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GeoReVi: A knowledge discovery and data management tool for subsurface characterization

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A B S T R A C T

Subsurface characterization is an interdisciplinary and multidimensional problem requiring contribution from numerous geoscientific and technical domains. In order to optimize and automate the process of subsurface characterization and structural modeling we developed a modular, open-source software system called GeoReVi (Geological Reservoir Virtualization). The tool implements the knowledge discovery in databases (KDD) process and utilizes techniques from visual analytics for interactive, interdisciplinary, database-bound knowledge discovery and communication. Multidimensional data sets – produced in subsurface and outcrop analog studies – can be imported, shared, transformed, projected, analyzed, modeled, grouped and visualized interactively in a custom-made graphical user interface. The underlying data model facilitates domain experts to efficiently work in multi-user environments. The knowledge discovery potential is illustrated with an exemplary case study.

Code metadata

Current code version	v1.0.1
Permanent link to code/repository used for this code version	https://github.com/ElsevierSoftwareX/SOFTX_2019_352
Legal Code License	GNU General Public License v3.0
Code versioning system used	git
Software code languages, tools, and services used	C#, XAML, WPF
Compilation requirements, operating environments & dependencies	Microsoft Windows, Entity Framework 6, HelixToolkit, Accord.NET, WPF, Caliburn.Micro, FontAwesome.WPF, DotSpatial, GeoAPI, ProjNET, LiteDB, MoreLinq, Extended WPF Toolkit, Math.NET
Support email for questions	contact@georevi.com

Software metadata

Current software version	v1.0.1
Permanent link to executables of this version	https://github.com/ApirsAL/GeoReVi/releases/tag/v1.0.1
Legal Software License	GNU General Public License v3.0
Computing platforms/Operating Systems	Microsoft Windows
Installation requirements & dependencies	Microsoft Windows
If available, link to user manual - if formally published include a reference to the publication in the reference list	https://github.com/ApirsAL/GeoReVi/blob/master/docs/GeoReViUserManual.pdf
Support email for questions	contact@georevi.com

1. Introduction

Subsurface characterization is a crucial step when planning its utilization. A prominent example is the development of natural resources hosted in a subsurface region. Here, with regards to geothermal, groundwater or hydrocarbon reservoirs, a region in the subsurface needs to be characterized in order to assess its petrophysical properties and to predict the performance of the resource exploitation process. Reservoir characterization is defined as '*the process of preparing a quantitative representation of a reservoir using data from a variety of sources and disciplines*' [1].

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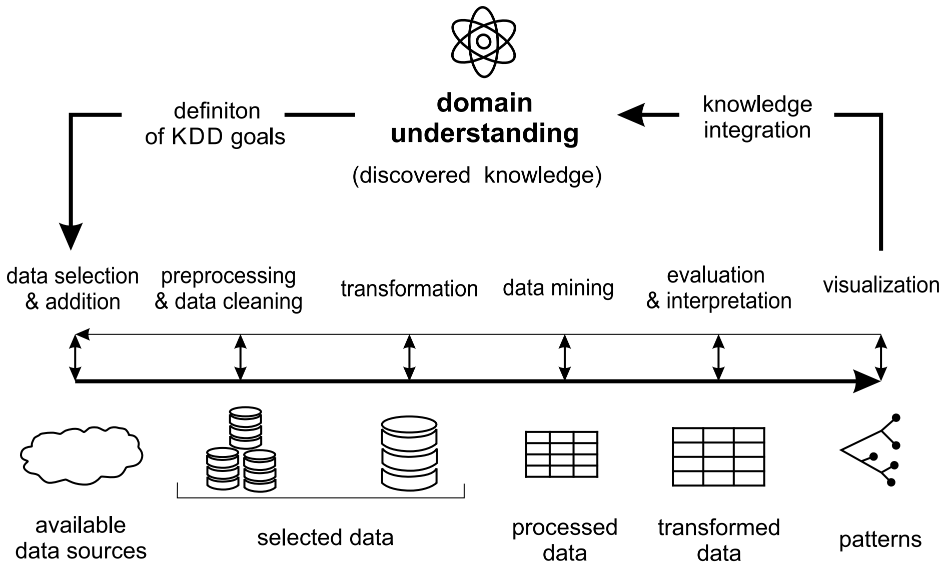

Fig. 1. Knowledge discovery in databases process after [2] and [3].

Accordingly, as numerous physicochemical rock and fluid properties contribute to a reservoir's potential, this problem can be considered being multidimensional with numerous contributing domains. However, any type of subsurface utilization requires a comprehensive knowledge of the subsurface architecture and the spatial distribution of relevant properties such as permeability and porosity for making profitable, business-critical yet sustainable decisions [4]. Consequently, modern automatized technologies for integrated exploration and modeling of subsurface-related data are required to increase subsurface predictability and to eventually optimize the subsurface utilization process.

Subsurface-related data are aggregated from multiple scales and numerous domains with contrasting ontologies [5]. These data are produced in well log measurements, in outcrop analog studies, drill core investigations, geophysical surveys or during development and can be both static (e.g. depth of lithological bodies) or dynamic (e.g. production rates). Numerous fundamental rock properties differ in their physical and mathematical nature. Rock properties such as permeability, stress, thermal conductivity/diffusivity are direction-dependent tensors [6–8] whereas porosity or grain density are scalar quantities. This diversity in mathematical and physical formats increases the effort to normalize reservoir-related data models and hampers data analysis and modeling of the properties. Often, these issues lead to inaccurate simplifications during flow and mass transport simulations such as assuming rock and fluid properties to be isotropic and homogeneously distributed in space and/or time.

With this study, we intend to bridge the gap between data collection, data management and integrated data analysis and visualization in the process of subsurface characterization. Therefore, we developed a software system called GeoReVi (*Geological Reservoir Virtualization*) with an internal implementation of the knowledge discovery in databases (KDD) process covering multiple aspects of visual analytics according to [9]. This software system enables domain experts to interactively manage and analyze any kind of spatial and multidimensional data sets through data processing, transformation, selection, import and mining algorithms.

1.1. Knowledge discovery in databases

The interdisciplinary field of KDD comprises a set of semi-automatic, non-trivial methods to extract novel, understandable, valid and useful patterns from domain-specific data sets stored in mature databases [3,10]. Those patterns are evaluated by the domain expert in order to extract '*knowledge*' [3]. The relationship between data and knowledge is commonly illustrated with the Data–Information–Knowledge–Wisdom (DIKW) hierarchy, which has been reviewed by [11]. The first conceptualization of the hierarchical representation of data, information and knowledge is defined in [12] and [13]. [13] defines data as '*symbols*', information as '*data that are processed to be useful*', knowledge as the '*application of data and information*' and wisdom as the '*appreciation of why*'. We will adhere to [13] and refer to knowledge as being '*know-how*' enabling information to be transferred into instructions. An example of this is planning a borehole for which we need information about the spatial distribution of stratigraphic units, structural elements and of physicochemical rock and fluid properties. Fig. 1 illustrates the iterative, 8-stage KDD process, which was conceptualized by [2] and redesigned and improved by [10]. The process starts with the domain expert's knowledge that is aimed to be maximized within the KDD process. The domain can be any discipline in which data are produced, managed and analyzed. Core of the KDD process is a set of data mining (DM) algorithms, which are deployed on a processed data set in order to find characteristic patterns or models. Prior to DM, data are selected, projected, cleaned, reduced and transformed by the domain expert. Pre-processing is supported by computer-aided process automation and intelligent pre-selections. DM algorithms in general comprise classification, summarization, correlation, regression, prediction and rule-discovery algorithms, whereby each DM algorithm is best suited to a specific problem.

2. Software description

2.1. Software architecture

GeoReVi is structured according to a client–server architecture. An illustration of the overall architecture is provided in Fig. 2a. GeoReVi is intended to be used in private, multi-user networks by using an application role authentication together with user credentials, which can be used to store and retrieve user-specific data. The server-side data storage is implemented as a relational database management system. However, GeoReVi can also be used in a local mode, where all data are stored in an integrated NoSQL database. GeoReVi targets the exploration

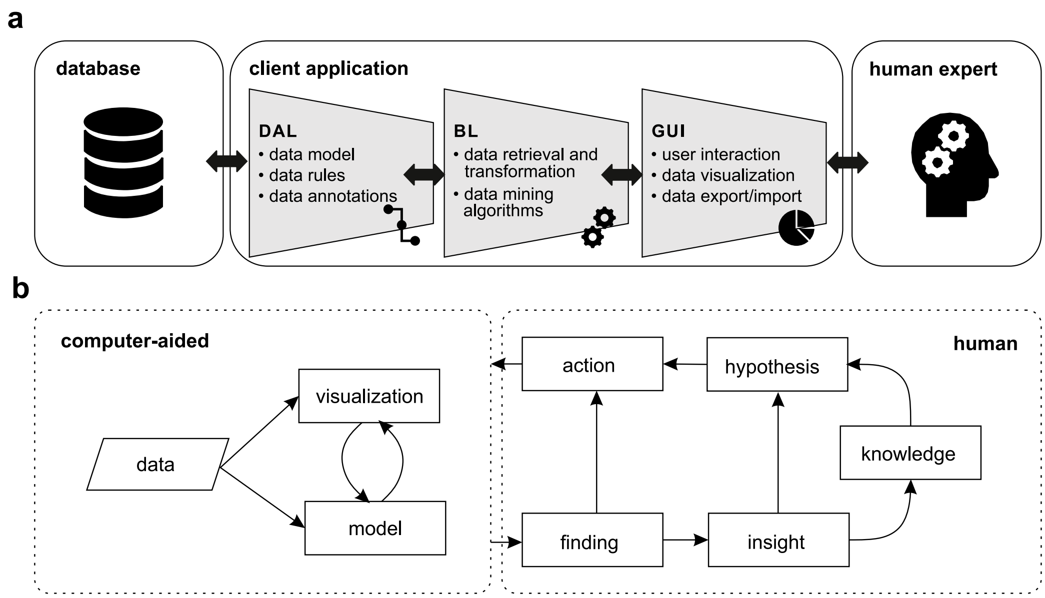

Fig. 2. (a) System architecture of GeoReVi (DAL = data access layer; BL = business logic; GUI = graphical user interface). (b) Knowledge generation model for visual analytics according to [14].

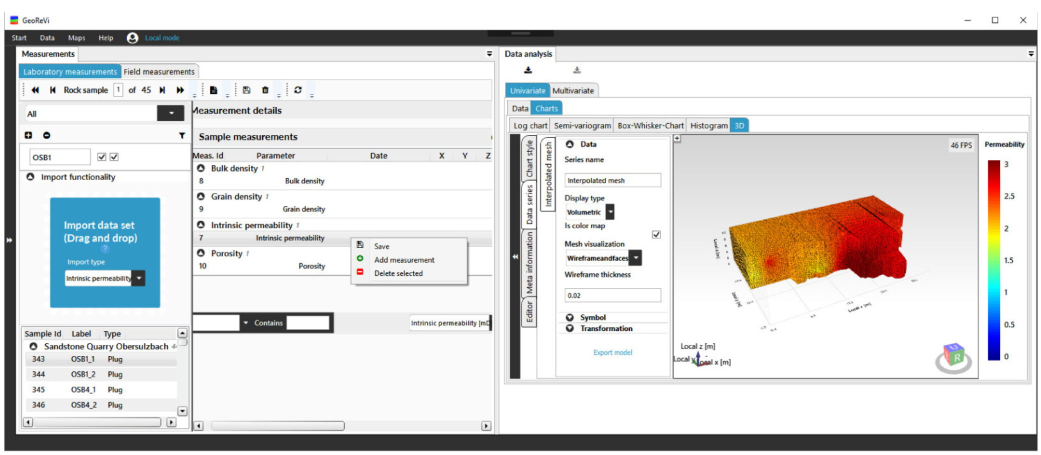

Fig. 3. Graphical user interface of GeoReVi. The measurements view is shown, where readings from laboratory and field measurements can be archived, analyzed and visualized.

loop of the knowledge generation model for visual analytics (KGMVA) after [14] (Fig. 2b). Within this model, a human expert extracts knowledge from huge data sets through interaction with a computer-aided feedback-loop of data selection, modeling and visualization. An important characteristic of a visual analytics system is the continuous interplay of automatic background processes and interactive visualization. With the provided architecture, a domain expert can manage and retrieve subsurface-related data while simultaneously analyzing and modeling a subsurface domain of interest.

2.2. System implementation

GeoReVi's client system has been developed with the *Windows Presentation Foundation* (WPF), which is included in the Microsoft .NET framework. We implemented the Model-View-ViewModel (MVVM) pattern that strictly separates the business logic from the graphical user interface and from the data model by dissociating these components into separated layers. For efficient MVVM-development the *Caliburn.Micro* framework was used. GeoReVi provides a modular structure using the *Managed Extensible Framework* (MEF), which makes the plug-in-based extension of the system easier for other developers.

In the Data Access Layer (DAL) the implemented data model is represented by a set of Plain Old CLR Objects (POCO) defined in the C# language. For database connectivity, we use the well-established *Entity Framework 6*, an object-relational mapper for the .NET framework, with the Code First approach. In order to provide compatibility to both relational and NoSQL databases, the POCO models were supplemented by data annotations from the *System.ComponentModel* assemblies. The database used for the local version is *LiteDB*, which is open-source and completely written in .NET C# managed code for offline data management. Business logic (BL) was developed with the object-oriented programming language C#. The business logic consists of view models and helper classes. The presentation layer or graphical user interface (GUI) displayed in Fig. 3 has been developed using the XML accent XAML (Extensible Application Markup Language).

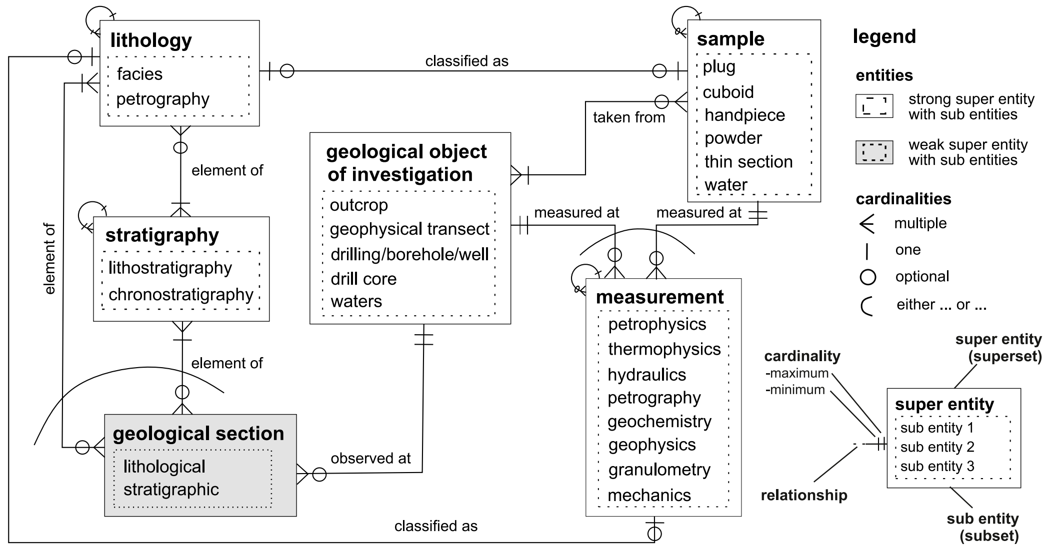

Fig. 4. Core data scheme of GeoReVi represented by an Entity-Relationship model. To provide a better overview, attributes were excluded from the model.

2.3. Software functionality

For a comprehensive overview of the functionality of GeoReVi, we refer to the user manual. However, in the following sections it will be briefly outlined how GeoReVi can be used to store, analyze, model and visualize geoscientific data.

2.3.1. Data storage

GeoReVi's logical data model (LDM, see Fig. 4) comprises the most common entities needed to assess the potential of subsurface geological media to store and extract heat or fluids sustainably. GeoReVi is specialized on geothermal rock and fluid properties, although the most important properties for oil and gas reservoir characterization are included as well. The basis for GeoReVi's LDM is built by the data collection of [15] that was remodeled into a relational data model according to the relational theory after [16]. Additionally, selected parts of the LDM for rock mechanics from [17] and the global geochemical database of [18] were used to extend GeoReVi's LDM. However, most data models are developed within a specific environment, wherefore each LDM had to be adapted to provide compatibility with the core scheme of GeoReVi.

For convenient data storage, custom drop-down menus, list boxes, data grids, color and date picker controls were developed that provide predefined domains. For manual data input, custom text boxes are provided. In order to reduce the number of controls in a view, sub-navigation is implemented via expandable menus or tab controls. To load bulk data sets into the database, a generic import procedure was developed that can semi-automatically assign data from .CSV, .XLS or .XLSX files to the entities in the database.

2.4. Statistical data analysis and subsurface modeling

For statistical data analysis and data visualization the user can load a set of univariate or multivariate measurement values of one or more samples or objects of investigation into the buffer memory, which are displayed in tabular format. Each data set loaded into the buffer memory is by default a mesh. A mesh consists of nodes, faces (quadrilateral or triangular) and cells (hexahedral or tetrahedral). GeoReVi covers individual functionality for 1-D, 2-D and 3-D mesh generation and for 3-D mapping. The user can select the meshes and create the visualizations and analyses with few commands. The meshes can be parameterized using both stochastic and deterministic algorithms such as inverse distance weighting (IDW), multiple varieties of kriging or conditional simulations. The quality of the models can be assessed with different types of cross-validation. Multivariate analyses in GeoReVi comprise k-Means cluster analysis, principal component analysis, self-organizing maps (Sammon mapping), bivariate regression and correlation analysis. The theory of the most important property modeling and statistical methods is explained in detail in the user manual, which also contains a detailed tutorial.

2.5. Data visualization

Custom controls were developed to visualize the data sets. Therefore, the dependency injection pattern has been implemented, which ensures that the properties of a control are loosely coupled with the properties of the instantiating class. This pattern simplifies the data binding of a view to its view model as well as the navigation between views. Chart controls comprise scatter charts, matrix charts, bubble charts, bar charts, line charts, box-whisker charts, ternary charts and combined line-bar charts. For 3-D visualization, the base functionality from the well-established *HelixToolkit.WPF* was used. In 3-D space, meshes can be visualized as point clouds, volume or surface meshes or as vector fields. Figures and charts can be exported in raster format (.PNG, .JPEG or .BMP) as well as in vector format (.EMF, .XAML or .PDF). 3-D objects can be exported as .OBJ, .X3D or .XAML files or in a custom, XML-based serialization with the extension .GMSH. GeoReVi enables to import and transform 3-D objects in .OBJ format and images in .PNG and .JPG format. Those may serve as target objects for mapping structures that can be used for surface interpolation. Moreover, this function includes ground-penetrating radar (GPR) and seismic datasets if they are provided in one of the aforementioned file formats.

3. Illustrative example

3.1. Spatial heterogeneity of a compartmentalized sandstone formation

In order to demonstrate the capability of GeoReVi to assist the knowledge discovery process connected to geoscientific problems, the intrinsic 3-D heterogeneity of fundamental petrophysical properties within a potential geothermal target formation was

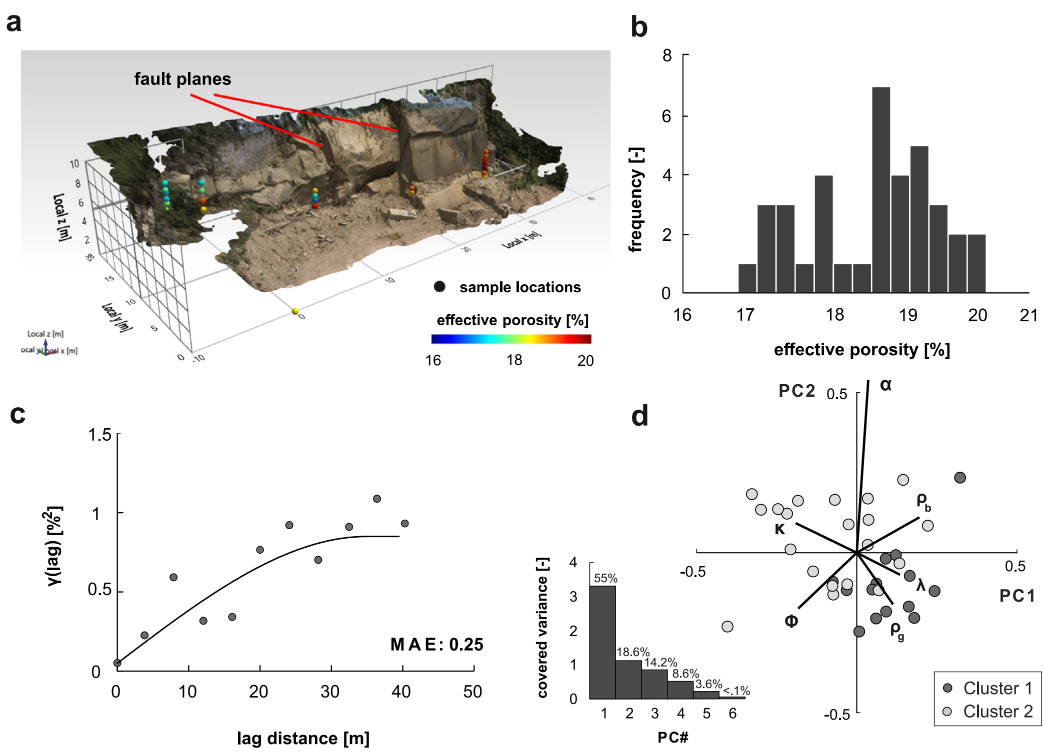

Fig. 5. (a) Photogrammetric model of the investigated sandstone quarry with marked sample locations and structural elements. The faults have a displacement of several meters. (b) Empirical distribution of the effective porosity in the Disibodenberg Formation. (c) Experimental semivariogram and variogram model of the effective porosity used for kriging and sequential Gaussian simulation (MAE = mean-absolute-error) (d) Principal component analysis in the form of a biplot and scree plot combined with a k-Means cluster analysis of the rock properties grain density (ρ_g), bulk density (ρ_b), effective porosity (ϕ), intrinsic permeability (κ), thermal conductivity (λ) and thermal diffusivity (α).

Table 1
Arithmetic mean ($\bar{x}$), minimum (*min*), maximum (*max*), variance (σ^2), coefficient of variation (c_v) and Dykstra–Parson coefficient (c_{dp}) of the measured rock properties: grain density (ρ_g), bulk density (ρ_b), effective porosity (ϕ_e), intrinsic permeability (κ), thermal conductivity (λ) and thermal diffusivity (α).

	ρ_g	ρ_b	ϕ_e	κ	λ	α
Unit	g/cm^3	g/cm^3	%	mD	W/(m · K)	10^{-6} m^2/s
$\bar{x}$	2.66	2.17	18.5	2.64	2.31	1.53
min	2.64	2.12	16.98	0.7	1.99	1.28
max	2.67	2.31	20.23	4.6	2.57	1.75
σ^2	2.1e−5	1e−4	0.6	0.6	0.01	0.01
c_v	0.003	0.015	0.04	0.31	0.07	0.11
c_{dp}	0.002	0.01	0.06	0.31	0.30	0.07

investigated in a quarry that is influenced by tectonic compartmentalization. The case study comprises numerous tasks that are involved in typical subsurface characterization workflows, including data integration, non-orthogonal mesh generation, statistical data analysis, spatial estimation and data visualization.

The investigated outcrop is located in Obersulzbach in southwestern Germany and contains sedimentary rocks from the Disibodenberg Formation (Glan Subgroup) belonging to the Permian Rotliegend Group in the Saar–Nahe-Basin. The Disibodenberg Formation in the quarry is an outcrop analog for the deeply buried formation in the northern Upper Rhine Graben [19]. Here, the deltaic sandstone bodies of the Disibodenberg Formation can be considered as potential hydrothermal reservoirs for power and heat production due to suitable permeability and porosity and sufficient thicknesses [20]. A low-offset strike-slip fault zone, which ranges from x = 14 m to x = 20 m, separates the outcrop into two major parts (Fig. 5a).

Measuring 50 × 15 × 10 meters, the extent of the outcrop is comparable to typical cell sizes of reservoir models built for industrial and scientific applications [21,22]. 36 cylindrical, oriented rock samples were taken from the outcrop wall and investigated in the laboratory determining the intrinsic permeability, grain and bulk density, effective porosity, thermal conductivity as well as thermal diffusivity (Table 1) of the rock matrix. Those properties can be considered key properties controlling heatflow in porous aquifers with regard to hydrothermal systems [23,24]. All samples and readings are documented in the local database of GeoReVi. The sampling strategy aims to simulate pseudo-wells in 3-D space in order to demonstrate the capability of GeoReVi to operate in 3-D environments.

The laboratory results were analyzed by descriptive and multivariate statistics for initial exploratory data analysis. Subsequently, the data sets were interpolated and simulated in 3-D space using inverse distance weighting (IDW), simple kriging (SK), ordinary kriging (OK) and sequential Gaussian simulation (SGS). For the parameter prediction, a 3-D hexahedral mesh with 80,000 cells was generated using an IDW interpolation of a photogrammetric model of the outcrop wall (Fig. 6a). The results were validated through leave-p-out cross-validation (LPO) providing the root-mean-square error (RMSE) and mean-absolute error (MAE). Each of those steps was performed with GeoReVi using the incorporated data mining and geostatistical algorithms and the interactive visualization capabilities.

3.1.1. Results

According to the classification provided by [21], the coefficient of variation c_v and the Dykstra–Parson coefficient c_{dp} indicate a very low heterogeneity of the sandstone formation (Table 1). However, the grade of heterogeneity varies among the considered rock properties. Intrinsic permeability owns a 100-times higher heterogeneity than grain density, which represents the most homogeneous rock property in turn. This is due to a homogeneous mineralogy of the sandstone. At the same time, secondary porosity, produced by feldspar dissolution [25], and non-pervasive

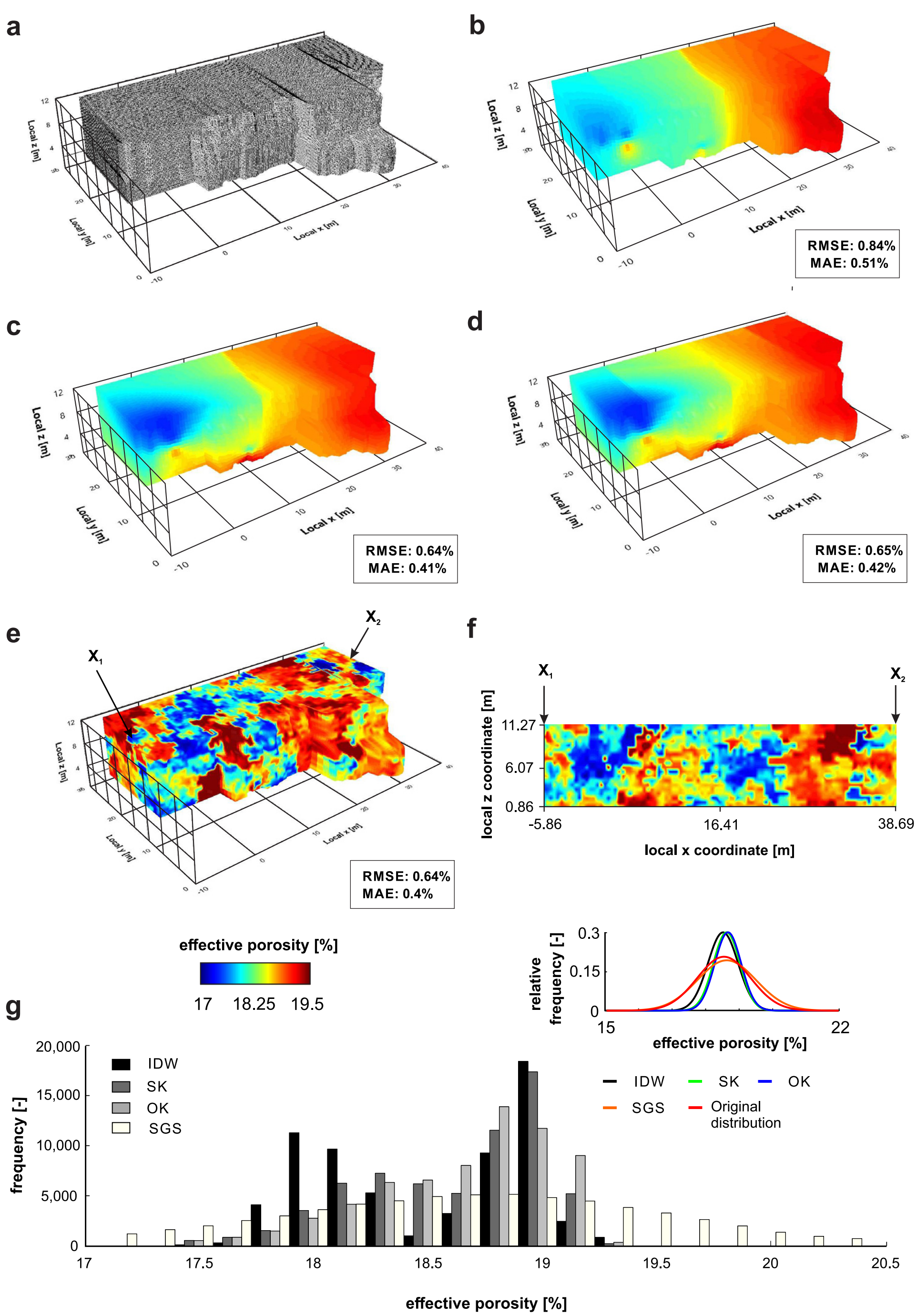

Fig. 6. (a) Hexahedral mesh generated by mapping the photogrammetric outcrop model. The model consists of 80,000 cells and has a volume of 8999 m^3. The mesh is used as a target for the interpolation and simulation processes. Comparison of IDW (b), SK (c) and OK (d) interpolations and SGS (e) simulation on the porosity data set of the quarry Obersulzbach. (f) Vertical cross section through the SGS realization (e) from point X_1 to X_2. (g) Empirical and theoretical distributions of the realizations in comparison to the original theoretical distribution.

cementation lead to a heterogeneous network of both closed and enlarged pore throats, strongly increasing the spatial variability of the permeability.

The cluster analysis (Fig. 5d) highlights the differences in the rock properties across the footwall and the hanging wall. Cluster one represents the samples east of the fault zone and cluster two the samples west of it. Five samples were categorized incorrectly with regard to their positions relative to the fault zone. Those samples, however, are located close to it and hence could be affected by tectonic overprint. Moreover, results from cluster analysis correspond well with the principal component analysis (PCA) where the categories derived from the cluster analysis are projected onto different regions in the biplot.

It can be seen that effective porosity shows a bimodal distribution between 17 and 20% (Fig. 5b). The effective porosity in the eastern part of the quarry is slightly higher than in the western part (Fig. 5a). The SK, OK and SGS realizations provide a low RMSE of 0.64, 0.65 and 0.64% respectively. The RMSE of the IDW realization (0.84%) is higher. Compared to the original histogram (Fig. 5b), IDW, SK and OK underestimate the original range whereas SGS reproduces the range appropriately (Fig. 6g). Contrary to the cross-validation results, IDW reflects the bimodal porosity distribution and hence the two-fold compartmentalization of the rock volume, which is exposed in the outcrop, more accurately than the other algorithms (Fig. 6b-e). SGS reproduces the observed variability best, which is also indicated by the sharp physical contrasts observable in the 2-D cross section which is taken from the SGS realization (Fig. 6f).

4. Impact

To the best of our knowledge, GeoReVi is the first open-source software system that incorporates the entire KDD process for subsurface characterization into one extensible application. The software system can be applied to address a wide variety of geoscientific research questions related to subsurface characterization — however, also general geoscientific problems can be addressed. This distinguishes GeoReVi from existing software solutions which are often tailored to meet the needs of specific disciplines such as hydrocarbon extraction or heat production. The modular architecture makes GeoReVi easily extendable for other researchers and the broad range of data mining algorithms and conventional geostatistics opens up new paths to go.

The system was tested in a series of outcrop analog studies [26] from both petroleum and geothermal research projects. GeoReVi allows researchers to produce optimized spatial property models through rigorous cross-validation and visual inspection of the results. Academic researchers can use GeoReVi as an integrated data repository, analytical platform and visualization system in the context of subsurface characterization. Thanks to the ability to handle local spreadsheet files, GeoReVi is not only limited to the data model provided by its database. Various types of spatial problems can be addressed by the generic yet simple spatial representation of geoscientific data sets.

5. Conclusions

GeoReVi constitutes an integrated software system that facilitates reservoir engineers, geoscientists, petrophysicists and other researchers to largely automate the subsurface-related data management and knowledge discovery process. The generic knowledge discovery potential of GeoReVi comprises statistical and spatial relationships among any kind of rock properties, optimized spatial predictions at any scale of subsurface investigations, uncertainty estimations and the discovery of multidimensional patterns in relational data sets. The normalized data scheme of GeoReVi makes the software robust to changes in the domain knowledge of subsurface characterization. Semi-automated preprocessing increases robustness of the data mining algorithms regarding sparse, erroneous or multidimensional data sets.

GeoReVi is able to overcome problems from existing open-source software packages related to geostatistics or geological modeling [27] such as the limited applicability of algorithms to 2-D features or regular lattices, restricted expert interaction, single-user environments and data storage limitations. Moreover, expensive commercial software packages – suitable to address those issues – are usually employed as black-box tools. With our work, we aim to contribute to the ongoing development of open-source, intelligent, automated data analysis systems by providing an intuitive and extensible geoscientific data management and analysis tool. Ongoing research will focus on the development of plug ins for finite element simulation of subsurface heat transfer and fluid flow.

CRediT authorship contribution statement

Adrian Linsel: Conceived and designed the analysis, Collected the data, Contributed data or analysis tools, Performed the analysis, Wrote the paper, Developed GeoReVi. **Kristian Bär:** Conceived and designed the analysis. **Joshua Haas:** Collected the data, Contributed data or analysis tools, Performed the analysis. **Jens Hornung:** Conceived and designed the analysis. **Matthias D. Greb:** Conceived and designed the analysis. **Matthias Hinderer:** Conceived and designed the analysis.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Sample availability

Samples are available at the Institute of Applied Geosciences in Darmstadt, Germany. Moreover, they are registered in the System for Earth Sample Registration (SESAR, www.geosamples.org) with the code names provided in Table A.1.

Table A.1
Rock samples taken from the outcrop in Obersulzbach with the associated International Geo Sample Number (IGSN).

Sample	IGSN	Sample	IGSN
OSB1_1	IEDAL0046	OSB25	IEDAL000P
OSB1_2	IEDAL0045	OSB26	IEDAL000O
OSB6	IEDAL0004	OSB28	IEDAL000M
OSB7	IEDAL0003	OSB29	IEDAL000L
OSB8	IEDAL0002	OSB30	IEDAL000K
OSB9	IEDAL0001	OSB31	IEDAL000J
OSB10	IEDAL001W	OSB32	IEDAL000I
OSB11	IEDAL001V	OSB33	IEDAL000H
OSB12	IEDAL001U	OSB34	IEDAL000G
OSB13	IEDAL001T	OSB35	IEDAL000F
OSB14	IEDAL001S	OSB36	IEDAL000E
OSB15	IEDAL001R	OSB37	IEDAL000D
OSB16	IEDAL001Q	OSB38	IEDAL000C
OSB17	IEDAL001P	OSB39	IEDAL000B
OSB19	IEDAL001O	OSB40	IEDAL0008
OSB21	IEDAL000S	OSB41	IEDAL0007
OSB22	IEDAL000R	OSB42	IEDAL0006
OSB23	IEDAL000Q	OSB43	IEDAL0005

Appendix B. Data availability

Data is available in the online repository and provided as a training data set for the GeoReVi tutorial. Also, the data is partly integrated into the local database that is shipped with the executable file.

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