plant \( k \) in a unit interval \( j \)

\( \epsilon_{PH} \) and \( \epsilon_{PH} \) - costs for the operation of hydro plants may be introduced in the model. These costs might include a complex structure like constant and variable components. In the current model formulation operation costs of hydro power plants are neglected

\[ \delta_i \] - permissible change of the output generation of a thermal unit \( i \) between two successive time intervals

\( a_i \) and \( \beta_i \) - rejection of renewable power for a time interval \( j \), \( 0 \leq a_i \leq 1 \) and \( 0 \leq \beta_i \leq 1 \)

The model aims to minimize the total operation costs in a short-term (day-ahead) interval of an EPS consisting of continuously operating thermal units (within their operation range \([P_{imin}, P_{imax}]\)), renewable stochastic generation form wind and solar power plants and \( k \) PHPS as peak generators with a strategy of maximum RES penetration.

\[ \min_J = c_i \sum f(P_{ic}) \] (1)

The balance constraint (2) will guarantee that the total production of both controllable and uncontrollable units and loads will equal the load forecasts for each time interval in the planning horizon:

\[ \sum_j P_{q,j} + \sum_j \sum_{i} P_{i,j} - \sum_j P_{r,j} = \Delta L_{Res,j} \] for each \( j \) (2)

The right-hand side of the balance constraint is the resulting load the has to be covered form the working controllable generation units:
\[ L_{P,\alpha,j} = D_i - (1 - \alpha_j) P_{\alpha,j} - (1 - \beta_j) P_{\alpha,j} \] (3)

It is clear that in some periods with peak RES production the resulting load will be less than the total minimum of operating thermal plants. In these periods excess renewable power should be rejected in order to sustain the power balance or this excess power has to be accumulated for further periods.

In order to avoid the modeling of the water balance constraints which is redundant and exhaustive for a short-term optimal coordination problem a single efficiency constraint for each PHPS \( k \) may be introduced.

\[ \eta_k \sum_j P_{P,k} = \sum_j P_{V,k} \text{ for each } k \] (4)

Water balance constraints (5) have to be formulated if not all hydro units are reversible of if a PHPS and a HPS use same water reservoirs. Further reduction of the number of the water balance constraints in achieved by formulating such constraints for those \( r \) that limit the hydro units operation in the given horizon (i.e. the limiting reservoir that is the smaller one). (5) is a general form of a water balance constraint for each reservoir \( r \) with modeling the work of all interconnected to \( r \) generators a pumps (feed-in and feed-out) as well as controllable and non-controllable inflows and outflows:

\[ V_j = V_{j-1} - \sum_{k \in \text{max}} \varphi_{mk} P_{mk} + \sum_{k \in \text{in}} \varphi_{nk} P_{nk} + \sum_{k \in \text{max}} \varphi_{mk} P_{mk} - \sum_{k \in \text{in}} \varphi_{nk} P_{nk} + Q_{r} + \sum_{k \in \eta} L_{r,k} - L_{r} - R_{r} \] (5)

\( \text{ffrom} \) and \( \text{ffrom} \) are the sets of plants (with their pumps and turbines) that drain water from \( r \) during \( j \). \( \text{in} \) and \( \text{in} \) are the sets of plants that feed in water in \( r \) during \( j \).

The following constraints model the physics of the accumulation-generation cycle, namely that no pumping and generation are possible simultaneously in a single time interval \( j \):

\[ P_{r,j} - v_{r,j} P_{P,\alpha,\max} \leq 0 \] (6)

\[ P_{r,k} - (1 - v_{r,j}) P_{P,\alpha,\max} \leq 0 \] (7)

Constraint (6) implies that the summary of the pumps is a controllable load whose power can be linearly controlled in a certain interval. Most pumps are considered controllable loads with a fixed power consumption. In order to model such particularity the following changes in the model may be introduced:

If using the number of pumps as groups (8) should be added:

\[ P_{r,j} - \sum_{\alpha} n_{\alpha,\alpha_j} P_{P,\alpha,\max} \leq 0 \] (8)

If using a respective modeling for each pump with a fixed level (6) will change because the summary pump consumption is determined by the work of each pump, i.e. \( P_{r,j} = \sum_{\alpha} P_{P,\alpha} \) and becoming (9) and adding (10) to keep each pump in the allowed power level (one of 0 and \( P_{P,\alpha,\max} \)):

\[ \sum_{\alpha} P_{P,\alpha} - v_{\alpha_j} P_{P,\alpha,\max} \leq 0 \] (9)

\[ P_{r,\alpha,\max} - v_{\alpha,\alpha_j} P_{P,\alpha,\max} = 0 \] (10)

Ramp-up and ramp-down constraints for the thermal units:

\[ \Delta P_{r,j} \leq \delta_j \rightarrow \Delta P_{r,j} \leq -\delta_j \text{ for each } i \text{ and } j \] (11)

If the duration of a unit time interval is greater than 30 minutes the ramp up and down constraints might be neglected, because most of the large thermal units can reach maximal operating value within 30 minutes.

Operation range for the thermal units is modeled with simple bonds:

\[ P_{r,\min,\text{max}} \leq P_{r,j} \leq P_{r,\max} \] (12)

The following simple bounds for the water reservoirs and the controllable outflows are introduced if water balance constraints (5) are implied in the model. The volume of each reservoir in every unit interval must be within the actual water level limits:

\[ V_{r,\text{min,usable}} \leq V_{r,j} \leq V_{r,\text{max,usable}} \] (13)

Values for the first (\( j=1 \)) and last interval (\( j=\text{max} \)) might be provided for the water level maintenance cycle:

\[ V_{r,1} = V_{r,1} \text{ and } V_{r,\text{max}} = V_{r,N} \] (14)

Thus this model allows for the analysis of the impact of different RES production in a short-term power balance as well as presenting in an appropriate way the specifics of hydro-power plant under consideration.

3. Conclusion

A model for optimized combined operation of thermal, PHPP and RES is formulated for short-term planning in the absence of the possibility of starting and stopping of the thermal generating units, resulting in a uniform operation of the base thermal plants and realization of the ideas of Energy Demand Management. The introduction of price indicators for the operation of storage capacities is justified from the point of view of the development and maintenance of these facilities, thus modifying investments in improving the installed facilities or their investments return policies. Differences in PHPPs may be modeled appropriately as general constraints using the efficiency coefficient for each storage plant or using water balance equations that allow for the estimation of natural resources in periods of high water and drought, as well as the quantitative and cost recovery of unprocessed water. Further the problem with the fixed operation level of pumps is discussed and appropriately solved in the model. It is built on a strategy for maximum production and utilization of RES energy, which is in line with environmental requirements as 100% RES power utilization, reduces the negative environmental impact of the thermal power plants. These models are especially useful in the case of generating power from renewable energy sources, which have a random nature of the generated electric power (wind turbines and photovoltaic power plants) and large amplitudes in the load schedules. In these cases, the optimal coordinated of conventional thermal power plants and storage capacities allows for an increase in the share of renewable production and hence the ecological operation of base power plants at small deviations. Without manageable loads and peak power, the balance of the EPS will be severely hampered. The approach of this model formulation to the different renewable stochastic resources allows for a deep analysis of the impact of the different RES production strategies and production/energy market penetration as well as it is a useful tool for the EPS optimization and development problems.

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1. Introduction

In the distant past people had practically no potential to influence the nature. However since the early 19-th century (the beginning of the Industrial Age) and especially since the rapid increase in the number of inhabitants of the Earth the technological potential for changing the natural resources has multiplied many times. The main cause of all problems is undoubtedly the increase in the world's population – more than 7 billion now, which means that it increased around 7-fold since the year 1800. Another several billion newcomers are expected by 2050, even with all the cataclysms and epidemics that can kill millions and depopulate entire regions. These epidemics (such as AIDS, for example) are a reality now in large areas of Africa and Asia, unlike Europe and North America where, despite their absence, population growth is about zero or negative. Six countries are currently "responsible" for over half of the annual human growth on Earth by 80 million people - India, China, Pakistan, Nigeria, Bangladesh and Indonesia [1].

If their economic (industrial) development follows their population growth at the same pace and their standard of living is close to that of the US and the European Union, this would mean almost immediate depletion of most resources such as oil, minerals, arable land and water. The Earth, which is currently sulfocating under the burden of its inhabitants, will have to absorb a new amount of carbon dioxide and harmful emissions.

The need of more and more resources (water, food etc.) for the continuously increasing amount of people worldwide leads to deforestation, related with clearance of forests for agriculture, building of cities, the fragmentation of forests, where large forest areas appear to be fragmented on numerous smaller plots located in agricultural lands or developing cities, which definitely affects forests and dependent species [2]. The deforestation leads to serious problems because the forests are very important to the health status of the environment. Forests provide numerous and vital ecosystem services for the environment and the climate. They help, for example, to regulate our climate and keep the river basins in a sustainable state by providing us with clean water. Forests contribute to purifying the air we breathe. The growth of the forest fund often helps capture large amounts of carbon dioxide from the atmosphere. This also helps to maintain and preserve biodiversity, as many species live in and depend on forests. The forests are also an important economic resource not only for the production of wood but also for other raw materials used for medicines and other products. Thus, forests have important functions for people's well-being and rest.

Methods of mathematical modeling are widely used for the study of complex processes, allowing mathematical description and an opportunity for performing numerical experiments. Investigation and modeling of complex phenomena are preceded by phenomenological observations and experimental work. After collecting the experimental data the investigation continues with interpretation and prediction of the behaviour of the system by identifying areas of independent variables, selection of the state parameters and definition of the parameters of the system under study. Thus one comes to the formulation of a model or to the description of the unknown and known variables and the relationships between them.

An interesting example of mathematical modeling is the work of Thomas Malthus “Essay on the principle of population” (1798) [3]. There Malthus mentioned the conflict between the growing population and the limited capacity of the environment, which has to satisfy the continuously increasing needs of natural resources. Due to Malthus, in certain moment of population development, its aspiration for growth should transform into “fight for survival”. The theory of Malthus had strong impact on Charles Darwin and his book “On the origin of species” [4] devoted to the theory of survival of the most adaptive individuals. In the early 20-s of the 20-th century Pearl [5], Lotka [6] and Volterra [7] separately developed mathematical models for studying populations. These models provoked conducting a series of experimental studies on predator-prey interactions, competitive relationships between species and the regulation of populations.

The aim of the present paper is to study a model proposed in [8]. It describes the temporary change of land-use in particular situations. We formulate the model and study some of its properties. Further we perform numerical experiments and give some of their results.

2. Mathematical model of land-use dynamics

Here we present a model of land-use dynamics proposed by Dobson et al. [8]. The usefulness of such models follows from the high rate at which natural habitats can be converted to other uses. For example, pristine or almost pristine habitats may be colonized by humans and transformed into agricultural land. Moreover, the agricultural land can be converted into degraded land or into housing developments, cities etc. [8]. In some situations conversion to agricultural land can be partially reversible. For example: the conversion of forests into farmlands can be followed by regeneration of forests over substantial areas after abandoning of the farms (transformations observed in some countries [8]).

The model proposed by Dobson et al. [8] describes the dynamics of the size of human population supported by agriculture, denoted by W, the amount of land under agriculture, denoted by Y, the amount of degraded land (in recovery), denoted by V, and the amount of pristine or recovered land (undisturbed forest), denoted by X.

The model is the following system of four ordinary differential equations:

\[
\begin{align*}
\frac{dX}{dt} &= sV - dWX \\
\frac{dY}{dt} &= dWX + bV - aY \\
\frac{dV}{dt} &= aY - (b + s)V
\end{align*}
\]
The meaning of the variables and of the parameters of the model is the following. The variable $X$ denotes the area of pristine forest habitat, which can be converted to agriculture land (area $Y$). Agriculture land transforms into unused land (denoted by $V$) after a time period $1/a$. It is also assumed that the unused land can be restored to agriculture land after an interval of time $1/b$. The variable $W$ denotes the number of people that use the land. The parameter $r$ denotes the growth rate of human population. Its dynamics is described by logistic expression with carrying capacity proportional to the land amount $h$ needed to support one human. The parameter $d$ denotes the rate of transformation of forests into agriculture land, while the parameter $s$ denotes the rate of recovery of degraded land to forest.

The parameters of the model are assumed to be non-negative. The problem has to be supplemented by corresponding initial conditions.

We study the Cauchy problem related to the model (1) – (4). The following theorems can be easily proved.

**Theorem 1.**
If the Cauchy problem (1)-(4) with non-negative initial conditions possess a continuously differentiable solution, then this solution is non-negative for every $t \geq 0$.

**Theorem 2.**
The system (1) – (4) with non-negative initial conditions possess a unique continuously differentiable solution for every $t \in [0, T]$, where $T$ is an arbitrary positive constant.

### 3. Numerical simulations

We solved the model numerically by using the code ode15s from the Matlab ODE suite. Ode15s is a multistep solver using numerical differential formulae [9].

We used the following values of parameters:

$s = 1, b = 0.2, a = 0.05, p = 0.2, r = 0.5, h = 0.9$

and initial values:

$X(0) = 10000, Y(0) = 0.1, V(0) = 0.1, W(0) = 30$.

We have analyzed the role of parameter $d$ for the dynamics of the system.

The result of the numerical solutions are presented in Fig. 1 – Fig. 4. In Fig. 1 we present the system dynamics for $d = 0.00005$, in Fig. 2 – for $d = 0.0001$, in Fig. 3 – for $d = 0.001$ and in Fig. 4 – for $d = 0.05$. 

\[
\frac{dW}{dt} = rW \frac{Y - hW}{Y}
\]
The numerical solution shows that when the initial patch of pristine forest is invaded by 30 people starting to use land for agriculture, whose area increases, the area of pristine forest declines, while the area of unused land increases. When the value of parameter $d$ is very small (e.g. Fig. 1, Fig. 2), the speed of these transformations is very small and it needs more time in comparison with situations with higher values of this parameters (e.g. Fig. 3, Fig. 4).

CONCLUSIONS

The presented model can be useful for prediction of the temporary dynamics of the various types of land and their change. Our future work will address the problem of estimation of parameters values by using specific field data.

BIBLIOGRAPHY

RESEARCHING THE CAPABILITIES OF INFORMATION TECHNOLOGIES FOR EDUCATION IN DESIGN, 3D MODELING AND VISUALIZATION OF THE WORKING OF COMPLEX MECHANISMS

ИЗСЛЕДВАНЕ НА ВЪЗМОЖНОСТИТЕ НА ИНФОРМАЦИОННИТЕ ТЕХНОЛОГИИ ЗА ОБУЧЕНИЕ ПО ПРОЕКТИРАНЕ, СЪЗДАВАНЕ НА 3D МОДЕЛИ И ВИЗУАЛИЗАЦИЯ НА ДЕЙСТВИЕТО НА СЛОЖНИ МЕХАНИЗМИ

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Abstract: This report explores modern means for researching automation of design and construction methods of engineering analysis and integrated production systems. The report is fully adapted for the need of knowledge and skills in the future work of engineering specialists in the field of machine-engineering.

Keywords: INFORMATION SYSTEMS, CLASSIFICATION, CAD SOFTWARE

1. Introduction.

The automation of the design is the systematic use of computer equipment and software in the process of engineering work (research, design, technological design, experimentation, planning and management of production processes) in the scientifically technical distribution of functions between the specialists and the electronic computing equipment (ECE). Additionally, including reasonably chosen methods for computer calculation of engineering tasks.

This means that the specialist is always leading in the design process. He solves the tasks that are creative. The ECE is tasked with the tasks that can be algorithmized i.e. provided with programs whose solving with the computer would be significantly more effective than manual execution.

As a creative process designing is an alternation of the mentally-creative and mentally-formal activities of the engineer. Formal types of activities are for example: information storage and search; processing the results of experiments; drawing up documentation, etc. These activities in the total design time balance can take up to 40-70% and are relatively easy to automate with the help of the ECE and appropriate software[13].


2. Researching the capabilities of information technologies for education in design.

Modern digital controllers (CNCs) offer advanced capabilities to increase productivity quality and implement an individual approach to each technical assignment. The programming and communication software based on a dialogue principle is the main focus. Undoubtedly the best form of organization of automated designing in the course of design training, 3D modeling, and visualization of the characteristic elements of armament are the automated design and manufacturing systems called Computer Aided Disign (Computer Manufacturing), fig. 1.

Information Systems for Computer Design and Engineering (CAD/CAE) with their capabilities facilitate the acquisition of knowledge and practical habits in working with engineering databases, engineering methods for calculation and analysis and simulation modeling in machine engineering.

The information support of the design and visualization of the distinctive armament elements is a set of activities for the creation and implementation in the work of machine-building organizations of computer networks and systems as well as various high-tech technical means (numerically controlled metal cutting machines, sensors, 3D printers, etc.) with corresponding information and programming capabilities in order to increase the efficiency and effectiveness of the management process and the life cycle of products.

**Fig. 1 Connections between automated design systems modules of engineering.**

The information support of the life-cycle management of the armament in the conceptual stage of designing of its individual details and mechanisms is expressed in assisting the engineering and designing activity by defining, forecasting and registering activities by assessing the suitability, feasibility and eligibility of the specified variants for the geometric description of digital models and computer simulation through the use of information systems[14].

CNC - computer (or computerized) numerical control
CMM - Coordinate Measuring Machines
The essence of the information systems in the private sector related to the maintenance of engineering solutions in the design of distinctive elements of the armaments in an organizational aspect can be defined as organizational-technical unification (complex) of bodies, automated workplaces, information resources (forces, means and systems), specialized peripherals, procedures and documents to ensure the handling, storage and provision of engineering support information at the design stage.

At this stage, there are many CAD/CAM/CAE systems that serve various functional areas of teams involved in the armament design process. The following section of the report presents the most used products for computer-engineered analysis and design.

2.1. Software products of Allplan Deutschland GmbH, Germany [1]:
- Allplan Engineering - integrated BIM / CAD design software.
- Allplan Architecture - object-oriented BIM/CAD software for designing all types of buildings.

2.2. Products of Altium, USA [2]:
- Altium Designer - CAD/EDA product for designing electronic circuits, embedded software, simulations, PCBs.

2.3. Autodesk Products, USA [3]:
- AutoCAD 2018 - a popular product for 2D and 3D design and construction on a global scale. The program offers innovations that provide more effective design and documentation that enables safer more accurate and seamless sharing of projects and drawings.
- AutoCAD LT 2018 - 2D drawing and detail design software with a focus on continuous productivity gain. Its comprehensive set of tools allows you to create, modify, and share drawings accurately and effectively. Using the original DWG file format ensures stability and interoperability when communicating with customers and colleagues.
- Autodesk AutoCAD Architecture 2018 - Special Software for Architects. Includes all the functionality of the standard 3D AutoCAD and adds specially designed architectural design tools that automate frequently recurring tasks and speed up the workflow. The DWG file format ensures seamless communication with colleagues and teams. Included visualization tools help ensure realistic presentation and early approval of the project.
- AutoCAD MEP 2018 - specialized CAD software for creating drawings in the water, electricity and HVAC section. Automates repetitive tasks by allowing engineers to create accurate documentation faster and communicate seamlessly with colleagues thanks to the DWG format.
- Advance Steel 2018 - a specialized product for designing structures. It allows the creation of BIM (Building Information Modeling) models and drawings of steel structures with integrated libraries and tools. Works as an AutoCAD upgrade. Version 2018 also includes AutoCAD 2018.
- Autodesk Revit - includes 3 modules with architectural, building and construction features:
  - Autodesk Revit Architecture Module 2018 - BIM for architects providing integrated tools for building design and analysis. Shows each distinctiveation, drawing, 2D, and 3D view from the same database, automatically coordinating changes at all stages of project design and deployment. Helps to make more informed decisions in the early stages of the project.
  - Autodesk Revit MEP 2018 Module - BIM for SIP, HVAC and HVAC Engineers. Provides special tools for design and analysis of building installations.
  - Autodesk Revit Structure Module 2018 - a BIM-based design solution that provides custom-designed design, analysis, and documentation tools. BIM helps coordinate drawings, reduce mistakes, and improves collaboration between the engineering and architectural team.
- Autodesk Revit 2017 includes Revit Architecture, Revit MEP, and Revit Structure as a single product for all majorities.
- Autodesk Robot Structural Analysis Professional 2018 - professional software for calculating building structures of all kinds. It offers functionality for thousands of analyzes, both static and dynamic, earthquake resistance analysis and hurricane winds.
- AutoCAD Plant 3D 2018 - 3D software for designing, modeling and documenting factory processes and industrial facilities (pipelines, equipment, bearing structures and other plant components, industrial buildings and wastewater treatment plants).
- Autodesk ReCap 2018 - Laser scanning data processing software initiated in digital CAD or BIM environments for building and refining specialized design software for renovation, reconstruction and rehabilitation projects.
- Autodesk Navisworks Manage 2018 - includes project review tools and more effective communication that combine multidisciplinary design data, including BIM or digital prototypes. Helps to detect inconsistencies prior to the construction phase, which reduces the cost and time to process the project.
- AutoCAD Mechanical 2018 [4] - Includes all the features of AutoCAD, as well as comprehensive automation tools for mechanical engineering tasks such as machine tool generation, sizing and distincteviation of materials. AutoCAD Mechanical has a library of over 700,000 standard elements, supports multiple international drafting standards, and allows users to create details and documents using Autodesk Inventor-created digital prototypes. AutoCAD Mechanical makes engineers more competitive by helping them save hours of effort they can use for innovation rather than drawing. AutoCAD Mechanical for machine design offers users up to 70% faster performance than AutoCAD.
- AutoCAD Electrical 2018 [5] - a specialized version of AutoCAD designed distinctly for electrical engineering and automation. AutoCAD Electrical incorporates all AutoCAD tools plus a complete set of CAD design features for electrical design. Extensive libraries with ready-made components and tools for automating tasks in electrical engineering and automation help save hours of effort to allow engineers to devote more time to innovation.
- Autodesk Inventor Professional 2018 - 3D Parametric Modeling Tool. The only product on the market that has a 100% garnet relationship with two-dimensional drawings in original DWG format. It enables the creation of a complete digital prototype allowing the machine to be tested and optimized before it is produced. Inventor provides a vast array of tools for easy 3D design, error elimination and machine and detail optimization. Provides users with tools for dynamic simulation, cable, tracking, and pneumatics in 3D, as well as the ability to create and test tooling. With Inventor's capabilities, you can be more effective, reduce errors and create innovative projects at times faster.
- Autodesk Fusion 360 - Cloud-based platform for 3D CAD, CAM and CAE design of machines and products. Fusion 360 combines mechanical design capabilities, simulations, tools to improve collaboration, and the ability to prepare components for CNC machines. The Fusion 360 works in iOS for Mac and Windows PCs, allowing the user of the client's preferred operating system. Fusion 360 is part of the AutoDesk product family for machine and product design and one of the core products in the Product Design Collection software package.
Autodesk Vault Family 2018 - The Vault Series products help support teamwork as well as individual designers. Autodesk Vault works directly from Autodesk applications, such as AutoCAD and Inventor, allowing for secure storage of engineering data, sharing and retaining previous versions, approving changes, and more.

Autodesk Nastran In-CAD 2018 - is a built-in CAD module for simulations using the Finite Elements method. Taken from Autodesk Nastran® Solver, this product offers users multiple analytics, including linear and non-linear stresses, dynamic simulations, and heat exchange. The product is available through network licensing, providing users with trouble-free work, eliminating the need for multiple individual simulation software. It delivers high-quality simulations in the CAD environment so you can test and create great products.

Autodesk Inventor HSM is a solution that works in addition to Inventor Professional software and provides users with an integrated CAM system with 2.5 and 5-axis processing for CNC machines.

Autodesk Alias 2018 - Product Designed for Machine Building and Product Design. Alias is used by 99% of all automotive manufacturers to create complex surfaces and shapes. In machine building, this program combines perfectly with the parametric model of Inventor and serves as a tool for modeling difficult by traditional methods such as propellers, screws, spirals.

Autodesk Moldflow 2018 - Specialized Plastic Product Simulation Software, part of Autodesk’s Digital Prototyping solution. This software offers tools that help manufacturers of plastics to test, optimize and validate their products and related manufacturing processes. Many companies use Autodesk Moldflow Adviser and Autodesk Moldflow Insight to reduce the need for costly prototypes, reduce the risk of potential manufacturing defects, and generally shorten the production process and bring their products to the market.

Autodesk CFD 2018 - Specialized fluid simulation software - heat pumps, streams, swirling, etc. Designed for designers in their day-to-day work with a menu in familiar AutoCAD and Inventor environments. Autodesk CFD offers the ability to make calculations both on a local computer and in Autodesk Cloud Space. Works with models from all three dimensional CAD formats.

Autodesk Manufacturing products that provide effective control over a wide range of NC machines - lathes, 2-5 axis milling centers, wire erosion machines, Swiss lathes, robots [6]:

- PowerMILL - a high-end control system for milling NC machines.
- FeatureCAM - control of milling, lathe, lathe and wire erosion machines.
- PowerSHAPE - modeling system for surface and solid geometric objects.
- PowerINSPECT - Product Inspection Product and Equipment.
- ArtCAM - a system for modeling and production of artistic forms.

2.5. Bentley Systems, USA [7]:

- MicroStation (MicroStation, MicroStation PowerDraft, Bentley View) - one of the most popular global 3D CAD / GIS infrastructure design solutions.

2.6. Products of Dassault Systemes, France [8]:

- CATIA - high-end engineering solutions for 3D design and manufacture. They allow users to simulate the whole cycle of industrial process modeling, from the original idea, through product design to virtual assembling.

3DEXPERIENCE - an engineering and business platform for managing development and production projects. Provides access to project information through regulations for all project participants (constructors, production technolo- gists, economists, project managers) as well as centralized storage and controlled information management.

SIMULIA - high-end simulations.

ENOVIA - Lifecycle and Management of Products.

DELMIA - Production Management.

2.7. Products of Dassault Systemes Solidworks Corp., USA [9]:

- SOLIDWORKS - SOLIDWORKS 'CAD solutions cover all aspects of a product development process with a seamless, integrated workflow - design, verification, communication and data management. The main SOLIDWORKS software applications are as follows:

PRODUCT DATA MANAGEMENT (PDM): Allows you to easily find and redirect files, details and drawings, automate workflow, and secure production with the correct version of the tech, product data.

ELECTRICAL DESIGN: Combines the functionality of electrical circuits from SOLIDWORKS Electrical Schematic with 3D design capabilities of SOLIDWORKS Electrical 3D.

SIMULATION: Allows you to simulate a different real environment for pre-production product testing in the virtual environment of the program.


2.8. Products of DP Technology Corp [10]:

- Esprit CAM - Automated, reliable and easy to use high-speed 3-axis and 5-axis CAM software. Using the knowledge of material handling, residual material, integrated simulation and ESPRIT testing provides fast, safe, and reliable CAM software for a wide variety of 3D operations. ESPRIT’s high performance and capabilities include processing of any kind of solid geometry (Solid, Surface or Wireframe), universal postprocessors generate a G code for any machine on the market, the ability to simulate and verify programs gives optimal quality and integrity detail. ESPRIT is 100% compatible with Windows and provides a convenient and familiar environment for maximum productivity.

2.9. Products of EPLAN Software & Service GmbH & Co. KG

- EPLAN Electric P8 - an electrotechnical CAD system for designing circuits in electrical design and automation. The product covers all the needs of the electric designer when preparing the technical and installation documentation. The program can be designed with multiple automated functions, has large array of macros and technical information for products that are used in such projects.

2.10. Products of HCL Technologies

- CAMWorks - a fully integrated SOLIDWORKS CAM control system for all types of CNC machine tools.

2.11. Products of SIEMENS PLM Software [11]:

- NX - a high-end CAD / CAE / CAM solution for 3D modeling, engineering analysis, CNC and CMM control. NX encompasses and accelerates the whole process chain in the creation and production of end-to-end products - design, design and system engineering, design, FEM / FEA simulation and optimization, production drawings, technical preparation, off-line programming CNC machines, measurement procedures and robotized production.

- ProX - the production and professional 3D printers offer the benefits of additive technology to produce a wide range of functional prototypes, spare parts, small and medium series of plastic details, dental and surgical products, and more. The 3D printing capabilities in metal, with solid, thermoplastic plastics and elastomers offer a real alternative to manufacturers looking for competition. 3D Printers ProX Direct Metal Printing produces metal parts and nodes with high precision and high metal density (96% - 100%) of a wide range of metallic powders with proven mechanical properties. The ProX DMP 100, 200 and 300 printers include the most flexible industry parameter control settings. The ProX DMP 320 complements the range of metal printers with the ability to build large-scale titanium alloy models and manage from one controller the parallel operation of 3 printers.

- Creaform's 3D scanners for reverse engineering and inspection

- 3D Stratasys printers - designed for conceptual design, prototyping and direct production, based on FDM and PolyJet technologies.

3. Conclusion.

The analysis of the listed products for computer-engineered analysis and design gives reason to summarize that different CAD/CAM products provide a variety of management databases, system and application software. However, they are compatible (or have integration capabilities) with Microsoft products as well as MS Project and MS SharePoint products, and this facilitates training, training and the work of engineering staff.

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COMPLEX SPATIAL MODELLING POSSIBILITIES OF THE SOCIO-ECONOMIC CHANGES OF HUNGARY - POTENTIAL APPROACHES AND METHODS

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Abstract: The paper overviews the possible methodological and practical approaches which can be used to create a custom-made toolset for the complex spatial modelling and forecasting of the socio-economic processes of Hungary for the 21st century. The author already participated in projects concerning land cover change and demographic modelling and gathered valuable experience in creating isolated models. In his three-year post-doctoral research programme, the author plans to take a more holistic approach with combining the elements of demography, economy and land use to create an integrated model with feedbacks between the consisting parts. The proposed methodology relies heavily on a scenario-based approach, creating a range of different forecasts from the business-as-usual ones to the highly improbable ones to explore the outer edges of future possibilities. Both local and global future assumptions will be considered during the formulation of the scenarios. An additional goal is to make the prepared modelling tool publicly available.

KEYWORDS: AGENT-BASED MODELLING, SPATIAL MODELLING, FORECAST, SCENARIO, HUNGARY, DEMOGRAPHY, ECONOMY, LAND COVER

1. Introduction

In the light of the looming challenges of the 21st century, the significance of socio-economical modelling and forecasting cannot be overstated. Besides global level, this need has been recognised in Hungary as well, and different sectoral predictions were prepared (Polónyi and Timár 2002, Király 2015, Koós 2015, Tagáti 2015, Vaszócsik 2017, Obádovics 2018).

I’ve also participated in some projects concerning land cover change modelling and demographic modelling (Long-term Socio-Economic Forecasting for Hungary – 2015, the further development of NATER (KEHOP) – the possible effects of climate change on internal migration processes (2017-2018), and the further development of NATER (KEHOP) – the methodological improvement of land cover modelling (2017-2018) (Farkas and Lennert 2015, 2016). During these research contributions, I’ve gathered valuable experience in creating isolated models, and I’ve also became familiar with the limitations of this approach. In my ongoing postdoctoral research project (PD 128372, from 2018.09.01 to 2021.08.31), focusing on the complex spatial modelling possibilities of the socio-economic changes of Hungary for the 21st century, I’d like to move toward a more holistic direction. The modelling toolset will constitute of three main components (demography, economy, and land use) forming an integrated model and thus provide more possibilities for feedback than the isolated ones. With heavily relying on a scenario-based approach, I want to extend the timescale of the forecast farther than before – and to explore the challenges and limits for Hungary in the 21st century. In order to achieve this, I am going to elaborate a custom modelling tool fit for my purposes. The existing professional software can be used to model the selected phenomenon (e.g. land use change) more or less universally – and I do not wish to compete with that feature. However, general applicability has a price – it cannot handle the regional/national irregularities of the investigated phenomena well, and it is hard (or impossible) to alter an existing toolset. However, if I build the modelling framework taking these regional characteristics into consideration from the beginning, I get much less generally applicable software as a result, but more fit to my purpose: the modelling of the selected socio-economic processes of Hungary. The aimed interconnectivity of the components also calls for a custom design.

Naturally, with these intentions, a marketable product cannot be prepared (the socioeconomic modelling needs of a single middle-sized country cannot be considered even as a niche market).

However, I still intend to make the prepared modelling tool publicly available in the suitable platforms (a dedicated website, and/or GitHub), in the hopes that the stakeholders and professionals can freely experience with the different scenarios and their territorial consequences, and to generate further research contributions.

The research project is still in the stage of conceptualisation (with results coming in 2021), so in the next pages, I’d like to summarise my previous experiences in modelling and forecasting, and present the insights that contributed to the conceptualisation of the recent research.

2. Results and discussion

In the project of the Long-term Socio-Economic Forecasting for Hungary, I created a land cover modelling and forecast with my college, Jenő Farkas. For the procedure, the Land Change Modeler for ArcGIS software was used and the Corine Land Cover maps were served as basemaps (1990 and 2006). According to the meta-analysis of Schrojenstein and his colleges, all simulation models of land use are based on at least one of the following four principles: continuation of historical development, suitability of land, result of neighbourhood interaction and result of actor interaction.

Also, they distinguished the following methodological concepts, which can be used for land use change modelling: cellular automata, statistical analysis, Markov chains, artificial neural networks, economic based models, agent based models (Schrojenstein et. al. 2011).

For predicting the amount of future land cover transformation, the LCM relied on Markov chains and on the historical trends (represented by the two basemaps). From the possible options for locating the sites of the transformations, we selected the Multilayer Perceptron neural network method, which uses a neural network, the basemaps explanatory variables (with the same spatial dimension) to determine the probability of change between each modelled land cover category. The available variables mostly emphasised the expression of the principles of suitability of land and neighbourhood interaction. Additionally, it was also possible to declare spatial constraints and incentives for certain transitions, which helps the expression of author interaction.

With the software, two types of predictions were produced, a hard prediction showing the land cover for 2030 and a soft prediction depicting the probability of change, which can be considered valid for a longer period. The results indicate an increase in the share of forests, artificial surfaces and vineyards and fruit cultivations, and a
favourable old-age dependency ratio. Also, without a feedback between the determination of the transition locations and the total amount of change, suitability does not necessarily translate to viability. In case of a shortage from a certain land use category, transitions will occur even in the highly improbable locations (except if absolute constraints had been declared). Generally, the Land Change Modeller software produces the best results in case long-term changes with few well identifiable location factors (like tropical deforestation and urban sprawl).

The planned recent research will take these limitations into consideration. The integrated execution with the demographic and economic component will make it possible to follow a more supply and demand based approach instead on relying on historical trends. And while the previous research experiences proved that Corine Land Cover is a good starting point for creating a basemap for modelling, but because of the presence of some unique features in Hungary (e.g. scattered farms and garden zones), some of the categories need revision (e.g. complex cultivation patterns).

In case of the preceding demographic modelling research (the further development of NATéR – the possible effects of climate change on internal migration processes), I used a self-developed modelling toolset coded in Python. The model integrates a lot of different theoretical-practical approaches of demographic modelling (e.g. cohort-component method, Lee’s push-pull theory, neoclassical theories, value-expectancy model, life course approach of migration, Enyedi’s urbanisation stages), but from methodological viewpoint, it can be considered as an agent-based model, which handles each inhabitant as an individual decision making agent. During each five-year modelling cycle, every person undergoes a multiple-step decision tree with seven possible outcomes (Passes away, gives birth, participates in university student migration, participates in labour migration, participates in suburbanisation, participates in amenity migration, remains in his/her former location without taking part in any of the former ones). The attractiveness of the areas are defined independently for each migration type, and probability for the actors to take part in either of the natural or migration movement depends on the age, sex and the socioeconomic status of the inhabitant. The model gives stochastic results.

During the research 33 scenarios were prepared, which differ from each other in three aspects: their fertility and mortality assumptions, the integrated climatic scenarios, and in their socioeconomic assumptions about transport, commuting, and the prevalence of atypical work. The results indicate that (further) natural decrease of the population of Hungary seems unavoidable, but the scenarios vary between moderate to drastic loss. Due to the current age structure, an increase in life expectancy can play a more significant role in reducing population loss than an increase in fertility. As a consequence, higher projected population number means a less favourable old-age dependency ratio. The results also point out, that the predicted changes will further increase the spatial differences of Hungary. While the agglomeration ring of Budapest will continue to grow, the larger part of Hungary faces significant to severe depopulation. The rate of decrease is average in the urban, below average in the commutable rural, and higher than average in the remote rural areas.

The different introduced climate scenarios only had minimal effect on the predicted migration patterns, while the differences in the socio-economic path caused more substantial alterations. The results also indicate that the effect of climate change on the internal migration patterns will depend more on the share of population who is able and willing to take the climactic parameters into account when changing residence than on the exact changes in the climatic parameters.

The created custom modelling tool provides a good starting point for the current modelling procedure. However, it still has three important shortcomings of which I plan to address this time.

The first concerns the agents: while they were created together with individual age and gender data from the population census of the starting year, municipality level data was used to describe their socioeconomic status – which affects their migration preferences and probabilities. This decision was a necessity stemming from the lack suitable data. While it provided acceptable results, it hindered the expression of the life-course approach. Also, the presence of different social strata within the same settlement is an important driving factor for some migration types (e.g. involuntary economic migration). These migration types could not be included without individually declared economic situation before, but the current project will remedy this. As the 0th step of the project, a more detailed database connected to agents will be assembled with the inclusion of socioeconomic data (the lack of suitable database still persists, so in some cases, I will have to rely on estimations based on cross-sectioned data).

The partial overlook of the meso-theories of migration shows a somewhat opposite shortcoming. While the previous one focused on the improvement of individual agents, the meso-theories emphasise the role of social connections in the migration decisions, especially family ties. In order to comply with this approach, the agents has to be formulated together with their respective relationship network (with the help of census data), and in some cases, migration decisions have to be taken in family level.

The importance of feedback was already emphasized between components. Within the demographic component, the changes of housing prices will also provide an important (usually negative) feedback, making migration from the depressed areas less probable. In the previous research, this phenomenon was taken into account using the settlement development level, but this time I aim for a more dynamic implementation. This will also help the inclusion of involuntary economic migration subtype to the model. To achieve this, a dynamic housing database has to be assembled, and joined to the agents. Also, the economic component has to take the housing market into consideration.

Without previous research experience, the elaboration of the economic component is the least certain. Economic actors (currently existing and potential fictional) determining the changes of the labour market (and thus the migration flows) surely have to be declared. The most important economic actor of Hungary is naturally the central government. It will be elaborated as a half-autonomous agent, with predefined preferences and condition-action rules which depend on the selected scenario.

3. Conclusion

The project aims to create projections till the end of the century. While it is a daunting aspiration, the previous research experiments pointed out its necessity. If we want the introduced socio-economic
paradigm shifts to play out in their full scale and create significant divergences from the business-as-usual scenarios, we have to consider a longer modelling period then a few decades. Naturally, it is increases the uncertainty of the projections. However, as the previous research results have pointed out, uncertainty appears in a spatially uneven pattern. While some settlements and regions face with a rather undetermined future, the fate of other areas seems to be more certain due to their path-dependency. Even without providing unquestionable predictions, the mapping of uncertainty is a valuable result in itself.

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AUTOMATIC GENERATION OF A NATIONAL DIABETES REGISTER FROM OUTPATIENT RECORDS

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Abstract: In this paper, we present the construction of Bulgarian National Diabetes Register, using pseudonymized outpatient records submitted to the Bulgarian National Health Insurance Fund. The automatic generation facilitates the construction because it does not burden any medical experts with additional paper work. The Register is a healthcare system integrating natural language processing in large scale and analytics functionalities that provide new views to the information concerning Diabetes Mellitus and diabetic patients in Bulgaria. This successful approach encouraged the authors to initiate a research programme in eHealth focused on collection and analysis of patient data, with the intention to assess the feasibility of secondary patient record use in evaluation of healthcare quality.

Keywords: HEALTHCARE SYSTEMS, BIG DATA IN HEALTHCARE, AUTOMATIC ANALYSIS OF CLINICAL TEXTS

1. Introduction

Diabetes prevention and cure in Europe have improved after 2008 because less people die [1]. Patient awareness is raising, self-monitoring becomes easier, and the variety of medications is growing. However, still a very high number of diabetic patients are undiagnosed and half of the European countries cannot provide reasonably good data concerning procedure indicators. It is claimed that \"as long as important data is not systematically reported and transformed into methodology, diabetes care will remain inefficient and, at worst, haphazard\" [1].

The Euro Diabetes Index 2014 lists seven European countries that support diabetic registers: Sweden, Denmark, Norway, Netherlands, UK, Switzerland, and Hungary [1]. Data input to the registers is ensured either by self-registration or by burdening medical professionals with additional documentation tasks. Practically, self-registration means that a significant percent of the patients remains unregistered. Even in Sweden, which is the country with the best diabetes care delivery in Europe according to the Euro Diabetes Index 2014, the register was constructed by self-registration. During its development phase 2001-2005 the self-registration rate of patients gradually increased and reached 75%, which in 2010 still remains stable and is one of the highest in the country [2]. No information is available about the procedures for register update and maintenance.

Availability of relevant data is of primary importance in diabetes prevention and treatment (\"no data, no cure\" according to the Euro Diabetes Index 2014). However, high-quality data is hard to collect. Information about diabetic patients is often not collected nationally but rather in hospitals or at regional level, with limited comparability of collected indicators. Moreover, data often come from isolated national projects or EU-funded initiatives with fixed duration. After the project ends, no strategic plans are built by the respective political or governing institutions and in this way projects that started and proved to be successful remain feasibility studies without practical effects.

All countries in Europe have national plans for discovery, treatment and prevention of Diabetes [3] but one hardly finds information about the execution of these plans, monitoring of various plan measures and evaluation of their success. Positive health outcomes are difficult to assess too, moreover this needs to be done dynamically at national level in order to improve the treatment plans. From a technological point of view, the general impression is that healthcare authorities lack understanding about the potential of modern Information and Communication Technologies (ICT) as an enabling tool that facilitates data collection, monitoring of indicators, knowledge discovery, early alerting and automatic sending of feedbacks, evaluation of updated indicators and automatic preparation of aggregated recaps.

Surprisingly, no attempts for automatic extraction of Registers from available Electronic Health Records (EHR) repositories are mentioned in the Euro Diabetes Index 2014. A recent book about secondary use of EHR [4] lists three types of users that utilize information from patient records: clinicians searching data for their daily work; clinical researchers who need to extract patient groups or cohorts, or patients with specific diseases for their research; and finally the hospital management that need to gather statistics and predict the future of the hospital activities. The book [4] states: \"Generally when asking users what type of systems they want, they do not know\". The suggested approach is to develop a prototype and show it to the users who give feedback. Thus, it somehow becomes clear that, apart from archiving purposes, the application of nation-wide EHR repositories is still limited and their potential as content repositories is not fully understood and exploited by the community of medical professionals.

In this paper, we sketch our approach to generate automatically an anonymous Diabetic Register from outpatient records, submitted to the only health insurance fund in Bulgaria – the National Health Insurance Fund. The construction took place in 2015 and later the Register has been updated. We show how the Register is used today, together with the underlying repository of pseudonymized outpatient records. Finally, we present ideas for future work in secondary use of patient records, to be performed within the National Research Programme \"eHealth\" funded by the Bulgarian Ministry of Education and Science in 2018-2021.

2. Generation of the Diabetes Register

The mandatory health insurance was introduced in Bulgaria in 1998. The National Health Insurance Fund (NHIF) was founded in 1999 with the mission to deal with the obligatory health insurance in the country. All General Practitioners and Specialists from Ambulatory Care produce reimbursement requests (Outpatient Records) whenever they contact patients and submit these requests to the NHIF. The Outpatient Records are semi-structured XML files with numerous fields containing structured and coded information about the patient and the examining medical expert, and sufficient clinical data to summarize the case. Many indicators in the Diabetic Register copy the structured data submitted to NHIF: (i) date and time of the visit; (ii) pseudonymized personal data, age, gender; (iii) pseudonymized visit-related information; (iv) diagnoses in ICD-10; (v) NHIF drug codes for medications that are reimbursed; (vi) a code if the patient needs special monitoring; (vii) a code concerning the need for hospitalization; (viii) several codes for planned consultations, lab tests and medical imaging.

The Outpatient Records contain also values of clinical tests and lab data, presented in the free text fields. Using software extractors for automatic text analysis of Bulgarian texts, which have been developed in our previous projects, we mine these values from four
3. Present Use of the Register

The main objectives of the National Diabetes Register are [5]:

- Assessing Diabetes Mellitus morbidity in Bulgaria;
- Providing views to patient care in long-term;
- Improving prevention by Diabetes risk stratification;
- Improving Diabetes patient care by comprehensive analysis of comorbidities, studies of Diabetes Mellitus complications and treatment side effect.

Here we show how the objectives listed above are met in various studies performed on patient groups.

Diabetes Mellitus morbidity assessment (Fig. 3) shows the trend of a steady gradual increase of prevalence of Diabetes Mellitus in the majority of Bulgarian demographic regions. The most significant increase (Fig. 3 – dark red) is observed in the regions with the poorest population and low quality of life. The average percentage 9.47% for Bulgaria looks relatively good in the European context. The distribution of patients per ICD-10 codes of diagnosis (Fig. 4) shows that in 2016 about 93.4% of the patients have Diabetes Mellitus Type 2 and approximately 5.28% - Diabetes Mellitus Type 1.

Lon-term studies of patient care have both economic and healthcare impact. They cover tasks like:

- Monitoring of treatment effect for new drugs and various combined therapies,
- Evaluation of Diabetes Mellitus glycemic control etc.

Treatment with new drugs like incretins achieves good effect on Diabetes glycemic control for most patients (Fig. 5). The statistical data show that the most popular combined treatment includes two types of Insulins and analogues for injection (Fig. 6). Three types of drug combinations are most popular for combined peroral therapy.

Fig. 1 Diabetes Register interface in USHATE – a general view

Fig. 2 Diabetes Register Web interface – public generalized and aggregated data enhanced with OLAP technology

Fig. 3 Prevalence of Diabetes Mellitus type 2 in demographic regions of Bulgaria in 2016

Fig. 4 Ratio of patients with different ICD-10 codes related to Diabetes Mellitus in 2016

1 https://usbale.org/bg/registr-zaharen-diabet/
Prevention is focused on reducing the risk factors associated with chronic diseases. Thus prevention related applications include comprehensive studies of Diabetes Mellitus risk factors. Risk stratification for prediabetes patients was shown in [6, 7, 8], which discuss risk factors and comorbidities between several socially important diseases like Diabetes Mellitus, Mental Disorders, Cardiovascular diseases and the Chronic Obstructive Pulmonary Disease (CORD). Several artificial intelligence approaches were developed and applied in these studies – like natural language processing, data mining, and machine learning. In [6] we report about experiments with the dataset of patients who were in prediabetes condition in 2013-2014 and with Diabetes Mellitus onset in 2015. The data mining techniques identify some well-known risk factors but new interdependencies among the indicators were discovered as well. The latter will need further investigation from healthcare point of view.

One of the primary objectives of the Diabetes Registers is better treatment of diabetic patients [3]. In order to achieve this goal, research in several directions was performed:

- Comprehensive analysis of Diabetes Mellitus comorbidities [6, 7, 8],
- Study of Diabetes Mellitus complications and treatment side effect.

We investigated the side effect of Schizophrenia treatment with first and second generation antipsychotics for triggering some prediabetes conditions. There is a wide range of diseases that have comorbidities with Diabetes Mellitus. One of the most discussed relation is between Diabetes Mellitus and Cardiovascular Diseases. Fig. 9 shows the dependency between Hypertension and Diabetes Mellitus. Hypertension is considered not only as one of prediabetes conditions but also as an important complication related to patients with Diabetes Mellitus. Another interesting finding is the relation between Malignant neoplasm of breast and Diabetes Mellitus [6], or Gonarthrosis (arthrosis of knee) [7]. An analysis of comorbidities between Schizophrenia, Diabetes Mellitus and COPD is presented in [8]. Etiology examination of the comorbidity between disorders is very important for mortality prediction and other outcomes. Diabetes as a chronic disease is considered a primary factor for increase of mortality (Fig. 10). The onset of Diabetes Mellitus for males happens a little bit earlier than for females. Thus Diabetes complications for male patients are usually developed in a younger age, the mortality percentage is higher and male patients die earlier than females with the same age, especially male patients with less contacts to doctors.
4. Future Work: the eHealth Programme

The European Commission’s eHealth Action Plan 2012-2020 [9] provides a roadmap to empower patients and healthcare workers, to link up devices and technologies, and to invest in research towards the personalized medicine of the future. The Action Plan aims to reduce the delay of introducing modern IT solutions in European healthcare and lists barriers that hamper the wider uptake of eHealth, among them:

- lack of awareness of, and confidence in eHealth solutions among patients, citizens and healthcare professionals;
- lack of interoperability between eHealth solutions;
- limited large-scale evidence of the cost-effectiveness of eHealth tools and services;
- lack of transparency regarding the utilisation of data collected by eHealth applications.

The Action Plan concludes that “the important issue concerning the lack of health data exchange can only be tackled by addressing in a coordinated way fragmented legal frameworks, lack of legal clarity and lack of interoperability”.

The Bulgarian National Research Programme eHealth2 has been initiated by the Bulgarian Ministry of Education and Science with the aim to address most of the barriers listed above by development of specialized research prototypes and demonstrators. Briefly, collecting pseudonymized patient records from various sources we aim to show that the EHRs of Bulgarian patients can be generated almost automatically from the collections of electronic documents that are exchanged between the National Health Insurance Fund, General Practitioners, medical specialists in Primary Care, Hospitals, Clinical Labs that perform tests and send lab results via internet, and so on. Each of these document is related to certain patient record collection itself given that in Bulgaria many important patient-related documents are standardized because they are all submitted electronically to the National Health Insurance Fund for reimbursement. Further our aim is to demonstrate, using the big data base of anonymous patient records, how the quality of healthcare procedures and treatments can be assessed at national level together with its costs.

It is expected that the project will deliver a methodology and technological solutions for providing semantic operability among the heterogeneous data generated by the healthcare sector and will demonstrate how the patient-related data can be integrated in complex clinical systems. These large-scale evidences will increase the confidence in information technologies and big data processing by healthcare systems. Last but not least, the public demonstration how to achieve improvements of patient cure and quality of life, together with optimization of costs, will pave the way to real application and practical adoption of the EHR in Bulgaria. We plan to apply in the forthcoming research efforts all lessons learned during the construction of the national Diabetes Register which is now supported by USHATE in Medical University Sofia.

Acknowledgements

We acknowledge the support of the National Research Programme eHealth, funded by the Bulgarian Ministry of Education and Science in 2018-2021 with grant DO1-200/16.11.2018. Gratitude is also expressed to the NHIF and the Bulgarian Ministry of Healthcare.

References


2 https://ez.mu-sofia.bg/home (in Bulgarian)
A MODEL OF BINDING OF DOXORUBICIN WITH HEPARIN AND ENOXAPARIN

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Abstract: Chemotherapy is one of the most successful methods of fighting with cancer, but like almost any kind of therapy, it has disadvantages such as severe side effects due to the high dose and/or unrestricted distribution within all body compartments. There have been numerous attempts to overcome these difficulties. The first option is to create a new active compound, what has shown to be very costly and, in many cases, ineffective. The other solution is to develop a new way to transport and release of existing drug in the organism using targeted drug delivery systems. Doxorubicin has been selected as a cytostatic substance that are already approved for medical use. The strategy is based on two features; entrapment of the active ingredient within the carrier by associating it with polymer and release it using external trigger guided by an imaging technique. The doxorubicin can be associated with heparin or enoxaparin. In order to implement the heparin/doxorubicin complex into the carrier structure, the thermodynamics of the aggregate formation need to be quantitatively described. The isothermal titration calorimetry has been used to extract the quantitative measures of its formation and stability, necessary for the designing both; pharmacological strategy and production process. To this end, the theoretical model of the binding has been developed and tested on well-defined experimental systems using heparins with different polymer lengths.

Keywords: HEPARIN, DOXORUBICIN, ITC, BINDING MODEL

1. Introduction

Chemotherapy is the well-established pharmacological approach in the treatment of cancer. Despite unquestionable successes application of chemotherapy carries serious risks of potentially dangerous side effects, which imposes a limitation on the drug dose. One of the ongoing efforts is focused on the designing pharmacological strategy, which is based on supramolecular devices. The strategy utilizes a well-established compound as an element of the device design to deliver and release it at the selected locations within the body. The main objective of our ongoing research is the construction of a new kind of carrier that will be injected to a patient body and a drug released by an external trigger such as ultrasounds. This approach will allow for a precise release of drugs at tumor location. The design of the effective release mechanism requires that the encapsulated drug is associated with a compound which will prevent its uncontrolled release.

For these purposes, the suitable polymer for the drug association needs to be selected and thoroughly described. At the first step, the binding stoichiometry will be determined. Next, the effect of different solvents on the aggregate stability will be evaluated. To this end, the calorimetric experiments have been performed and obtained thermograms analyzed.

For purpose of this research, the doxorubicin has been selected as an active compound and heparin and enoxaparin as polymer scaffolds for doxorubicin association. Doxorubicin is a substance that is widely used in oncology, hence its application as an active ingredient has already been approved by authorities.

2. Measurements

In order to collect the high-quality experimental data for model fitting, we test the variety of experimental arrangements. Base on these studies doxorubicin at concentration 1.84 mM as titrant was selected. As substance in the cell, we use 0.045 mg/mL of both heparin and enoxaparin dissolved in 10 mM HEPES. The doxorubicin and heparin solutions were prepared before each experiment. Before use, every solution was degassed for 30 min with mixing at temperature 22 °C. All measurements were performed using ITC calorimeter (TA Instruments NanoITC 2G). The volume of the sample cell and the titrating syringe were equal to 1019 µl and 250 µl respectively. Each experiment consisted of 25 injections of 10 µl volumes, except the first one, which was equal 1.14 µl and discarded in the subsequent analysis. Times between injections were set to be 300 s. All measurements were performed at 22 °C.

Results

Example of thermograms, obtained in the experiment when enoxaparin was titrated with doxorubicin, are shown in Figure 1, whereas the same experiment performed with heparin is shown in Figure 2. Left panel shows row experimental data, whereas right panel the same data corrected for the baseline. When 0.045 mg/mL heparin was titrated with 1.84 mM doxorubicin similar but not identical thermograms were collected (Figure 2).

![Figure 1. Example of thermograms obtained when 0.045 mg/mL of doxorubicin dissolved in 10 mM HEPES buffer (pH = 7.4) was titrated by 0.045 mg/mL of heparin.](image1)

![Figure 2. Example of thermograms obtained when 0.045 mg/mL of heparin dissolved in 10 mM HEPES buffer (pH = 7.4) was titrated by 1.84 mM doxorubicin.](image2)

Quantities of heat flow in titration experiments were appropriately corrected for the heat of dilution. Example of such data is presented in Figure 3, where doxorubicin was titrated into the 10 mM HEPES buffer alone.

![Figure 3 Example of thermograms obtained when 10 mM HEPES buffer (pH = 7.4) was titrated by 1.84 mM doxorubicin.](image3)
3. The model

The doxorubicin-polymer binding process was approximating with the binding model, in which binding seats are independent and ligands are not interacting with each other. The binding is mainly driven by electrostatic interaction, which is described by the Stern model since doxorubicin and polymers are charged (Figure 5 and Figure 4).

Figure 1 Single heparin monomer.

Figure 5 Chemical structure of doxorubicin.

4. Model fitting to experimental data

All fitting procedures were done using NanoAnalyze v.3.8.0 software made by TA Instruments. Experimental data was fitted to the equation 3, that is a one of model contained in software that we use. Fitting quality was assessed on basis of Monte Carlo simulation checking the susceptibility of the model to random disturbance s. The average deviation of \( \Delta H \) was determined to be about 5 % of the determined value and the \( n \) deviation was between 2 and 5 %.

\[
Q = \Delta H \times 10^{-9} \times (L_{\text{Bound},i} - L_{\text{Bound},i-1} \times (V_i - V_t)) / V_t,
\]

Where \( V_t \) – total volume, \( V_i \) – volume of ith injection.

\[
L_{\text{Bound},i} = \frac{a - \sqrt{(a - 1019 \times 10^{-6})^2 - 4 \left( \frac{1}{K_d} \right)^2 L_i T_i n}}{2 K_d}
\]

Where \( K_d \) - \( L_i \) - concentration of ligand after ith injection, \( T_i \) - concentration of cell after i-injection, \( n \) – stochiometric number.

\[
a = -\frac{1}{K_d} (L_i - T_i n)
\]

Where \( K_d \) - \( L_i \) - concentration of ligand after i-injection, \( T_i \) - concentration of cell after ith injection, \( n \) – stochiometric number.

The heat flow after each injection was calculated as an area under the peak calculated from thermograms.

Examples of experimental data along with fitted functions, for bot enoxaparin and heparin, are presented in Figure 5 and Figure 6. In both cases the difference between heats of binding and dilution are fitted.

Figure 6 Example of fitting the heat flow generated by interaction between doxorubicin and heparin with the independent binding seat model.

Figure 7 Example of fitting the heat flow generated by interaction between doxorubicin and enoxaparin with the independent binding seat model.

The average value for results of fitting experimental data determined for both polymers is presented in Table 1. Association of heparin with doxorubicin is accompanied by larger enthalpy change than that obtained for enoxaparin indicating stronger binding. This is accompanied by the large difference in a number of binding seats per heparin molecule and smaller dissociation constant.

Table 1 The average value of parameters retrieving from fitting of experimental data to the model.

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Unit</th>
<th>( n )</th>
<th>( \Delta H )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Heparin</td>
<td>M</td>
<td>98,68</td>
<td>-7,84</td>
</tr>
<tr>
<td>Enoxaparin</td>
<td>M</td>
<td>28,44</td>
<td>-6,55</td>
</tr>
</tbody>
</table>

5. Conclusion

Calorimetric data shows that the doxorubicin interacts with negatively charged polymers and that the interaction depends on the size (number of binding seats) on a polymer. Specifically, doxorubicin binds to heparin almost an order of magnitude stronger than with smaller enoxaparin. In addition, there are three times less binding seats on enoxaparin than heparin. The determined quantities are critical for the design of a carrier with tuneable parameters, which are important for an aggregate stability.

6. Acknowledgments

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7. References

MODELLING THE RELATIONSHIP BETWEEN SATURATED OXYGEN AND DISTOMS' ABUNDANCE USING WEIGHTED PATTERN TREES WITH ALGEBRAIC OPERATORS

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Abstract: Machine learning has been used in many disciplines to reveal important patterns in data. One of the research disciplines that benefits from using these methods is eco-informatics. This branch of applied computer science to solve environmental problems uses computer algorithms to discover the impact of the environmental stress factors on the organisms' abundance. Decision tree type of machine learning methods are particularly interesting for the computer scientists as well as ecologists, because they provide very easy interpretable structure without any practical knowledge in mathematics or the inner working of the algorithm. These methods do not rely only on classical sets, but many of them are using fuzzy set theory to overcome some problems like overfitting, robustness to data change and improved prediction accuracy. In this direction, this paper aims to discover the influence of one particular environmental stress factor (Saturated Oxygen) on real measured data containing information about the diatoms' abundance in Lake Prespa, Macedonia, using weighted pattern tree (WPT) algorithm. WPT is a decision tree method variant that combines fuzzy set theory concepts, like similarity metrics, fuzzy membership functions and aggregation operators, to achieve better prediction accuracy, improve interpretability and increase the resistance to overfitting compared to the classical decision trees. In this study, we use Algebraic operators for aggregation. One WPT model is presented in this paper to relate the saturated oxygen parameter with the diatoms' abundance and reveal which diatoms can be used to indicate certain water quality class (WQC). The obtained results are verified with the existing knowledge found in literature.

Keywords: ECOLOGICAL MODELING, ENVIRONMENTAL DATA, DIATOMS, FUZZY LOGIC, WEIGHTED PATTERN TREE (WPT), ALGEBRAIC OPERATORS

1. Introduction

The machine learning algorithms are more frequently used to discover underlying drivers of the environmental stress factors that affect organisms' abundance. This is very important in ecological science that studies ecosystems that are threatened by pollution or they are under recovery program. In this case, monitoring is very important, as well as the data analysis. Data analytics usually is done by statistical algorithms, like canonical correspondence, detrended correspondence or principal component statistical analysis. These techniques provide useful understandings of the underlying ecological processes. However, they are limited in terms of interpretability and in most cases, they suffer from subjective opinion of the domain expert. This is because the results are plotted on graph, from which the biological expert draws interpretations of the distances between groups and clusters of diatoms related with the environmental factors based on his previous knowledge. That gives the final model interpretation a degree of expert self-opinion, which should not be the case. That’s why more and more experts use modelling techniques where the expert opinion is reduced to minimum, instead, an underlying statistical procedure takes over to confirm the prediction model accuracy.

In this direction, the well-known ID3 [1], C4.5 [2] or CART [3] decision tree algorithms leave no room for expert influence, only in the stage when the model results needs to be verified with the existing knowledge found in literature [4]. Moreover, the decision tree algorithms produce easy interpretable model for which no mathematical knowledge is required, unlike the neural networks. There are various subgroups of decision tree algorithms, some of them differ on the type of heuristics used, some of them are different on how the model is learnt with different data partitioning strategies, and some of them on what type of sets is used to extract the knowledge (classical or fuzzy set theory). Fuzzy decision tree algorithm [5] is in a subgroup of decision tree algorithms that uses fuzzy set theory to improve descriptive and predictive performance of the models, as well as improve the interpretability of the models using fuzzy linguistic terms. Fuzzy linguistic terms play important role in interpretation, due to their similarity with the human language when transforming the model tree into rules. Beside this, the fact that in many research studies the fuzzy decision trees reported to have better performance than the crisp decision tree algorithms [6] at the expense of small increase of the time needed to build the model.

Further research is done in improving the fuzzy decision tree algorithms. In that direction, the authors in [7] give detailed description of the pattern tree algorithm, which further improves the accuracy of the fuzzy decision tree algorithm. This is done by combining different types of membership functions and aggregation operators with various similarity metrics to achieve not only multi criteria decision-making, but also improving predictive accuracy and producing a model that is more resistant to overfitting. The pattern tree algorithm produces fuzzy rules with linguistic terms that can be obtained from the traditional hierarchical tree like structure. Furthermore, for each branch, a similarity between the target attribute and the input attribute is obtained, which evaluate the level of confidence of predicting the output attribute with that input attribute. Since each dataset may contains multi-class target attributes, one pattern tree model is built for each class of the target attribute. In this way a forest of pattern tree models is obtained, without knowing which tree holds the highest confidence of predicting the target class from the descriptive attributes. In this direction, the authors in [8] have presented the weighted pattern tree algorithm (WPT), which weights each pattern tree model to a class of the target attribute. In this way, the decision-making expert can select which output model is confident of predicting a given class. The WPT algorithm uses the similarity value between the target class attribute placed at the root of the model tree and the fuzzy term of the input attribute on the root branch. The membership degree of each input attribute is obtained using the process of fuzzification, which transforms the crisp attributes into fuzzy attributes by using different mathematical functions (triangular, trapezoidal, Gaussian, etc.). These membership functions are widely used for fuzzification, depending on the nature of the input dataset and the purpose of the fuzzy system. Consequently, many researchers found out [9] that the fuzzification process has high influence on the accuracy of the classifier. Beside the different membership functions that WPT algorithm uses to build the final model, the WPT also uses different similarity metrics to find the most informative attribute related to the target class. Additionally, the WPT algorithm uses aggregation operators that relate each input attribute to the output attribute as operation between two fuzzy sets to narrow the search space. In both cases (similarity metrics and aggregation operators) there are many metrics and operators that may fit the modeler’s needs to obtain high predicting accuracy. We use the recommendations that we suggested in [10], which are based on the experimental evaluation with different membership functions.
In this paper, we obtain one WPT model that consist from four sub-models to predict the relationship between the diatoms abundances as indicators of water quality classes based on saturated oxygen parameter. The mathematical modelling is performed on ecological dataset that is comprised with ten input attributes and one output attribute. The ten input attributes represent the ten most abundant diatoms found in Lake Prespa water ecosystem [11] and one output target attribute that describes the ecological water quality class based on saturated oxygen parameter [12]. In this way, the obtained WPT model relates the diatoms’ indicator status with the certain water quality class based on saturated oxygen parameter.

The rest of the paper is organized as follows: Section 2 provides description of the WPT building blocks: membership functions, similarity metrics and aggregations operators, as well as dataset description. In Section 3, we present the WPT model, we discuss the results and verify the obtained knowledge with the existing knowledge found in literature. The main conclusions and our future work are outlined in the Section 4.

2. Algorithm Concepts and Data Description

The WPT algorithm relies on the fuzzy theory concepts like membership functions, similarity metrics and aggregation operators, same as the pattern tree algorithm. However, the WPT uses additional information from the tree root similarity value to assign a degree of confidence or weight each model. The performance of the model depends on the membership function that is used, as well as the type of the similarity metric and aggregation operator. Following the recommendation that we gave in [10], we use the Bell membership function for building model.

The Bell membership function is defined with three parameters \(a\), \(b\) and \(c\). In order to achieve complete evenness between the fuzzy terms, we replace the parameter \(a\) with 10, \(b\) is replaced by \(\sigma\) calculated using (1), while \(c\) is replaced with \(\mu\) (mean value of the range of each fuzzy term).

\[
\sigma = \sqrt{\frac{\ln(10)}{2 * \ln(0.5 + r)}}
\]

In equation (1), \(r\) stands for the length of the fuzzy range. After all these changes take place, the calculation of the Bell membership function fuzzy terms is made by

\[
f(x; \mu; \sigma) = \frac{1}{1 + \left(\frac{x - \mu}{10}\right)^b}.
\]

Additionally, very important factor that influence the model accuracy is the number of fuzzy terms used per attribute. This has effect on the interpretability of the models as well as on the type of analyses that is conducted on the obtained knowledge. That is why selecting the number of fuzzy terms can be done on basis of the needs of domain expert or based on experimental evaluation of the model. For this purpose, we use five fuzzy terms which corresponds with the number of classes used in the European Water Framework directive (Directive 2000/60/EC of the European Parliament) for water quality classification, where there are five categories (poor, bad, moderate, good and high).

The next component of the WPT model building process is selection of the appropriate similarity metric. The similarity metric can greatly affect the accuracy of the model as well as the selection process of the most confident model for prediction. For this purpose, we consider the same metric used in [10]. However, we want to note that maybe other similarity metrics, like Jacquard, Cosine or Squared Euclidean, could be more adequate for this purpose. The similarity metric \(\text{Sim}_{\text{RMSE}}\) used in [10] is based on the RMSE (Root mean squared error) distance metric and calculates the similarity between two fuzzy sets \(A\) and \(B\) as

\[
\text{Sim}_{\text{RMSE}} = 1 - \frac{2 \times \sum_{i=1}^{n} (\mu_A(x_i) - \mu_B(x_i))^2}{\sigma^2}.
\]

The results of the calculations using (3) reside in range between 0 and 1. To calculate this, the \(\text{Sim}_{\text{RMSE}}\) similarity metric uses the membership degrees for a given crisp value \(x_i\) in two fuzzy sets \(A\) and \(B\), which are denoted as \(\mu_A(x_i)\) and \(\mu_B(x_i)\). The value of the \(\text{Sim}_{\text{RMSE}}\) similarity is propagated in each branch all the way up to the root of the model tree. Using only the similarity metric for estimating the relationship between the input and output attributes leads to low performances of the models. Therefore, the WPT algorithm also uses fuzzy aggregation operators, which are operations over two fuzzy sets to learn better models. Typically, triangular norms and conorms are used in fuzzy induction algorithms, and also in fuzzy decision tree algorithms. In [10], we used two fuzzy aggregation operators: Algebraic AND (T-norm) and Algebraic OR (T-conorm), which are defined as

Algebraic AND = \(\mu_A(x) \times \mu_B(x)\)

Algebraic OR = \(\mu_A(x) + \mu_B(x) - \mu_A(x) \times \mu_B(x)\).

It is important to note that also some other Triangular T-norm or T-conorm aggregation operators can be used here, that may have influence on the performance of the model and its interpretation of the model.

The dataset used for modelling the relationship between saturated oxygen and diatoms’ abundances is obtained from the EU funded TRABOREMA [11] project. The goal of this project was to assess the ecological status of the Lake Prespa. During the monitoring stage, valuable data about the physico-chemical parameters as well as organisms’ relative abundance was collected. Overall, sixteen parameters were measured and 116 different diatom species are counted. For each sample, the relative abundance for all 116-diatom species is obtained. Using this type of monitoring, the relationship between the influencing factors and diatoms’ relative abundance can be discovered. In the ecological literature [4], the relationship between environmental stress factors and diatoms as bio-indicators is well established, but for many diatoms, this relationship remains unknown. The environmental stress factors in the established ecological literature are represented with water quality classes (WQCs) based on a certain physico-chemical parameter. These classification systems can be found in the ecological literature, like the classification systems for Conductivity [13], pH [13], [12] and Saturated Oxygen [12]. The saturated oxygen classification system defines five classes for the target attribute, which are given in Table 1.

| Table 1: Water quality classes for the saturated oxygen physico-chemical parameter. |
|---------------------------------|-----------------|
| **Name of the water quality class** | **Parameter range** |
| Oligosaprobous | > 85 % |
| β-mesosaprobous | 70% - 85% |
| α-mesosaprobous | 25% - 70% |
| α-meso / polysaprobous | 10% - 25% |
| Polysaprobous | < 10% |

Since WQC Polysaprobous doesn’t contain any values in the measured dataset, this class was removed. Therefore, the final dataset contains 4 WQCs based on the saturated oxygen parameter. Considering this classification system, it is obvious that using machine learning algorithms we face with typical classification problems, where the saturated oxygen WQCs are the possible values for the target or predictive attribute, while the relative abundances of the top ten most abundant diatoms are the input or descriptive attributes. By using the parameters’ settings described in the previously, in the next section we present the WPT model in order to describe the relationship between Saturated Oxygen and the diatoms as bio-indicators.
3. Results and Verification

Four models are obtained, one for each WQC, and for each model the highest similarity is given in Table 2.

Table 2: The highest similarity that is obtained from the WPT models for the WQCs.

<table>
<thead>
<tr>
<th>Name of the water quality class</th>
<th>Highest similarity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Oligosaprobous</td>
<td>0.5249</td>
</tr>
<tr>
<td>β-mesosaprobous</td>
<td>0.5620</td>
</tr>
<tr>
<td>α-mesosaprobous</td>
<td>0.6897</td>
</tr>
<tr>
<td>α-meso/polyosaprobous</td>
<td>0.8253</td>
</tr>
</tbody>
</table>

Based on the results in Table 2, the highest similarity is obtained for the WPT model for α-meso/polyosaprobous WQC. The model for this class is presented on Fig. 1. The highest similarity obtained with this model shows that it has highest confidence to predict the corresponding WQC. The model depicts the diatoms that can be used to indicate this WQC.

![Fig. 1 WPT model for the α-meso / polyosaprobous WQC for Saturated Oxygen. In brackets, the similarity between the membership degrees for a given fuzzy term for a diatom and the WQC is given. According to the model, the Cavinula scutelloides (CSCU) and Cocconeis placenta (CPLA) diatoms can be used as excellent indicators for α-meso / polyosaprobous WQC. The two other diatoms Cyclotella juriljii (CIUR) and Cyclotella ocellata (COCE) can be also used as excellent indicators since the similarity value between these two diatoms and the α-meso / polyosaprobous WQC is higher compared to the similarity values for bad indicating properties. For verification of the results, we compared them with the ecological preferences found in [4]. For the CIUR and NPRE diatoms no records exist for their ecological preferences because they are newly described taxa. The CPLA diatom is eutrophic with medium oxygen demand according [4], while the model shows that the CPLA diatom is an excellent indicator for waters with low values of saturated oxygen. On the other hand, the CSCU diatom is alkibiontic, freshwater to brackish water species, being oligosaprobic indicator with eutrophic preferences according [4]. The model gives directions that this diatom is an excellent indicator for α-meso / polyosaprobous class opposite from which the known ecological literature directs. And finally, according the model the COCE diatom is excellent indicator of α-meso / polyosaprobous WQC, which if also obtained by other models that we generated with other experiments, thus this could add additional knowledge in the literature for this diatom. According [4], the trophic ecological preferences are the only one known for this diatom and since the trophic state index classification is out of the scope of this paper, adding new knowledge regarding the saturated oxygen demand for this diatom, could enrich its indicating properties.]

4. Conclusion

In this paper, we presented a technique based on fuzzy set theory that could reveal the relationship between the saturated oxygen α-meso / polyosaprobous WQC and the ten most abundant diatoms found in Lake Prespa. We built a model that presents which diatoms can be used for indicating the WQCs for saturated oxygen. The results from the WPT model are compared with the known ecological preferences found in the literature.

In future, we plan to investigate the influence of other similarity metrics and aggregation operators to further improve the accuracy of the models. Other type of membership functions could be more suitable for diatom modelling, thus revealing more valuable knowledge from the measured data. Also, modelling other water quality classes or trophic index classes could increase the applicability of the algorithm.

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References