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Aiwlib library as the instrument for creating numerical modeling applications

A. V. Ivanov[1], S. A. Khilkov[2]

Keldysh Institute of Applied Mathematics
[1] ORCID: 0000-0001-5132-3748, aivanov@keldysh.ru
[2] ORCID: 0000-0003-2702-5630, khilkov.s@gmail.com

Abstract

Aiwlib library is a library for **C++11** and **Python** languages, which is aimed for the development of high-performance computing numerical simulation applications running under **GNU/Linux OS**. It also provides means for batch calculations, search through results using multiparametric filters and visualisation of results.

The visualization is supported of data given on uniform rectangular grids of high dimension in the form of two-dimensional slices with an effective change in the position and orientation of the slice; data given on spherical grids; arbitrary surfaces in three-dimensional space defined on triangular unstructured grids; voxel visualization of data given on uniform three-dimensional grids; visualization of the magnetization distribution under micromagnetic or atomistic modeling.

The library was applied for development of software packages for seismic, plasma physics and turbid medium optics. It was also turned useful for solving fundamental and applied problems concerning the magnetic materials study and creating spintronics devices, simulation of field development for the oil reservoir that contains kerogen with in-situ combustion taken into account, simulation of poroelastic medium problems and hydraulic fracture problems.

Keywords: numerical simulation, visualization, HPC applications.

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1. Introduction

There are at least three different ways to speed up a process of development of an numerical simulation application: choosing the right architecture, using high level libraries and metaprogramming (code generation), with help of computer algebra systems among other things.

Last decades shown that development on interpreted languages which has dy-

namic typing (so called "duck typing", for example Python, Ruby) is faster by an order of magnitude than development with aid of traditional compiler-based languages with static typing (C/C++, Pascal, Fortran). On the flip side, the resulting application performance is low, Python application is 10-30 times slower than C++ one depending on the problem type.

A numerical simulation program usually can be divided into two parts the computational core and the interface. The computational core is written with care. Its modifications are arguably rare since it has to provide the best performance. Yet the interface is modified continually to match different setups and its performance is of no importance since the most part of computational costs fall on the computational core activities.

The ideal architecture for the numerical modelling application is the combination of the interface written an interpreted language with dynamic typing (we chose Python [1, 2]) and the computational core written in an traditional compiler-based language which uses the static typing (aiwlib is written in C++11). To connect the parts we are using SWIG tool [3]. The core is compiled as the shared library and is imported to python as custom module. This approach, for one, allows us to solve the calculation parameters assigning problem efficiently. In the simplest case parameters values are listed in the control file, which is written in Python, and they are edited on an as-needed basis. The aiwlib library has its own build system based on GNU Make [4]. It provides short (3-4 lines) user Makefile for such projects.

There are packages based on a similar architecture. A well-known system Matlab uses its own interpreted language, which is focused on implementing complex algorithms in terms of linear algebra, carrying out calculation and visualizing the results. However, it is possible to implemented an individual function in the C language and load it as shared library. The numpy library includes a number of algorithms applied

mathematics written in C and advanced visualization tools that are called from Python.

However, the Matlab system is commercial (with a fairly expensive license). On top of that implementing an C extension to Matlab is not an simple task. The numpy library is widely used (and in fact it is a full-fledged replacement for Matlab), but the overhead for implementing complex algorithms only in Python are too high, even if we take the calls of high-level functions on C into account. Unlike analogues, the aiwlib library instantiates main classes and function of the kernel written in C++11 to Python, which makes it possible to use almost the same code in both languages, choosing the optimal decomposition of the application from the ratio "code performance / development speed" point of view.

There is a persistent myth that numerical modeling applications written in C++, are inferior in performance to applications written in Fortran. In reality, it is much easier to write inefficient applications in C++ than in Fortran, but obeying several simple rules [5], erase the difference in performance. On the contrary, quite a few tools, provided to the developer in modern C++ language, significantly speed up effective implementation of complex computational algorithms. In particular, LRnLA (locally recursive non-local-asynchronous) algorithms, which provide extremely high performance in problems of numerical simulation [6, 7, 8, 9], were implemented on combination of C++ and Python languages with heavy use of the C++ templates mechanisms.

The choice of C++11 standard in aiwlib is explained by the fact that, on the one hand, this standard gives a number new features (for example, variadic templates), and on the other hand, it is already well established and is supported by quite old compilers on most current clusters and supercomputers.

The second way to accelerate the creation of a numerical simulation applications is making use of high-level libraries. At the moment there is a huge number of libraries that implement both complex data structures (containers, for example, lists and various trees), and computational algorithms (SLAU solvers, fast Fourier transform, etc.). Even if we limit ourselves to

C++ libraries we can mention boost, Eigen, gmm++ and MTL4 as examples. The core of the aiwlib library is close to the library blitz++.

The aiwlib library complements the traditional functionality of similar libraries with developed debugging tools, elements of linear algebra with a number of specific operations, various containers (including arrays of arbitrary dimension based on the Morton Z-curve and unique spherical grids based on the subdivision of a dodecahedron), means of carrying out mass calculations and developed means of visualization.

Visualization tools consist of the shell for a standard gnuplot plotter,

allowing with minimum effort to build a print quality graphic, and a number of specific utilities for visualizing data on a spherical grids,

surfaces, distributions of magnetic moments, etc. Unlike standard tools

(eg paraview), aiwlib library viewers have a relatively poor window interface (which is partly compensated by the developed command-line interface) and are focused on handling large amounts of data.

The third way to accelerate the creation of numerical simulation applications is the metaprogramming (automatic code generation) and various systems computer algebra [10, 11]. There are some tools in the aiwlib library for implementation of this approach (in particular, converting algebraic expressions from Python language to gnuplot, C++ and LaTeX formats is used in the gplt utility), but this is rather complex topic and is beyond the scope of this article.

The previous version of the library aivlib (with the letter "V", [12]) was successfully developed for over ten years, until it became clear that the elimination of the accumulated list of drawbacks requires breaking of the backward compatibility. This article is devoted to the second version of the library which is referred to as aiwlib (with the letter "W", [13]). Versions are incompatible but they can be applied to one project simultaneously (from the point of view of the compiler those are different libraries).

2 Library core

2.1 Debugging tools

The aiwlib library provides advanced debugging tools which take into account the specific nature of numerical simulation applications. The <aiwlib/debug> header file in C++ consists of init_segfault_hook() function definition, the debug output macros WOUT and WERR, the macro

WCHK, checking the values of expressions for nan and inf, WEXT and WEXC macros, which allow print information from the stack when an exception is raised or a segmentation fault occurred, and WASSERT and WRAISE macros to trigger an exception.

All macros print messages, which mention the source file, line number and function, to the standard output stream or the standard error stream. The macros (except the WRAISE macro) only work if the EBUG macro is defined, for example, by using the "-DEBUG" compilation option or the "debug=on" argument of make, otherwise, the macros are ignored by the compiler. The macros listed can take as arguments an arbitrary number of expressions. Here is the fragment of code

int a = 1; double b = 2.5; WOUT (a, a + b, a * b + 3);

which after compiling and running will print to the standard output stream the text

 # test.cpp main () 14: a = 1, a + b = 3.5, a * b + 3 = 5.5

The WERR macro outputs information to the standard error stream. It accepts any expression which result can be printed to the stream std::ostream with the aid of the operator "<<".

The WCHK macro checks the values of its arguments (which should be the results of evaluation of floating point number expressions) on the values of inf and nan. If at least one argument did not pass the check, an error message is displayed, and an exception is raised.

Macros WEXC and WEXT form special objects based on templates std::tuple on the stack. Those objects contain copies of

the arguments, that practically does not affect the performance. When the stack frame is destroyed (for example, the normal return from the function) objects with copies of macro arguments are destroyed without side effects. When an uncaught exception is raised or segmentation fault occurred the accumulated information is printed to the standard error stream. The WEXC macro is thread ignorant thus it may be used in multithreaded mode, but it does not handle segmentation faults. WEXT macro works similarly, but it registers objects in the global table, hence it is thread unsafe. If an segmentation fault occurs information from all the objects registered in the global table is printed to the standard error stream. To enable the processing of segmentation faults you must call the function

init_segfault_hook();

This approach is often more convenient than a memory dump analysis with the help of debugger. To begin with, the debugger can not show the history of changes for arbitrary variable, while the WEXC and WEXT macros can (this requires calling several macros). Secondly, when you run your application on a supercomputer, the amount of memory to dump may become too large for analysis.

When the processing of segmentation faults is enabled, a call stack is also displayed. It can be analyzed by the standard addr2line tool.

The first argument for the WASSERT macro should be a condition. If its value is false, an exception is raised.

2.2 I/O Streams

The aiwlib library provides I/O streams (abstract base class aiw::IOstream and its successors aiw::File and aiw::GzFile), based on the standard FILE streams and the zlib library. Aiwlib streams differences from standard std::iostream streams are larger performance (due to the elimination of an extra buffering), the availability a type-safe analog of the printf method, the ability to map fragments of a file with automatic garbage collection and operations "<" and ">", which are overloaded as binary IO operations for all current data types and containers, including STL types.

2.3 Elements of linear algebra

The aiwlib library defines the template for the vector aiw::Vec<D, T=double>, parametrized by dimension (length) D and cell type T (double is default). For this type traditional operations addition, subtraction, scalar multiplication and comparison operations (for an effective checking if the point lies in a D-dimensional parallelepiped), componentwise multiplication, a module and maximum calculations and so on are overloaded. The Vector type with int as the cell type has an alias named aiw::Ind<D>. It is used as an index when accessing cells of multidimensional grids.

A multidimensional area traversal operation (D nested loops) is implemented:

aiw::Ind<D> N = ...; // size of an area

for (Ind <D> i; i ^= N; ++ i) {...}

Typically, instantiating C++ templates to Python with SWIG requires a special SWIG instruction for each instance of the instantiation. The Instantiation is accompanied by the automatic generation and the compilation of the large amount of C++ code, while the SWIG capabilities to handle C++11 standard extensions are limited. However, any alternative which allows binding C++ and Python is significantly harder for an end user. Since the internal representation of data in objects of the type Vec<D, T> is trivial, the aiwlib library implements a special mechanism for instantiating such object, based on the interaction with the SWIG type control system. Eventually for vectors no instantiation is required: in Python it is enough to import a module aiwlib.vec to get transparent access to objects Vec<D, T> (for all current types T) which are present in the C++ code with all their capabilities.

In order to instantiate containers described further (multidimensional and spherical grids) to Python, it is necessary to assemble a separate module for each type and dimension using the make utility, for example

make MeshF3-float-3

leads to the assembly of the module aiwlib.MeshF3, containing a three-dimensional grid with float as the cells type.

2.4 Multidimensional Grids (Arrays)

The most efficient approach for implementing multidimensional arrays is to create in memory a traditional one-dimensional array (vector) and emulate the multidimensionality with aid of an address arithmetic. For this to happen it is necessary to define a one-to-one correspondence between the index of the cell of the multidimensional grid $I=(I_x,I_y...)$ and the offset in one-dimensional array *f*.

Obviously, there are many different solutions to this problem, however the traditional way is the dictionary order of cells

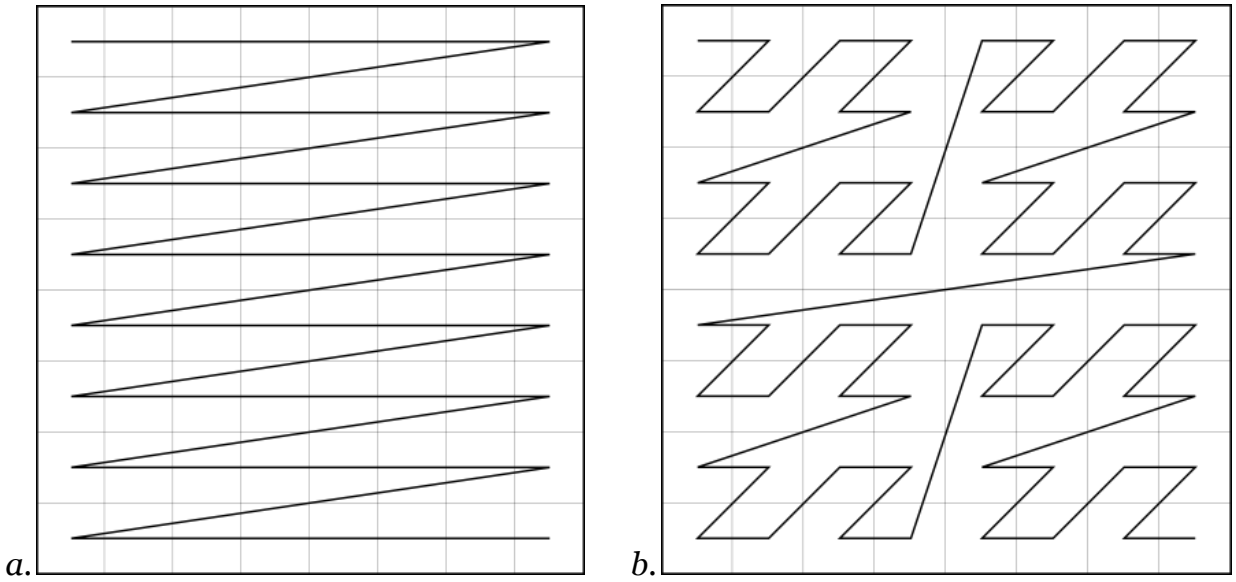
$$f = I_x + N_x I_y + N_x N_y I_z ..., \quad (1)$$

where the x-axis is the "fastest", the data in memory is localized along the x-axis.

There are different axis orders available, for example, in traditional multidimensional arrays of language C of the form T arr [Nx][Ny]... the x axis is the "slowest". In general case, the traditional solution can be written as

$$f = p_0 + \vec{I}\cdot\vec{S}, \quad (2)$$

where p_0 is the offset of the zero cell, $\vec{S}$ is the offset vector of the cell with the index (1,1,1...).



a. *b.*

Fig. 1. Traditional traversal of multidimensional array (a) and traversal based on Morton Z-curve (b)

If a multidimensional array is a *D*-dimensional hypercube with side size equals 2^R cells the traditional approach is reduced to constructing the offset *f* in the form

$$f = I_x\cdot\mathbf{2^0} + I_y\cdot\mathbf{2}^R + I_z\cdot\mathbf{2}^{2R} + ... = \sum_{k=0}^{D-1} I_k\cdot\mathbf{2}^{kD} = \overbrace{...\underbrace{i_z^{R-1}...i_z^0}_{R\ бит}\underbrace{i_y^{R-1}...i_y^0}_{R\ бит}\underbrace{i_x^{R-1}...i_x^0}_{R\ бит}}^{D\ групп\ бит}, \quad (3)$$

where *k* is the coordinate axis number (from 0 to *D*), i_k^l is the l-th bit in I_k. One can suggest alternative order *f*

$$f = \overbrace{\underbrace{i_{D-1}^{R-1}...i_y^{R-1}i_x^{R-1}}_{D\ бит}...\underbrace{i_{D-1}^{1}...i_y^{1}i_x^{1}}_{D\ бит}\underbrace{i_{D-1}^{0}...i_y^{0}i_x^{0}}_{D\ бит}}^{R\ групп\ бит}, \quad (4)$$

resulting in an order based on a fractal Z-curve of Morton (Lebesgue) [14], Fig. 1.

In contrast to the traditional traversal, one based on Z-curve significantly facilitates the construction of various adaptive-recursive grids and ensures high locality of data (the nearest neighbors in the configuration space, as a rule, are located close in memory). That may increase the efficiency of calculations in the so-called memory-bound problems [7, 8]. A fixed set of array sizes and low random access efficiency are drawbacks of the Z-curve traversal. The calculation of the offset f by the multivariate index of cell I is an fairly expensive operation from the computational cost point of view.

The aiwlib library provides two array classes Mesh<T, D> and ZCube<T, D>, parameterized by the type of the cell T and the number of dimensions D of the array. The Mesh class implements the traditional traversal and ZCube implements traversal based on the Z-curve. Both classes have random access operator by multidimensional cell index (an object of the type aiw::Vec<D, int>); efficient traversal for the array and efficient access to the nearest neighbors of the cell, including the periodic boundary conditions option; adjustment of uniform grids (limits and step) and logarithmic scale on some axes, allowing to calculate the coordinates of cell centers and cell corners in configuration space; piecewise-constant, linear, local cubic and B-spline interpolation (can be adjusted independently for individual axes); transposition (change of order) and flip for axes; efficient saving data to disk and loading data from the disk in binary and text formats in order to analyse or to visualize it later.

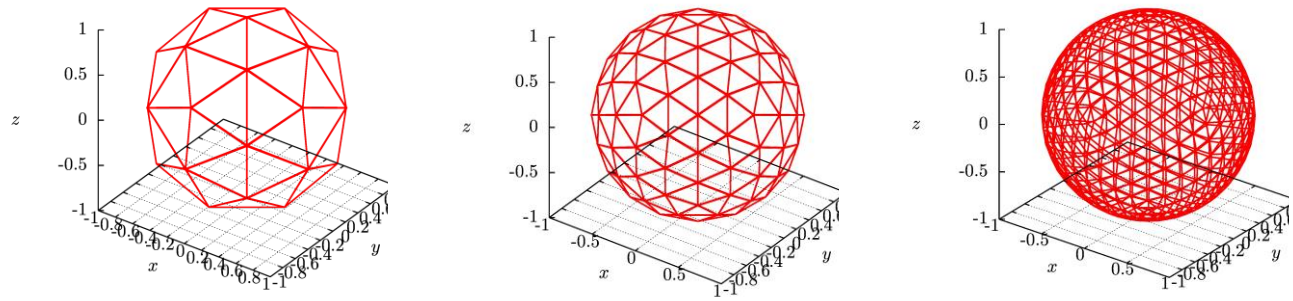
In addition, the Mesh class also allows you to cut rectangular subdomains (grids of the same type, but smaller) and build slices (meshes with less number of dimensions). Any grid conversion (transposing, axis flipping or subdomain and slice cutting) returns a new grid object which provides alternative access to the same data area. The memory allocation and move operations for large amounts of data are not performed. In addition to increase of the performance, that introduces extra opportunities for data processing, for example, a two-dimensional section of a three-dimensional grid may be filled with new data, which will lead to a change of the original three-dimensional grid.

Furthermore, if necessary, it is possible (by connecting the appropriate header file meshop) to overload the "unary minus" operator, binary +, -, *, /, ^ (like in degree) operators and functions abs, acos, asin, atan, ceil, cos, exp, fabs, floor, log, log10, sin, sinh, sqrt, tan, tanh, atan2, fmod, pow over instances of Mesh <T, D> classes.

Expressions of arbitrary complexity are allowed, so they may contain overloaded operations and functions whose operands are instances of Mesh<T, D> classes or any other data for which the expression will make sense if the instances of classes Mesh<T, D> are substituted with values from one cell (type T).

The expression itself does not lead to any action unless the operator "<<==" occurred, the left operand of which must be an instance of the class Mesh<T, D> and the right is the expression. In this case, a cycle is started on grid cells, on the left hand side of the operation "<<==", for each grid cell on the left the result of the expression on right hand side is calculated and is written separately. The implementation is close to the grid-operator approach, developed, for example, in [15].

2.5 Spherical meshes



$R = 0$ $R = 1$ $R = 2$

Fig. 2 Spherical mesh based on the recursive subdivisions of the dodecahedron with different numbers of division steps (ranks).

The aiwlib library provides a mesh on a sphere composed of almost regular

triangles constructed by recursive decomposition of the dodecahedron [16, 17], Fig. 2. Compared to traditional spherical coordinates with two strong singularities on poles, a spherical mesh based on a dodecahedron has 12 weak inhomogeneities corresponding to centers of the dodecahedra faces. At these points the mesh nodes are incidental to five cells, in contrast to six for all the remaining nodes, and these cells are also most distorted (one of the angles is 72° instead of 60°).

The mesh contains 60*4^R cells and 30*4^R+2 nodes, where R≥0 is the rank of the partition. A search for the cell into which a three-dimensional vector points algorithm, the operations for traversing the mesh and accessing to the neighbors of the cell, the algorithms for calculation the coordinates of vertices, centers and areas for cells are efficiently implemented.

The mesh is provided as the Sphere<T> template, parameterized by a cell type, The template also includes methods for writing and reading data in a binary format. In addition, there is an utility for visualizing such data in the library. In numerical simulation a spherical mesh is usually a convenient substitute for traditional spherical coordinates, apart from the absence of strong singularities, a spherical mesh with the same fineness (maximum cell size) requires approximately half the number of cells due to absence of condensation of nodes near the poles.

Data from a spherical mesh can be saved to and loaded from a disk in a binary format, and can also be visualized using the uplt viewer described below, Fig. 3.

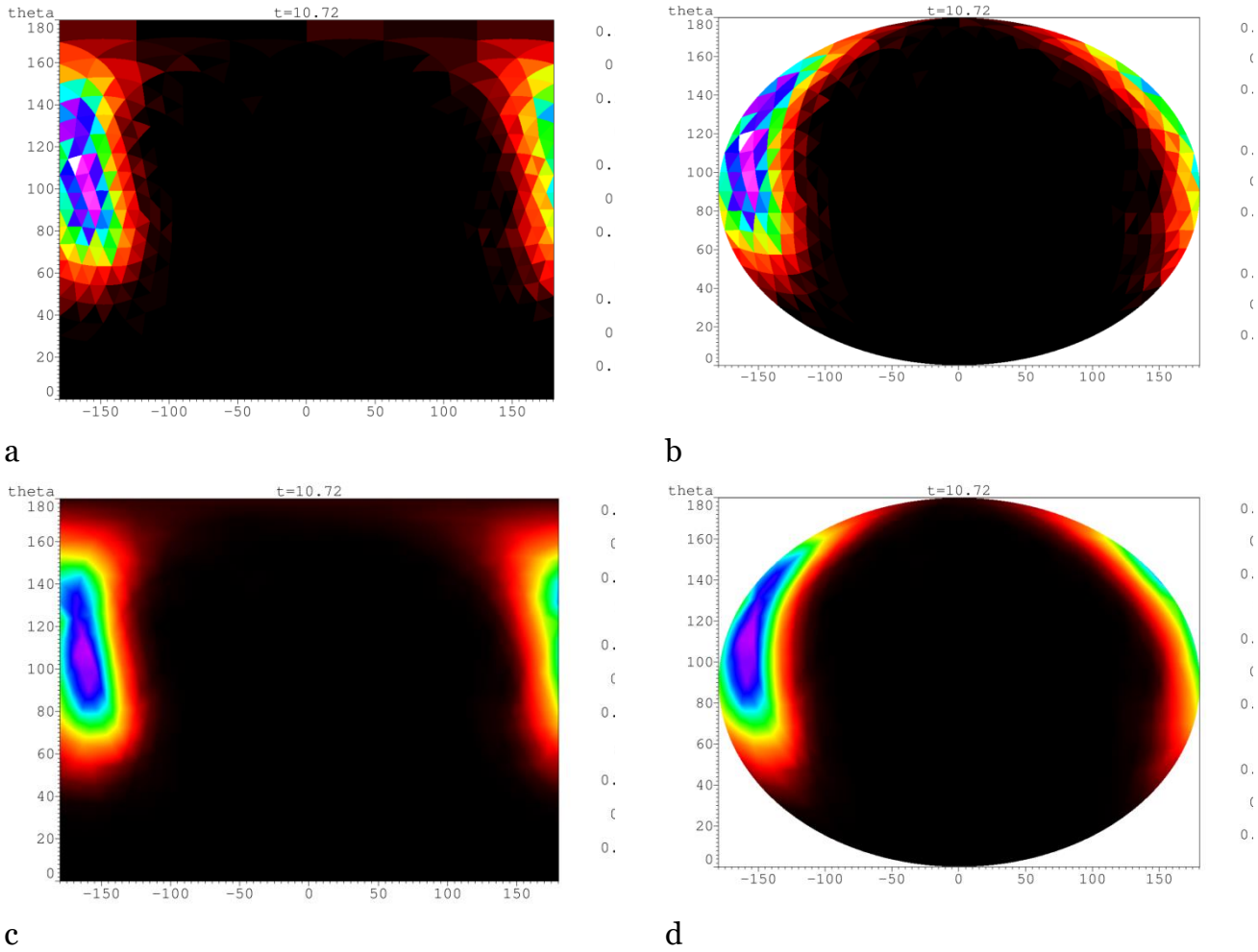


Fig. 3. Visualization of the distribution function of magnetic moments on a spherical mesh of the third rank in the coordinates θ,φ without interpolation (a, b) and with linear interpolation in cells (c, d) with aid of Mercator projection (a, c) and with aid of Mollweide projection (b, d)

3 The batch start calculations and analysis of results

While performing numerical simulation, the results of each calculation should be saved with the information on the calculation parameters used and algorithms. Otherwise, the results tend to turn into an abstract picture after a while. If there are quite a number of methods and libraries to store parameters, yet saving of an algorithm is a problem, and the only acceptable solution for it today is to store the source code of the application as well.

When performing batch calculations (for example, in the analysis of the behavioral dependence of a device on several parameters and the calculation of its phase diagrams) requires a mechanism, which allows us to start the application multiple times with different parameters automatically. It also preferable to have control over the allocation of resources within the framework of local network or a cluster.

To analyze the results, a multiparametric search through the calculations is required. Thus the results of calculations should be kept in special, ordered way. It should be possible to search for specific versions of the source code. This problem may be solved manually, for example, placing the results of calculations on a well structured directory tree, but this approach requires a strict self-discipling of a user and is tangled by the fact that during the calculation the order criteria may expand and change dramatically.

For large series of calculations, a neat solution to the above problems may take considerable amount of time and effort. Several working groups have developed their own libraries, providing the means to simplify the process of writing the environment [18, 19, 20], but there is no unified approach for the problems.

The RACS system described in this section (Results & Algorithms Control System, the system to control results and algorithms) provides:

• setting the calculation parameters at startup for applications written in Python and C++;

• automatic saving parameters and source codes for each calculation;

• batch execution of calculations (cycled by parameter values) and load balancing both on local machines and on clusters with MPI;

• control points manipulation for C++ applications, even on clusters with MPI;

• advanced tools for multi-parametric searches, analysis and results processing.

The following points were in focus while the RACS was developed:

• easy usage (minimal modification of the debugged code is required);

• concise and intuitive syntax when starting calculations;

• the ability to process results using the operating system and third-party utilities without losing the data integrity;

• Integration with other utilities, printing the data in gnuplot format with gplt headers, reading metainformation about calculations by other utilities.

Even for a low-skilled user, RACS automatically provides necessary "minimum" of the calculation self-discipline (storing of source codes and

parameters). As a result, the user is able to fully concentrate on

dealing with his problem.

While developing the RACS system, special effort was taken to facilitate the application of RACS on the finished program. RACS is written in Python and is primarily aimed on applications, written in C++ (high-performance computing core) and Python (upper control layer of the application and the interface parts) linked together by the SWIG utility [3]. In order to start calculations, RACS can be attached to applications written only in C++ without using Python.

As a rule, the calculation starts from the current (working) directory containing the source codes of an application, main executables in Python or C++, etc. For each calculation in repository (some directory) an unique directory is created. Calculation parameters, source codes and simulation results are stored there. The set of calculation parameters in form of a dictionary is saved as a file .RACS located in the calculation directory. The format of .RACS is defined by the standard Python module named pickle.

In addition to the .RACS file .src.tgz file may be created in the unique calculation directory (archive containing the source code of the application which performed the calculation) and in case of "daemonized"

calculation the logfile (standard output and standard error streams combined) is also placed there.

The repository can be structured in an arbitrary manner, i.e. it is the directory tree where calculations are grouped according to user requirements (for example, by values of key parameters).

Individual calculations and repositories can be moved by OS tools, sent over the network, etc.

The application is started as command line instruction, but loading the RACS system adds extra command-line arguments which make it possible to change the calculation parameters, to start batches and to change the service parameters of the RACS system. It is possible to start calculations batch looping through the list of the parameters values and to balance the computer load induced automatically.

In order to analyze the simulation results the racs command-line tool is introduced. There were attempts to create a version with a GUI in 2010. However, it quickly became clear that the GUI does not provide any advantages, but it complicates the interaction with other command-line

utilities essentially. It also introduce problems with remote work through ssh.

The tool allows you to display the dictionary of parameters for a separate calculation (contents of .RACS file), to select the calculations that meet different criteria, to print selected results in various formats, to modify selected calculations, or to delete them.

In fact, calculations placed under RACS form a non-relational database, where individual calculations are the records in the database, and repositories are the tables.

The racs tool is able to jointly process multiple repositories. Repositories are processed sequentially (in the order in which they were mentioned). Results are mergeed into a common selection (set of calculations).

The racs tool gives the user broad opportunities for multiparametric searching, analysing, joint processing and visualizing the large volumes of numerical simulation results. To date (the first versions appeared in 2003, the first publication [21] in 2007), RACS has proven itself useful to organize large series of calculations in various fields, i.e. seismic, modeling of the field development for kerogen-containing reservoirs with in-situ combustion taken into account, modeling of magnetic systems [22] and the development of spintronics devices [23], gasdynamics of the combustion [24], the study of resonant properties of nonlinear systems [25], etc.

4 Visualization utilities

4.1 The gplt tool, the typographic quality plotter based on gnuplot

The gnuplot application is one of the oldest visualization tools attributed to GNU project. Despite a number of shortcomings (primarily the low performance, especially for surface plots) gnuplot is still popular due to the flexibility, a variety of output formats and good graphs appearance. The plotting graph of typographic quality (with the correct fonts, axes labels, etc.) requires quite a lot of work. The gplt tool parses command-line arguments, generates a set of instructions, and runs make. Since the fact that many necessary parameters are set by default, and due to the concise syntax, a minimum of actions (keystrokes) is required to obtain a typographic quality plot in .pdf format with LaTeX fonts and formulas. In addition gplt-file containing the arguments of the corresponding call is formed for each plot. One can edit the file to change the plot if it become necessary.

The gplt tool is written in Python. It reads the comments in .dat files (text files with data to render). Special Comments (starting with #:) allows you to specify names for data columns, declare additional numerical constants, customize the column names displayed on plots for different output formats. The gplt tool is capable of using wide variety of expressions (Python code snippets) containing the column names for plotting. The gplt utility can also use metainformation (contents of .RACS files) about calculations in expressions while plotting graphs for calculations controlled by RACS system. The expression may be converted through abstract syntax tree in make, LaTeX, EPS, and other formats.

4.2 The uplt tool, the visualization of data on multidimensional and spherical grids as a set of two-dimensional slices

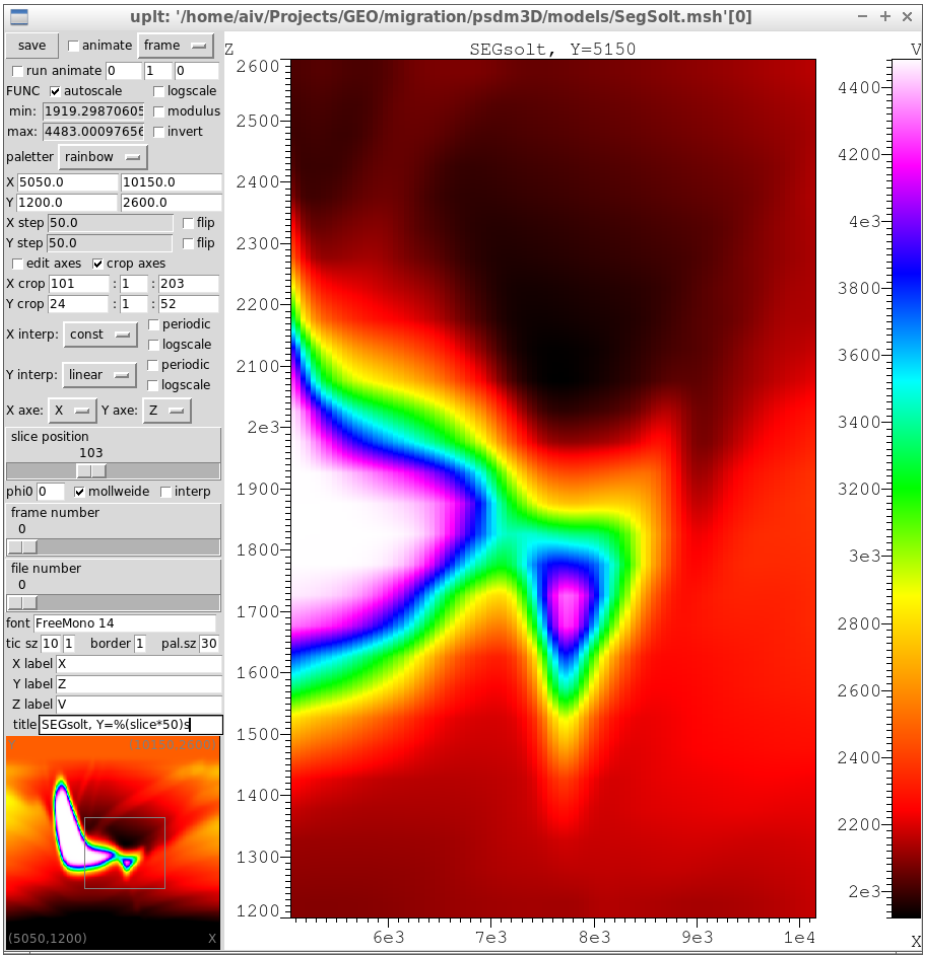


Fig. 4. Vertical slice of the depth-velocity model for well known international synthetic seismic dataset SEGsalt.

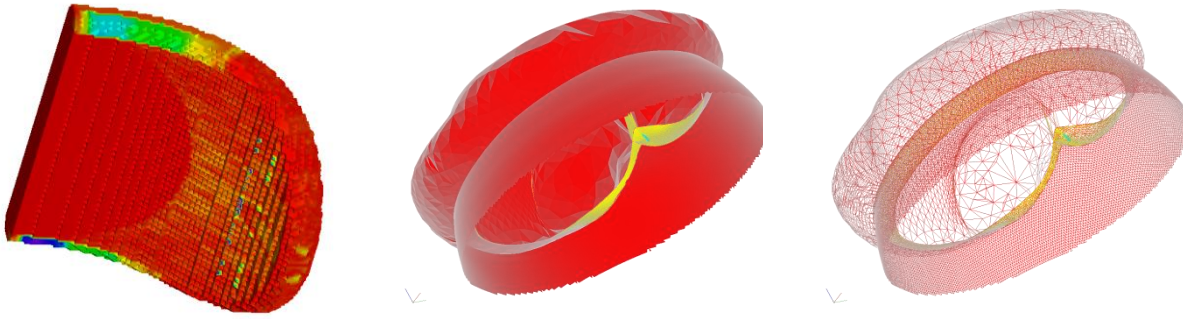
The uplt viewer is used to visualise the scalar functions of the form f(x, y), defined on uniform rectangular meshes or spherical meshes stored in the binary formats of the library aiwlib, Figure 4. The viewer is implemented in C++11 and Python languages. It uses Tkinter library and Python Image Library. In uplt viewer it is possible to adjust the palette and limits of the image in many ways. Uplt also supports logarithmic scales for any axis and different interpolation types. When the data written in one file as the sequence of independent frames (each frame contains data from one mesh), viewer allows you to navigate through the frames. For uniform meshes with number of dimension greater than two, two-dimensional slices are displayed instead of the full mesh. However the viewer makes it possible to select the orientation and position of the cut. It is possible to start animation (sequential drawing of files, frames in one file or movement of a slice through one frame) and automatic video compiling with the ffmpeg utility.

Rendering options are set in two ways from the graphical user interface and when the application starts with help of command line arguments. Uplt also supports PDF as image output format.

Despite the fact that the viewer does not utilise a graphics accelerator,

viewer achieves acceptable drawing speed for large (gigabytes or more) volumes of data.

4.3 The utility splt, the visualization of surfaces defined by unstructured triangular grids.



a b c

Fig. 5. Error level on an unstructured tetrahedral grid during the evolution of a surface with a movable boundary (a) and a wave front in the form of a surface during migration on SEGsalt international seismic dataset (b) and a so-called "wire" form for the same wave front (c)

The three viewers described below (splt, mplt and fplt) are built with help of a separate package AbstractViewer, which is not included in the aiwlib library. The package is focused on developing new 3D viewers in C++ and Python languages using OpenGL library and glut. It also permits to embed viewers in numerical simulation applications for displaying and analysis results during the calculations on GPGPU. The package was developed by S. Khilkov and is distributed under the GPL-v3 license.

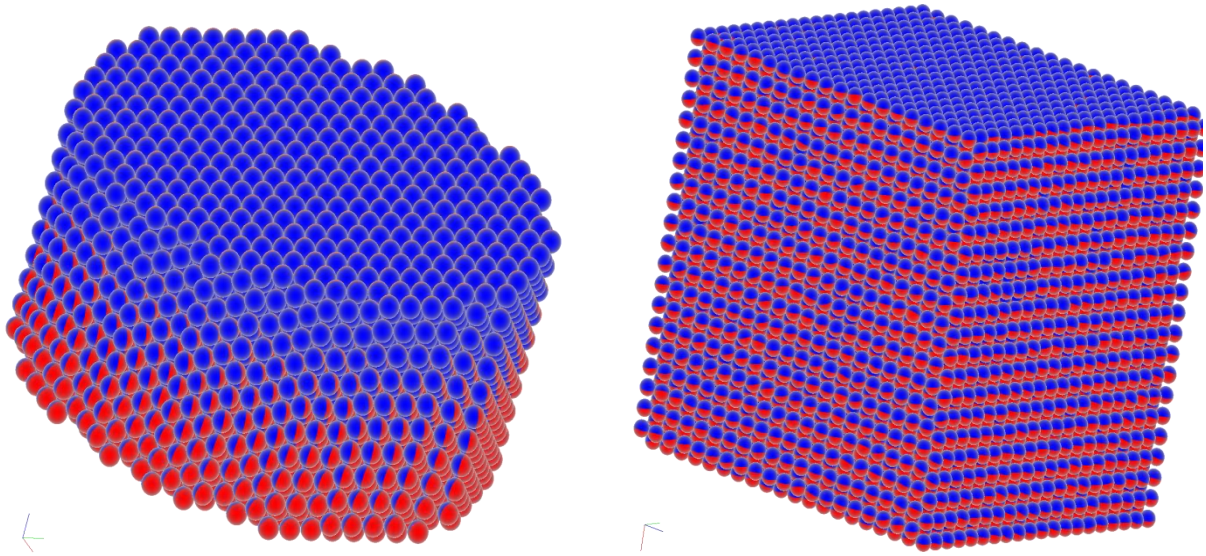
Due to the efficient use of a discrete video card, viewers have high performance. The interface is made in a deliberately "Spartan" style, the manipulator "mouse" allows you to rotate the image, all other actions are performed with aid of hotkeys and command line interface in the terminal. The command line uses the readline library, which provides autocomplete feature for the input buffer and access to the commands history. Terminal commands are executed in Python language, which makes it possible to to run scripts for generation a series of images, creation of the animation, etc.

All viewers supports palettes switching and color range limits adjustments. They implement clipping planes, scaling and rotating transformations of the image.

The splt viewer can display quite an arbitrary surface defined by an unstructured triangular grid (Figure 5), while tetrahedral grids are specified as sets of faces. Grids are stored in a binary format of aiwlib library. An arbitrary number of independent frames (instant grid states) could be placed in a single file consecutively. Grids in different frames may have different numbers of nodes and vertices. Viewer implements an efficient switching between frames.

Arbitrary data sets of type float4 may be associated with vertices and cells of a triangular grid (for example, coordinates and components are associated with vertices speed, and density is defined at cell centers). Each data field has an unique text name. During the visualization, it is possible to select arbitrary combinations of fields, the values of three fields are plotted along the axes xyz, the value of the fourth field is shown as the color. It uncovers broad potential for visualization and analysis of complex data, the detection of various dependencies and then studying their evolution in results of calculations.

4.4 mplt tool, the visualization of magnetic moments distributions and vector fields



a b

Fig. 6. Distribution of magnetic moments in the cylinder made of antiferromagnetic material which has incomplete fcc lattice (a) and for a cube made of ferromagnetic material with bcc lattice (b)

In order to visualize the distribution of magnetic moments, the aiwlib library provides the mplt viewer. The magnetization of a single cell/atom is represented by red and blue sphere (similarly to compass arrow) which blue pole is oriented along the magnetic moment direction. A three-dimensional array of such spheres conveys the distribution magnetization on the surface of the sample well (inner spheres are virtually not visible, Fig. 6).In order to study the magnetization distribution within the sample it is necessary to use slices and/or cut-off planes.

The viewer works with the data stored in a special binary format of the aiwlib library. The simulation results are stored in one file, which consists of a header describing the spatial distribution of the magnetic moments and data frames after it. Each frame contains the values of the magnetic moments at some point in time. To store the orientation of a single magnetic moment one can use either a vector of three float4 numbers (12 bytes), or the cell number on the spherical grid built with help of a recursive decomposition of a dodecahedron of the rank five (2 bytes, the accuracy is approximately 1°). The viewer efficiently displays arrays of up to 10^9 magnetic moments, the only limit is the video memory size.

4.5 fplt tool, the voxel visualization of three-dimensional uniform grids

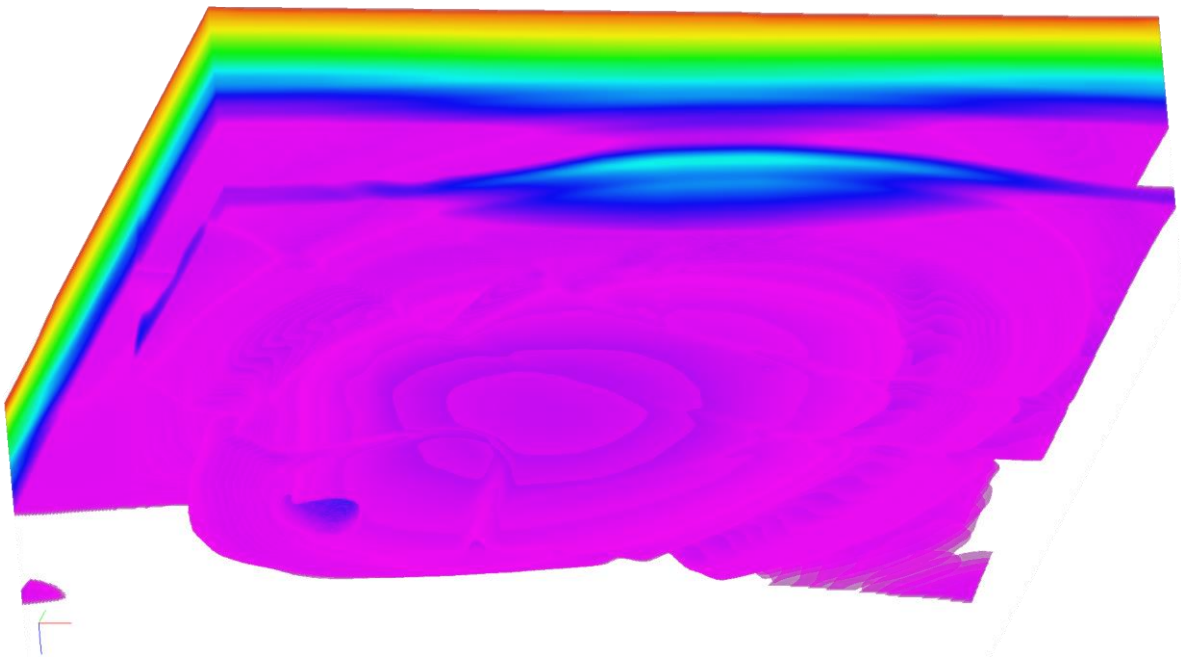


Fig.7. Three-dimensional image of a velocity-depth model of a known international synthetic seismic dataset SEGsalt.

The fplt viewer provides the voxel visualization of uniform 3D meshes saved in aiwlib library formats, figure 7. A pixel shader traces rays with an increment of the order around the grid cell size, taking transparency into account. The initial value (color) is considered invisible (completely transparent), the tracing of each ray is completed after achieving a given value in the pixel α-channel (default value is 0.95) [26] or if the ray escapes the data area.

5 Other modules

The aiwlib library has a number of additional modules for solving various specific tasks.

The construction of isolines which is implemented in C++; control points for stopping and continuing the calculation; serialization of data in the pickle format; the discretization of a Voronoi partition; means to collect and to store the metainformation about custom data types (structures) to use in postprocessing of calculations results; some elements of linear algebra and analytical geometry, including the projection construction and rotation operations; means for reading/writing test configuration files and configuring user objects.

An efficient way to parse the command-line arguments, allowing you to create your DSL (Domain-Specific Languages) implemented in Python; high-level module to work with date and time; the automatic detection of files containing the source code of the application written in C++ and Python languages, combined by the SWIG utility and compiled with make; the cost effective protocol for transferring data through sockets and high-level tools for developing simple network client-server applications; the conversion algebraic expressions from the Python language format into other formats with aid of the abstract syntax tree.

6 Conclusion

The first version of the aiwlib library was written in 2008, and some of its parts (the RACS system and the gplt tool) appeared in 2003. Over the years the library code evolved dramatically. The kernel code

became simpler, smaller, more stable, and its capabilities significantly expanded.

The aiwlib library and its previous version aivlib were used successfully in a number of projects: development software packages for the seismic prospecting [27, 28, 29], the physics of plasma [6] and the optics of turbid media [30]; solutions to fundamental and applied problems in analysing of magnetic materials and thecreation of spintronics devices [22, 23]; the research on resonance properties of superparamagnets [25]; simulations of the gas dynamics and the combustion [24], processes of the field development for kerogen-containing oil reservoirs, taking the in-situ burning into account, the material degradation and the blistering in the subsurface layers under the influence of the ion bombardment [31]; modeling of problems of poroelasticity and hydraulic fracturing of the formation [32]. In the meantime, the developed of visualization tools of the library played the important role in those projects. Due to efficient analysis of simulation results, debugging code and the adaptation of numerical schemes to the problems in question were greatly simplified.

The core of the library is distributed under the license Apache-2 (which permits to apply it in commercial projects with a closed source code), and visualization utilities are distributed under the GPL-3 license.

The aiwlib library development is continuing actively. We are intended to include in the library modules for the CUDA language, as well as templates (frameworks) for creating magnetic materials simulation codes and various variants of FEM/XFEM, since we have acquired sufficient experience in those areas.

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