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NPJSC «Abylkas Saginov Karaganda Technical University»,
Karaganda, Kazakhstan.
E-mail: sea_kitten_1@mail.ru

ANALYSIS OF THE USE OF THE PYTHON PROGRAMMING LANGUAGE FOR GEOLOGICAL MODELING OF SOLID MINERAL DEPOSITS

Ponomareva Marina Victorovna – Candidate of Technical Sciences, Associate Professor of the Department of Geology and Exploration of Mineral Deposits, NPJSC «Abylkas Saginov Karaganda Technical University», Karaganda, Kazakhstan, E-mail: mv_ponomareva18@mail.ru, https://orcid.org/0000-0001-8652-9607;
Ponomareva Yekaterina Vadimovna – PhD, Acting Associate Professor of the Department of Geology and Exploration of Mineral Deposits, NPJSC «Abylkas Saginov Karaganda Technical University», Karaganda, Kazakhstan, E-mail: sea_kitten_1@mail.ru, https://orcid.org/0000-0003-1322-6773;
Shirokaya Yekaterina Dysembekovna – Master's student of the Department of Geology and Exploration of Mineral Deposits, NPJSC «Abylkas Saginov Karaganda Technical University», Karaganda, Kazakhstan, E-mail: zernisska@gmail.com, https://orcid.org/ 0009-0007-8147-7917;
Tungushbayeva Ainash Tagaibekovna – PhD student of the Department of Geology and Exploration of Mineral Deposits, NPJSC «Abylkas Saginov Karaganda Technical University», Karaganda, Kazakhstan, E-mail: ajnastungusbaeva@gmail.com, https://orcid.org/ 0000-0002-4749-7785.

Abstract. Purpose. The main task of modeling is to identify the main, characteristic features of a phenomenon or process, its defining features. Geological modeling of deposits is one of the ways to organize, to structure and to visualize large arrays of obtained geological and geophysical data.

Methods. This paper deals with the process of developing a structural 3D model of the Nurkazgan Vostochny field using the Python programming language based on geological data obtained from the results of geological exploration within various periods with the use of the Geone library, the methods of which allow using both ordinary kriging and stochastic interpolation methods (extrapolation) of the initial data.

Findings. As a final result, it is possible to evaluate the distribution of lithological varieties in the modeled block and to export each of them in a convenient digital format for subsequent processing.

Originality. The Python programming language, unlike commercial implementations of 3D modeling programs, pro-vides complete control over the workflow and at the same time, due to the presence of a large number of modules for geological modeling and data visualization, is in no way inferior to them.

Practical implications. At the present stage of the geological science development, 3D modeling methods have be-come widespread, making it possible to develop realistic models of geological structures based on the use of various geophysical, geochemical and geological data. This circumstance is conditioned by the rapid development of computing facilities, and at the moment the geologist is provided with various tools that increase the efficiency of his work in the area under consideration.

Keywords: geological modeling, deposit, programming language, interpolation, Python, ore field, database, model, lithology.

М.В. Пономарева, *Е.В. Пономарева, Е.Д. Широкая, А.Т. Тунгушбаева, 2025.

КеАҚ «Әбілқас Сағынов атындағы Қарағанды техникалық университеті», Қарағанды, Қазақстан.

E-mail: sea_kitten_1@mail.ru

ҚАТТЫ ПАЙДАЛЫ ҚАЗБАЛАРАРДЫ ГЕОЛОГИЯЛЫҚ МОДЕЛЬДЕУ ҮШІН PYTHON БАҒДАРЛАМАЛАУ ТІЛІН ҚОЛДАНУДЫ ТАЛДАУ

Пономарева Марина Викторовна – техникалық ғылымдар кандидаты, «Пайдалы қазбалар кен орындарын геологиясы және барлау» кафедрасының доцент міндетін атқарушы, «Әбілқас Сағынов атындағы Қарағанды техникалық университеті» КеАҚ, Қарағанды, Қазақстан, E-mail: mv_ponomareva18@mail.ru, https://orcid.org/0000-0001-8652-9607;

Пономарева Екатерина Вадимовна – PhD, «Пайдалы қазбалар кен орындарын геологиясы және барлау» кафедрасының доценті, «Әбілқас Сағынов атындағы Қарағанды техникалық университеті» КеАҚ, Қарағанды, Қазақстан, E-mail: sea_kitten_1@mail.ru, https://orcid.org/0000-0003-1322-6773;

Широкая Екатерина Дюсембековна – «Пайдалы қазбалар кен орындарын геологиясы және барлау» кафедрасының магистранты, «Әбілқас Сағынов атындағы Қарағанды техникалық университеті» КеАҚ, Қарағанды, Қазақстан, E-mail: zernisska@gmail.com, https://orcid.org/0009-0007-8147-7917;

Тунгушбаева Айнаш Тагайбековна – «Пайдалы қазбалар кен орындарының геологиясы және барлау» кафедрасының докторанты, «Әбілқас Сағынов атындағы Қарағанды техникалық университеті» КеАҚ, Қарағанды, Қазақстан, E-mail: ajnastungusbaeva@gmail.com, https://orcid.org/0000-0002-4749-7785.

Аннотация. Мақсаты. Модельдеудің негізгі міндеті – құбылыстың немесе процестің негізгі, сипатты белгілерін, оның анықтаушы белгілерін анықтау. Кен орындарын геологиялық модельдеу – алынған геологиялық және геофизикалық мәліметтердің үлкен массивтерін ұйымдастыру, құрылымдау және бейнелеу тәсілдерінің бірі.

Әдістемесі. Бұл мақалада бастапқы деректер бойынша қарапайым кригинг және стохастикалық интерполяция әдістерді қолдануға (экстраполяция) мүмкіндік беретін Geone әдістері кітапханасының көмегімен әртүрлі кезеңдерде геологиялық барлау нәтижелерінен алынған геологиялық деректер негізінде Python бағдарламалау тілін қолдану арқылы Нұрқазған Шығыс кен орнының құрылымдық 3D моделін құру процесі қарастырылады.

Алынған деректері. Соңғы нәтиже ретінде модельделген блокта литологиялық айырмашылықтардың таралуын бағалауға және олардың әрқайсысын кейіннен өңдеу үшін ыңғайлы цифрлық форматта экспорттауға болады.

Түпнұсқалығы. Python бағдарламалау тілі, 3D модельдеу бағдарламаларының коммерциялық енгізулерінен айырмашылығы, жұмыс процесін толық бақылауды қамтамасыз етеді және сонымен бірге геологиялық модельдеу және деректерді визуализациялау үшін көптеген модульдердің болуына байланысты олардан ешбір кем түспейді.

Практикалық маңызы. Геология ғылымы дамуының қазіргі кезеңінде әртүрлі геофизикалық, геохимиялық және геологиялық мәліметтерді пайдалану негізінде геологиялық құрылымдардың шынайы модельдерін жасауға мүмкіндік беретін 3D модельдеу әдістері кеңінен тарады. Бұл жағдай есептеу қуатының қарқынды дамуына байланысты және қазіргі уақытта геологқа қарастырылып отырған салада оның жұмысының тиімділігін арттыратын әртүрлі құралдар беріледі.

Түйін сөздер: геологиялық модельдеу, кен орны, программалау тілі, интерполяция, Python, кен орны, мәліметтер базасы, модель, литология.

М.В. Пономарева, *Е.В. Пономарева, Е.Д. Широкая, А.Т. Тунгушбаева, 2025.

НАО «Карагандинский технический университет имени Абылкаса Сагинова», Караганда, Казахстан.

E-mail: sea_kitten_1@mail.ru

АНАЛИЗ ПРИМЕНЕНИЯ ЯЗЫКА ПРОГРАММИРОВАНИЯ PYTHON ДЛЯ ГЕОЛОГИЧЕСКОГО МОДЕЛИРОВАНИЯ МЕСТОРОЖДЕНИЙ ТВЕРДЫХ ПОЛЕЗНЫХ ИСКОПАЕМЫХ

Пономарева Марина Викторовна – кандидат технических наук, доцент кафедры «Геология и разведка месторождений полезных ископаемых» НАО «Карагандинский технический университет имени Абылкаса Сагинова», Караганда, Казахстан, E-mail: mv_ponomareva18@mail.ru, https://orcid.org/0000-0001-8652-9607;

Пономарева Екатерина Вадимовна – PhD, исполняющий обязанности доцента кафедры «Геология и разведка месторождений полезных ископаемых» НАО «Карагандинский технический университет имени Абылкаса Сагинова», Караганда, Казахстан, E-mail: sea_kitten_1@mail.ru, https://orcid.org/0000-0003-1322-6773;

Широкая Екатерина Дюсембековна – магистрант кафедры «Геология и разведка

месторождений полезных ископаемых» НАО «Карагандинский технический университет имени Абылкаса Сагинова», Караганда, Казахстан, E-mail: zernisska@gmail.com, https://orcid.org/0009-0007-8147-7917;
Тунгушбаева Айнаш Тагайбековна – докторант кафедры «Геология и разведка месторождений полезных ископаемых» НАО «Карагандинский технический университет имени Абылкаса Сагинова», Караганда, Казахстан, E-mail: ajnastungusbaeva@gmail.com, https://orcid.org/0000-0002-4749-7785.

Аннотация. Цель. Основная задача моделирования выявить главные, характерные черты явления или процесса, его определяющие особенности. Геологическое моделирование месторождений является одним из способов упорядочить, структурировать и визуализировать большие массивы получаемых геолого-геофизических данных.

Методика. В данной работе рассмотрен процесс построения структурной 3D модели месторождения Нурказган Восточный с помощью языка программирования Python на основе геологических данных, полученных по результатам проведения геологоразведочных работ за различные периоды с использованием библиотеки Geone методы которой позволяют использовать как обычный кригинг, так и стохастические методы интерполяции (экстраполяции) исходных данных.

Полученные данные. В конечном результате возможно оценить распределение литологических разностей в моделируемом блоке и экспортировать каждую из них в удобном цифровом формате для последующей обработки.

Оригинальность. Язык программирования Python, в отличие от коммерческих реализаций программ по 3D моделированию, предоставляет полный контроль над рабочим процессом и в то же время, благодаря наличию большого количества модулей по геологическому моделированию и визуализации данных, ни в чем им не уступает.

Практическое значение. На современном этапе развития геологической науки широкое распространение получили методы 3D моделирования позволяющие создавать реалистичные модели геологических структур, основанных на использовании различных геофизических, геохимических и геологических данных. Данное обстоятельство обусловлено бурным развитием мощностей вычислительной техники и на текущий момент геологу предоставлены различные инструменты, повышающие эффективность его работы в рассматриваемой области.

Ключевые слова: геологическое моделирование, месторождение, язык программирования, интерполяция, Python, рудное поле, база данных, модель, литология.

Introduction. The ore field of the Nurkazgan deposit is located in the outer zone of the latitudinal branch of the Devonian volcanic-plutonic belt and is confined to the junction of large Caledonian structures: the Erementau-Niyaz anticlinorium, the Semizbugy and Shakshan synclinoriums. This structural position determines the widespread development of volcanic, intrusive and volcanogenic-sedimentary formations of Devonian age in its structure. They make up the Tyulkuly ring volcano-plutonic struc-ture with the intrusive massif of the same name in the central part (Ponomareva, et al., 2023).

According to their structural position, the nature of the structure and lithological composition, the volcanic-sedimentary deposits are classified as the Zharsor formation of the Lower Devonian age.

The Zharsor formation (D_1žr) based on petrochemical and lithological features, is divided into lower and upper subformations.

The lower subformation (D_1žr1) is most widespread in the central part of the deposit. Within the subformation, two units have been identified.

The lower unit (D1žr11) is composed of agglomerate tuffs, less commonly lavas and automagmatic breccias of basaltic andesite composition with rare horizons of coarse tuffs of andesitic composition and thin lens-shaped interlayers of tuff siltstones or tuffites. In the upper part of the section there is a horizon of pelitic tuffites up to 100 m thick. The rocks have a greenish-gray and dark green color. They are largely hydrothermal-metasomatically altered, in some areas to full-blown beresites. The thickness of the unit is at least 550 m (Ivadilinova, et al., 2023).

The upper member (D_1žr1_2), whose lower boundary is conventionally drawn along the roof of the horizon of pelitic tuffites, at the base of the section is composed of alternating lens-shaped layers of pelitic-psammitic tuf-fites and tuff conglomerate breccias that form a unit with the thickness of about 170 m. Higher in the section, there is coarse-grained, less commonly, lithocrystallineclastic tuffs and lavas of andesidacite composition, including rare lenses of tuffaceous sandstones and conglomerates. All the rocks of the upper unit are subjected to hydro-thermal-metasomatic alterations, in some sites up to full-blown beresites. The thickness of the unit is more than 360 m.

Upper subformation (D_1žr_2). The deposits of the sub-formation are widely distributed in the western, northern and eastern parts of the field area a form the wings of the Tyulkuly structure. Most of the area of their development is covered by loose sediments (Levin, et al., 2021).

The subformation is composed of red tuffaceous sandstones of different grains alternating with lens-shaped layers of boulder-pebble conglomerates, gravelites and less commonly siltstones. Interlayers of gray-colored tuffaceous and volcanic-canomictic sandstones are of sharply subordinate importance in the section. In the lower part of the section, a horizon of coarse tuffs of dacitic-andesidacite composition is distinguished. The thickness of the subformation is at least 850 m.

Subvolcanic formations of the Early Devonian associated with volcanism of the Zharsor period, are widespread in the southern part of the ore field. They are similar in composition to the volcanic rocks of the formation and are represented by small bodies of various shapes ranging in size from 100 x 150 m to 500 x 1000 m; dike-like bodies with the thickness of no more than 10-11 m and the length of up to 150 m are rare. According to their composition, leucocratic basaltic, basaltic andesite and rarely andesidacite porphyrites are distinguished.

Cenozoic sediments in the form of a loose cover overlay the Paleozoic formations on approximately 50% of the field area. They are divided into the Kalkaman and Pavlodar formations of the Neogene and parts of the Qua-ternary system. The Neogene deposits are mainly represented by clays with rare interlayers and lenses of sands and pebbles; the Quaternary system: by loams, clays, polymictic fine- and medium-grained sands and less fre-quently pebbles (Kubich, et al., 2024).

Weathering crust. Weathering crusts of linear and area types are widely developed. On the surface, products of weathering crusts are rare, as they are overlaid with a cover of loose Cenozoic sediments. They are mainly developed from hydrothermally and tectonically processed rocks. The products of the weathering crust are clayey-crushed and clayey variegated formations. Their thickness varies from a few meters to 30 m, rarely, along fault zones, up to 50 m.

Intrusive formations in the territory of the Nurkazgan deposit are closely related to the Devonian volcanism, which led to the formation of the orebearing Tyulkuly volcano-plutonic structure. Among them, the Early Devonian- Karamenda complex of quartz diorites and the Middle Devonian complex represented by small intrusions and dikes of granite porphyries, subalkaline granite porphyries, and dikes of subalkaline diabases are conven-tionally distinguished.

The Early Devonian Karamenda complex of quartz di-orites ($q\delta_1D_1km$) of the first phase and granodiorites ($\gamma\delta_2D_1km$), granodiorite porphyries ($\gamma\delta\pi_2D_1km$), dike-shaped bodies of quartz diorites ($q\delta_2D_1km$) of the second phase of intrusion makes up the Tyulkuly massif and two small-sized massifs in the northwestern and northeastern parts of the field area (Isatayeva, et al., 2024).

The first phase of intrusion is represented by quartz diorites and quartz diorite porphyrites. They are the most widespread and for the most part are almost completely hydrothermal-metasomatically processed, which makes it difficult to resolve unambiguously the issues of the composition and age of the rocks. The least altered varieties are represented by medium-fine-grained quartz diorites of the soda series, which is characteristic of the Early Devonian intrusions. Increased alkalinity is closely related to intense potassium metasomatism. The formations of the second phase include massive and fluid granodiorites and granodiorite porphyries. Along the contact of rocks of the first and second phases of intrusion, orebearing intrusive breccias are developed, completing the formation of the intrusion (Cameron, et al., 2017).

Materials and methods. Based on the analysis of the initial information, about 84 exploration wells were drilled in the Nurkazgan eastern area, using which a geological description of the core was made. When processing the results of the description of core samples, the main lithological varieties were identified that were assigned individual codes (Figure 1). The methodology for constructing a structural 3D model using the Python programming language based on geological data obtained from geological exploration conducted over different periods was also applied in studying the geological structure of the northeastern part of the Zhezkazgan Basin with the aim of identifying polymetallic ore deposits. (Turner, et al., 2021).

The initial data is presented in the form of a database consisting of three tables (Figure 2):

- collar: the position of the exploration well mouth;
- survey: the spatial position of the wellbore;
- litho: intervals of tracking rocks along the borehole (Lamotte, et al., 2021).

lithe	code	color	color
weathering crust	1	burlywood	
clay	2	gold	
ferruginization in the WZ	3	darkslategray	
sandstones, siltstones, alluvium	4	saddlebrown	
tuffs and volcanomictic clastic rocks	5	yelow	
quartz diorites	6	pink	
quartz diorite rocks	7	purple	
granodiorites	8	green	
os-undiivided	9	orange	
quartz-diorite dike	10	gray	
granite-porphyry dike	11	red	
Middle-Devonian post-ore dike complex	12	indigo	

Figure 1 – Basic lithological varieties and their codes

Drillhole Name	Easting	Northing	Elevation	Target Depth
NE_801	357891	558684	539.86	1521.6
NE_802	357990	558680	543.48	1591
NE_803	358090	558677	546.86	1543.7
NE_804	358190	558674	554.81	1541.7
NE_805	358291	558673	566.42	1511.6

Drillhole Name	Distance	Dip	Azimuth
NE_801	1521.6	89.9	173
NE_802	1591	89.48	286
NE_803	1543.7	88.94	271.29
NE_804	1541.7	89.92	359
NE_805	1511.6	88.73	307

holeid	from	to	Lith	code
NE_801	0	931	tuf	5
NE_801	931	1403	O-S	9
NE_801	1403	1521.6	kvarcdioryt	6
NE_802	0	939.98	tuf	5
NE_802	939.98	1371.22	O-S	9

Figure 2 – Example of the collar, survey, litho database tables

At the first stage, it is necessary to prepare the initial data for further interpolation (Figure 3).

For this purpose, the Pygslib library was used that has been designed for rock analysis and geostatistical modeling, with the help of which the lithology distribution across the wells at equal intervals was obtained; in that case it was equal to 5 m. Thus, a table was obtained containing the coordinates of the central point of the interval, each of which was assigned a lithological code included in that interval (Groshong, 2006).

At the next stage, all the calculations were performed using the methods of the Geone library (Appendix 1). At the first step, codes corresponding to the lithology were determined and each of them was assigned a specific color. Next, a covariance model was defined that set the main parameters of interpolation using the simple kriging method (Turner, 2007).

To set the initial data of the interpolation method, it is necessary to determine the dimension of the modeling area:

• Origin: the anchor point of the modeling area (ox, oy, oz = 357300, 558600, -1300);

• Dimension: the number of cells along the axes (nx, ny, nz = 170, 160, 1900)

• Spacink: the cell size (dx, dy, dz = 10, 10, 10).

The initial data for points with specific lithology are loaded into the Points variable using the Pandas library methods (Bilibin S. I., et al., 2004).

At this stage, there is all the necessary information to transfer the data to the simulateIndikator3D() method of the Geone library (Demyanov, et al., 2010; Zakrevsky, et al., 2008):

• Category_values: lithological codes;

• Cov_model: a covariance model (it should be noted here that for each lithology category one can set one's own covariance model; in that case, to simplify the calcu-lation, only one covariance model was used to all the lithology categories);

• X: coordinates of points with the original lithology;

• V: a lithology category value;

• Method: interpolation (extrapolation) method, in our case "simple_kriging";

• searchRadiusRelative: an average search radius — 10;

• NneighborMax: thenumber of search points—12.

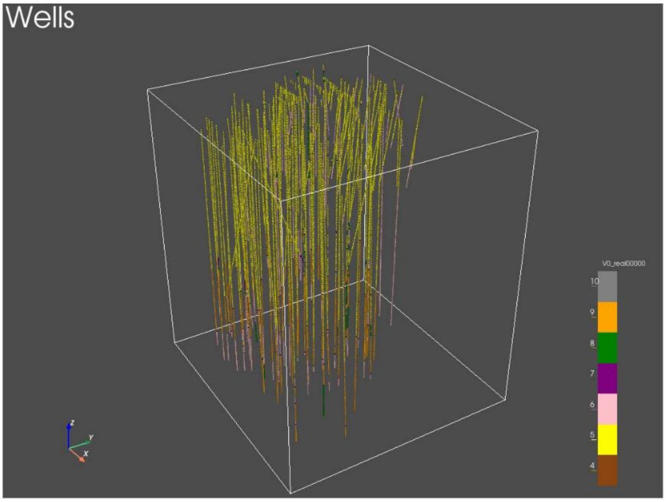


Figure 3 – Well lithology

Results and discussion. After performing the calculations, the results of the implementation are retrieved by assigning the “image” attribute to the variable. Visualization of the obtained modeling results is carried out using the drawImage3D_surface method (Kovalevsky, 2020; Michel, 2022):

• Custom_scalar_bar_for_equidistant_categories: the image of the lithology category scale (true or false);

• Custom_colors: a set of predefined colors in the li-thology category;

• Filtering_value: a category value that will be dis-played when printed.

This method additionally has a large number of set-tings for detailed visualization of certain modeling results obtained (Figures 4, 5).

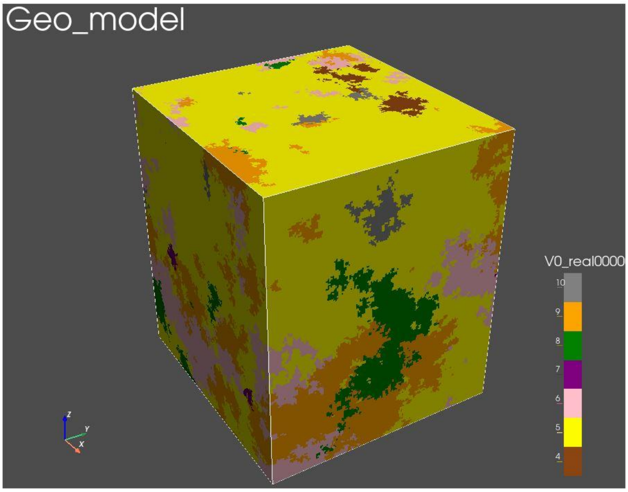


Figure 4 — General view of the modeling results

1)

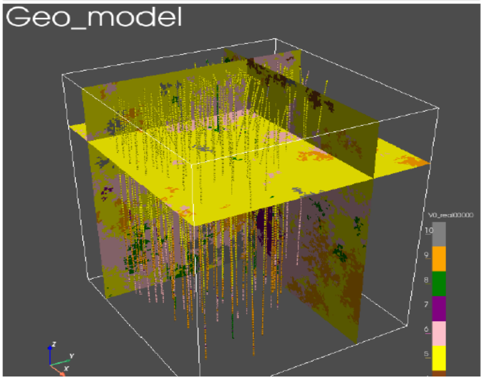
```
pp = pv.Plotter(shape=(1,1), window_size = [700, 700])

pp.subplot(0, 0)
data_points = pv.PolyData(x)
# ... set color for data points according to their value
data_points_col = [matplotlib.colors.to_rgb(
    categCol[np.where(np.asarray(category_values) == i)[0][0]]) for i in v]
    # color for data points according to their value
data_points['colors'] = data_points_col

pp.subplot(0, 0)
gn.imgplot3d.drawImage3D_slice(simul, plotter=pp,
                               slice_normal_x=x[10,0],
                               slice_normal_y=x[0,1],
                               slice_normal_z=x[50,2],
                               custom_scalar_bar_for_equidistant_categories = True,
                               custom_colors = categCol,
                               # categActive=[True, True, True], # by default...
                               scalar_bar_kwargs={'title_font_size':10, 'vertical':
                               text='Geo_model')
pp.add_mesh(data_points, rgb=True, point_size=2., render_points_as_spheres=True)

pp.link_views()

pp.show(cpos=(165, -100, 115)) # position of the camera can be specified
```



2)

```
pp = pv.Plotter(shape=(1,1), window_size = [900, 700])

pp.subplot(0, 0)
gn.imgplot3d.drawImage3D_surface(simul, plotter=pp,
                                 custom_scalar_bar_for_equidistant_categories = Tru
                                 custom_colors = categCol,
                                 filtering_value = (7,8),
                                 scalar_bar_kwargs={'title_font_size':20, 'vertical
                                 text='Geo_model')



pp.link_views()

pp.show(cpos=(165, -100, 115)) # position of the camera can be specified
```

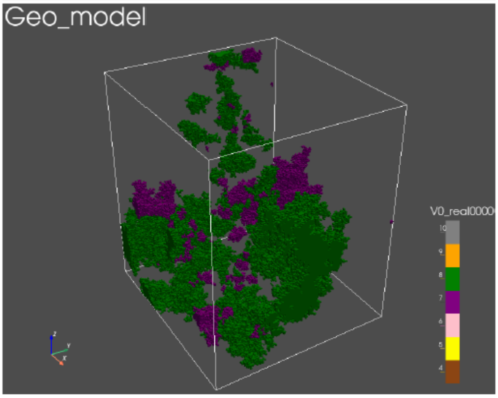


Figure 5 – The data preparation script and geological modeling process using the Python programming language: 1) import of necessary libraries; 2) designation of the necessary categories and color palette; 3) covariance model; 4) dimension of the modeled block; 5) loading source data; 6) solving the model using the simple Kriging method; 7) implementation; 8) display of wells and selected resulting planes; 9) display of selected categories (quartz diorites)

Conclusions. As a final result, it is possible to evaluate the distribu-tion of lithological varieties in the modeled block and to export each of them in a convenient digital format for subsequent processing (Kessler, et al., 2021).

After obtaining the first modeling results, the further task of the geologist is to determine the covariance model parameters for each lithological variety, which makes it possible to determine in more detail the boundaries of their distribution in the modeled block.

In general, the Geone library has an extensive set of implementing geostatistical methods, which allows geologists to configure accurately their geological models, including modeling various geological features, such as the content of components, processing the results of geophysical methods and much more.

The Geone library provides a number of advantages:

• flexibility and customizability of modeling geologi-cal data;

• the ability to model various geological structures, in-cluding ore deposits, layered rocks and others;

• access to a variety of modeling methods, including geostatistical and machine learning methods;

• open source and active support from developers and community;

• simple and convenient interface for use by both ex-perienced professionals and beginners.

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