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SECTION 2. Applied mathematics. Mathematical modeling.

A MODERN APPROACH FOR SOFTWARE CONSTRUCTION OF TOOLS FOR MATHEMATICAL MODELING OF MASS TRANSFER PROCESSES IN CATALYTIC POROUS MEDIA

Abstract: This article discusses the main problems of software construction of mathematical modeling systems of underground processes on the investigation of the architecture of a number of well-known programs. There are different ways to construct software that might be more or less suitable depending on the nature of the physical problem to be solved. In this paper, we acknowledge the importance of methodology, architecture and object-oriented programming approach. A modern way for creating computer modeling systems of underground processes is provided. It includes a range of tools, software architecture, design patterns, a list of actual libraries and other hints. We demonstrated usage of this solution on our tool NanoSurface.

Key words: NanoSurface, software construction, mathematical modeling, mass transfer, nanoparticles

Language: English

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Introduction

The number of scientists during the investigation of processes of mathematical physics uses application packages. In particular, most widespread are Matlab, Maple, MathCAD. These packages allow to carry out experiments concordantly to the beforehand chosen numeral method. Such integrated environments appeared with intensive development of mathematical and computer design, as Comsol, RSOFT FemSIM and other. They allow to decide the different applied tasks of theory of resiliency, electromagnetism, dynamics of liquids and gases, design mechanical cooperation, mass transfer and others like that by means of both mathematical raising of task (system of equalizations) and from the physical point of view (choice of physical model, for example model of diffusion). These packages are universal and well adapted for engineers that want to apply the prepared mathematical model to the certain terms.

Next to that, for the design of difficult run-time processes scientists aim to perfect the existent mathematical models of geophysics. They present the big collectives of scientists, job of that performances is creation of own software products (NADRA - 3d [1], ORCHESTRA [2], PHREEQC [3], HPx [4],

PHT3D [5], OpenGeoSys (OGS)[6], HYTEC [7], HYDRUS [8], TOUGHREACT [9], eSTOMP [10], HYDROGEOCHEM [11], CrunchFlow [12], MIN3P [13], PFLOTRAN [14] and other). Development of such software products requires additional knowledge from planning and constructing of software.

Common description some of the marked software products, their historical development, the list of the applied mathematical models, property and comparing to other programs is driven in the scientific articles and technical documentation [15], [11].

The purpose of this article is to review the major software systems of computer simulation of underground processes and analyze their components from the standpoint of software design, as well as a description of its approach to implementation of the software system.

Thus, an analysis of the above software systems has allowed to identify a number of shortcomings. The main ones are the following:

- Lack of an object-oriented approach when designing mathematical models or a large number of fields of classes, which are contrary to the approaches of managing complexity [16].



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• Program complexes of mathematical models are mainly represented by linear differential equations. This simplifies the use of numerical methods, but however, to describe real physical processes eliminates the complex relationships between equations are needed.

• Code a number of software systems not available for analysis. Also missing are a detailed history of changes in the open program code for tracking the evolution of development and easier understanding of the program.

• Awkward interface. There is no single standard input of the task boundary conditions.

The success of the development of any software product is choosing the right methodology, instrumental development and architecture of the program complex.

The development methodology

Some ideas of the technological approach to automating the calculations of mathematical modeling were proposed by Sergienko I. V., Skopetsky V. and Deineka V. S. [17].

It is noticeable that the mentioned software systems dynamically changed for a long time of development. This means that the classical waterfall development model is not suitable for these products through the study of new physical phenomena and continuous improvement of existing mathematical models. Therefore, for this class of problems well suited such an advanced and flexible development methodology like Agile Scrum & TDD.

Development tools

In the case when the project involves a large team, there is a need for the clear structuring of the changes made by every member, control over the execution of tasks, elimination of faults. For this purpose use special programming tools. Knowledge and use of such tools can increase productivity by more than 50%.

The main tool in development programs is an integrated programming environment (IDE). It usually includes a code editor, a compiler and debugger. The choice of IDE depends on the programming language. The most common programming languages for scientific computing – is a C/C++, Fortran, Python, Java, C#.

Another important tool for team development is version control system, which allows you on the same time work on a project for several developers and once this is corrected to accurately specify exactly which code it was. In this case, programmers are not prone to the syndrome of "works - do not touch", because I can safely delve into the most complex experiments with the program and at any time to return to the "code that worked" regardless of the number of experiments that were performed. Moreover, if the user suddenly wants to make a

slight change when the program is promising, but not completely operational, all that will need to switch to stable branch, to make the necessary changes to satisfy the user request and to switch back to the main trunk of development. Popular version control systems are GIT, SVN, Mercurial. These systems are free. To work with them developer need to have the repository (where the code will be stored). The following services are available free of charge on the web services <https://github.com>, <https://bitbucket.org>, etc.

For setting goals, monitoring their implementation and discussions with team, programmers, mathematicians and testers we recommend to use the project management system. For small projects widely popular free system trello (<https://trello.com>).

Software Architecture

Lately, there was a talk about the unification approach to the creation of software products, the standardization of mathematical models and create a unified registry [18]. This will allow to combine efforts of many groups of scientists to create a more versatile software complexes. However, not all developers decided to publish on public the source code. Only three of all of the above programs contain the public source code (HYDRUS, PFLOTTRAN, PHREEQC). Only one of these, indicated current latest version (PFLOTTRAN).

It is obvious that to ensure code reuse, you should separate the logic of the numerical simulation from the view (input and output) data. In the design of software systems using high-level languages this is achieved using classes and design patterns. It is worth noting that this is the most critical part when designing the architecture.

NanoSurface

Try to consider the above shortcomings in the programming of software systems for mathematical simulation of underground processes and correct approaches to developing them when creating your own software complex NanoSurface. This complex developed in the study of mathematical modeling of mass transfer of salt solutions in catalyst and dispersion media.

Consider the class hierarchy of NanoSurface. The first version of this software package carried out computer modeling of the process of migration of saline solutions in a catalytic porous medium in the presence of filter traps [19]. For a numerical solution to the boundary value problem we used the method of finite differences. The obtained finite difference analogs of the differential equations. For finding the values of unknown functions used sweep method. This built the corresponding differential equation in prorating. The program code includes an implementation of the sweep method, and all



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mathematical operations for output coefficients of the sweep carried out before beginning programming.

The next versions of NanoSurface simulated vertical migration of radionuclides in catalytic porous medium in linear and nonlinear cases [20, 21], taking into account the diffusion of the skeleton

of the soil [22] the non-isothermal conditions [23], the porosity of particles [24] in unsaturated porous media [25], as well as other factors the technical implementation of numerical modeling, describing mathematical model, it is difficult to realize the ideal software.

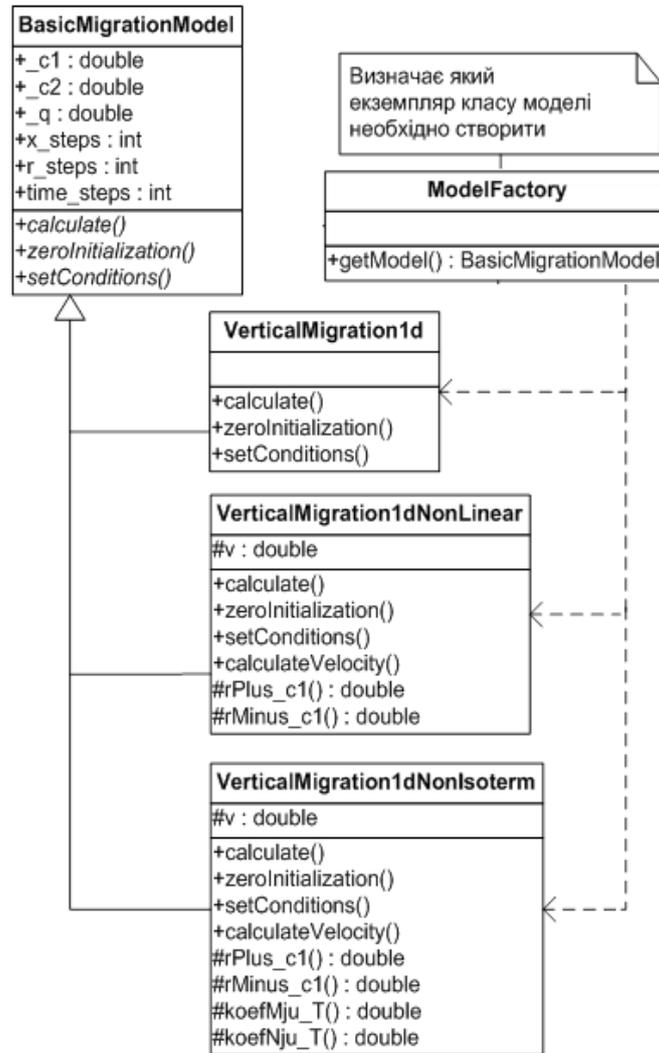


Figure 1 - The hierarchy of the main classes of mathematical models NanoSurface.

At the same time for numerical experiments is important to compare the obtained results with the previous one. Therefore, based on the original model [19] was designed BasicMigrationModel base class and all subsequent classes formed a hierarchy of classes (figure. 1). And user interface has simple selection of necessary mathematical model.

In the UML diagram (figure. 1) shows a portion of a class to understand the overall structure of the complex. The basic logic of the mathematical model located in abstract class BasicMigrationModel with virtual methods for setting boundary conditions required data fields and calculations. Derived classes for specific models implement the appropriate

methods and enhance the functionality of the base. In order to decide which class instance must be created, used design pattern "Parameterized factory method" (Factory Method). It is in the concealment of a particular class must be created and returned under the guise of a common abstraction. In our case, the class factory method ModelFactory presented by getModel(), which depends on the user's choice selects the desired class of mathematical models.

The class hierarchy of the user interface to specify initial and boundary conditions programmed mathematical models organized in a similar way. There is a parent class with a minimum number of controls and its child classes extend the functionality.

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When you click the start calculation is called a factory method for creating a common abstraction model, and further work is going on with it.

Thus, don't need to remember an instance of a class has been created. All requests happen with a pointer to the model (table. 1), and call methods of required classes is done using virtual functions setConditions(), calculate() etc.

Table 1
Examples of the use of General abstract mathematical model

```
// Initialization
model->zeroInitialization();
// Assignment of boundary conditions
model->setConditions(...);

// Calculate
model->calculate();

// Plotting
graph1 = new GraphWidgetSimple("Concentration c1",
model->_c1, ...);
graph2 = new GraphWidgetSimple("Concentration c2",
model->_c2, ...);
```

Architectural pattern for separating logic and user interface. Special attention is paid to the NanoSurface method calculate() that is responsible for numerical calculations. In the first versions of the program, this method had the form given in table 2.

Table 2

Method calculate()

```
// The basic cycle time
for (int k = 0; k < time_steps; k++) {
// Calculation of rate of filtration
/* Calculation of the equations with q
Factors driving direct and reverse*/
// Calculation for the equation
with c2
alfa[1] = 0; beta[1] = _c2[0][k];
// The coefficients of the sweep
for (int i = 1; i < x_steps; i++) {
a[i] = ...; b[i] = ...; c[i] = ...; f[i] = ...;
}
// Directly
for (int i = 1; i < x_steps; i++) {
alfa[i+1] = b[i] / (c[i] - alfa[i] * a[i]);
beta[i+1] = (a[i] * beta[i] + f[i]) / (c[i] - alfa[i] *
a[i]);
}
// Reverse
for (int i = x_steps - 1; i > 0; i--) {
_c2[i][k+1] = _c2[i+1][k+1] * alfa[i+1] + beta[i+1];
}
```

```
// Calculation for the equation of c1
//The coefficients of the sweep
//Direct move , reverse
// ...etc for all other equations
} // end of loop over time
```

It is noticeable that the code of the mechanism of the sweep method is repeated for each equation. In this regard, it is placed in a separate class to address the problem of code reuse. It is also allowed to choose and explore different methods of sweep to compute (ordinary, counter, block, etc.). After the corresponding refactoring code method, calculate() has acquired the following form (table 3): The software package NanoSurface is written in the programming language C/C++ using the Qt framework. This gives the opportunity to prepare the program without significant source code changes to work in such operating systems as Windows, Linux, MacOS. In the user interface (figure. 2) signing input fields is carried out using the library Qwt MathML Renderer". It allows the use of the mathematical markup language MathML (Mathematical Markup Language). This greatly simplifies the understanding of the interface of the complex, as provided by the full graphic compatibility of field names with their counterparts in the mathematical model.

Table 3
Method calculate() after refactoring

```
ThomasBaseAlgo * thomasAlgo =
ThomasFactory::getAlgo(algoUserSelected);
// The basic cycle time
for (int k = 0; k < time_steps; k++)
{
// Calculation of rate of filtration
/* Calculation of the equations with q
The coefficients of the sweep
The use of the sweep selected by the user */
// Calculation for the equation with C2
//The coefficients of the sweep
for (int i = 1; i < x_steps; i++)
{
a[i] = ...;
b[i] = ...;
c[i] = ...;
f[i] = ...;
}
// The use of the sweep selected by the user
thomasAlgo->performSweep(_c2,k,a,b,c,f);
/* Computation of the equation with C2
The coefficients of the sweep
The use of the sweep selected by the user*/
// ...etc for all other equations
} // end of loop over time
```



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The results of numerical experiments can be represented as 2D/3D graphs and tables. Table data presentation is typical and implemented via standard QTableWidget class. We inherited this base class by our own TableWidget to provide additional functionality to export data to a file and a table view with concentration values data. Graphics in 2D view are represented in the widget GraphWidgetSimple that is a wrapper class for QwtPlot. This class is part of the Qwt library which includes a variety of graphical elements (dials, compasses, thermometers, etc.) for programs that require graphical representation. NanoSurface wrapper provides

additional functionality in the choice of time step scaling, grid, comparison of many graphs, the choice of display style etc. Similarly, Graph3DWidgetSimple implemented by a widget that is a wrapper class for Q3DSurface. This class is part of the Qt Data Visualization module, whose main purpose is to visualize data in three-dimensional space, includes the construction of 2D cross sections of 3D data interaction with the mouse (zoom, rotation, selection of data), perspective and orthographic projections, it uses OpenGL engine for rendering, settings themes.

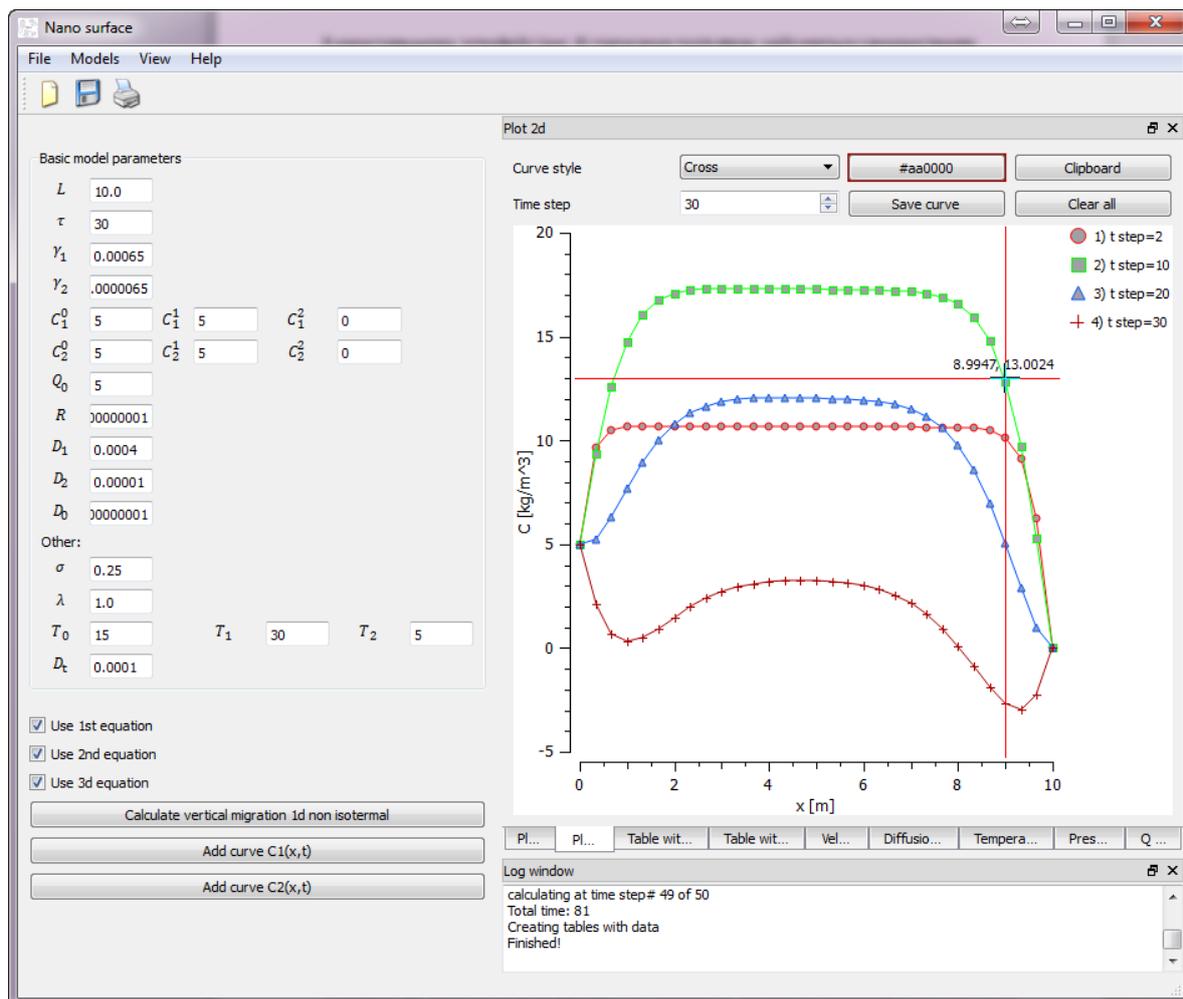


Figure.2 - The program interface of NanoSurface.

The main menu contains items for loading and saving the boundary and initial conditions, choice of the mathematical model, view, help working with the program and a description of the mathematical models.

Conclusion

During the last two decades have witnessed the rapid development of software tools for

mathematical simulation of underground processes. This led to the emergence of a variety of software systems for the numerical solution of problems modeling physical, hydrological, biological and geochemical processes in the porous media vadose zone.

However, progress does not stand still and requires addressing new challenges, in particular, to

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consist the development process of such complexes coordinated with each other.

This article conducted a brief analysis of several software solutions from the point of view of design and construction. A new approach to the creation of a program complex of mathematical modeling on the example of cross-platform software complex NanoSurface, which includes a selection of tools, building architecture, use modern patterns of software design and use of relevant libraries are provided.

The complex relationship between the equations of the mathematical model in NanoSurface

done through the mechanism of virtual functions and a pattern of the factory method.

Abstracted interface to the concrete implementation of the selected user mathematical model provided by a model pointer to abstract class. It allows to unify display and analysis, regardless of the selected mathematical model.

However, the issue of creating a user-friendly interface for selection of parameters of the mathematical model remain open. Therefore, the work on software product NanoSurface requires further improvement.

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