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Version 2.5 - TOUGH2Viewer 2.0: A multiplatform tool for fully 3D Voronoi TOUGH grids

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A R T I C L E I N F O

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A B S T R A C T

This paper introduces new geostatistical features implemented in TOUGH2Viewer, a pre and post processing tool for the TOUGH family of codes developed in the Java programming language. The main additions in version 2.5 are the introduction of features for the automatic generation of numerical models with spatial variability of porosity and permeability. These features are described in detail within the paper, enabling researchers to address fundamental questions in the field of geostatistical petrophysical variability of the reservoir characteristics. The generation of spatial variability (variogram) and statistical distribution (histogram) are obtained by using the Spectral Simulation method 2D models, and the Sequential Gaussian Method for 2D and 3D models. Starting from a full functioning input for TOUGH, directly from the TOUGH2Viewer environment, it is possible to automatically generate and run several geostatistical different realizations of the same numerical model in a very easy way and with a minimum of input by the user. Emphasizing ease of installation, usability, and extensibility, the code's structure is presented alongside illustrative examples that demonstrate key functionalities.

Metadata

Nr	Code metadata description	*Metadata*
C1	Current code version	v2.5
C2	Permanent link to code/repository used for this code version	https://github.com/stebond/TOUGH2Viewer2.5
C3	Permanent link to reproducible capsule	none
C4	Legal code license	Apache License, Version 2.0
C5	Code versioning system used	GIT
C6	Software code languages, tools and services used	Java
C7	Compilation requirements, operating environments and dependencies	NetBeans 8.1 IDE, Java JDK 1.8 or higher, Java3D, JFreeChart.
C8	If available, link to developer documentation/manual	https://github.com/stebond/TOUGH2Viewer2.5
C9	Support email for questions	stefano.bondua@unibo.it

1. Description of the software-update

Over the past few years, development efforts have been directed toward the implementation of new features in TOUGH2Viewer [1], including the integration of the Geostatistical Parameters Generator (GPG). Geostatistical tools are of fundamental importance for the correct assessment of uncertainties and sensitivity analyses performed in numerical modeling.

GPG introduces the geostatistical features in TOUGH2Viewer, allowing the generation of distributions of model parameters with a given statistical and spatial correlation, useful for TOUGH [2] numerical modeling. It is worth mentioning that TOUGH have a built-in feature for the generation of permeability modifier with a given statistical distribution (keyword SEED; for further information refer to [2], but it does not include features for automatically generating multiple distributions of spatial variability of model parameter.

Geostatistical Simulations allows the generation of several realizations of the so-called regionalized variables. Each realization represents one possible spatial distribution of the parameters of the system

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(herein after referred as scenario). By processing the entire set of scenarios, it becomes possible to derive powerful probabilistic measures that cannot be obtained from a single, smoothed spatial distribution, like those obtained using a classical interpolator method (inverse weighted distance method, geostatistical kriging, etc. …). The capability of considering the spatial uncertainty of the parameters collectively, rather than one by one, is the definitive advantage of numerical simulation for modern risk assessment and decision-making [3–5]. Among the several geostatistical methods available in the literature, it is worth mentioning the Sequential Gaussian Simulation method [6], the Turning Bands method [7], the Dilution method [8], the Tessellation method [9]. A complete review of the geostatistical method can be found in [10]. Previous work on the use of the GS methods for TOUGH was presented by [11].

Two are the Geostatistical Simulations algorithms implemented in TOUGH2Viewer, the 2D Spectral Simulation [12] and the Sequential Gaussian Simulation [13]. The original codes were ported and refactored from Fortran to Java and incorporated in TOUGH2Viewer. The geostatistical simulated data (GSD) computed via the two algorithms are used to assign to the blocks of the numerical grid the permeability modifiers and the porosity.

Therefore, directly from the TOUGH2Viewer environment (i.e. via the "*MultiSimulation generator*" GUI), it is possible to automatically generate and run several different geostatistical realizations of the same TOUGH numerical model in a very easy way.

The generated GSD can be also easily used outside TOUGH environment, as they are saved in csv file format.

2. The working flow

To assign a GSD of the desired parameters, such as permeability and porosity, to the TOUGH model, it is necessary to start from an existing TOUGH model by loading its file MESH into TOUGH2Viewer. Using the GPG features (i.e. the graphical interface of TOUGH2Viewer called *MultiSimulation generator*) several GSD scenarios can be automatically generated and used to modify the MESH section (permeability modifier) and the INCON section (porosity) of an existing TOUGH input file, in order to create multiple TOUGH input files, one for each scenario, allocated in separated folders.

2.1. The 2D spectral simulation method

The original SPECSIM2 code from [12] has been implemented in Tough2Viewer maintaining his main structure and input format. Through a simple and intuitive Graphical User interface (GUI), it is possible to set the grid parameters and the geostatistical parameters, like the variograms structures and additional parameters, like the seed number and the number of realizations (see Fig. 1). The GSD are generated by clicking the "run" button from the Tough2Viewer's menu. Once the GSD scenarios have been generated, it is possible to verify them by means of the same GPG window, displaying the variogram related to the GSD (Fig. 2a), histograms (Fig. 2b) and 2D simplified maps (the 2D projected values of the geostatistical simulated fields). As the Spectral Simulation Method generates a random distribution of data following a Gaussian function, then it is possible to modify the range of existence of the generated random data between a minimum and maximum values, with a given mean and variance; it is also possible to generate a lognormal distribution. In the first case, the transformation of the Gaussian variable is computed using the approach proposed by [14]. Briefly, let $X \sim N(\mu, \sigma_X^2)$ and let $a = min$ and $b = max$, with $a < b$, using the logistic sigmoid $\delta(t) = \frac{1}{1+e^{-t}}$, obtaining $Y = a + (b - a)\sigma\left(\frac{X-\mu}{s}\right)$,

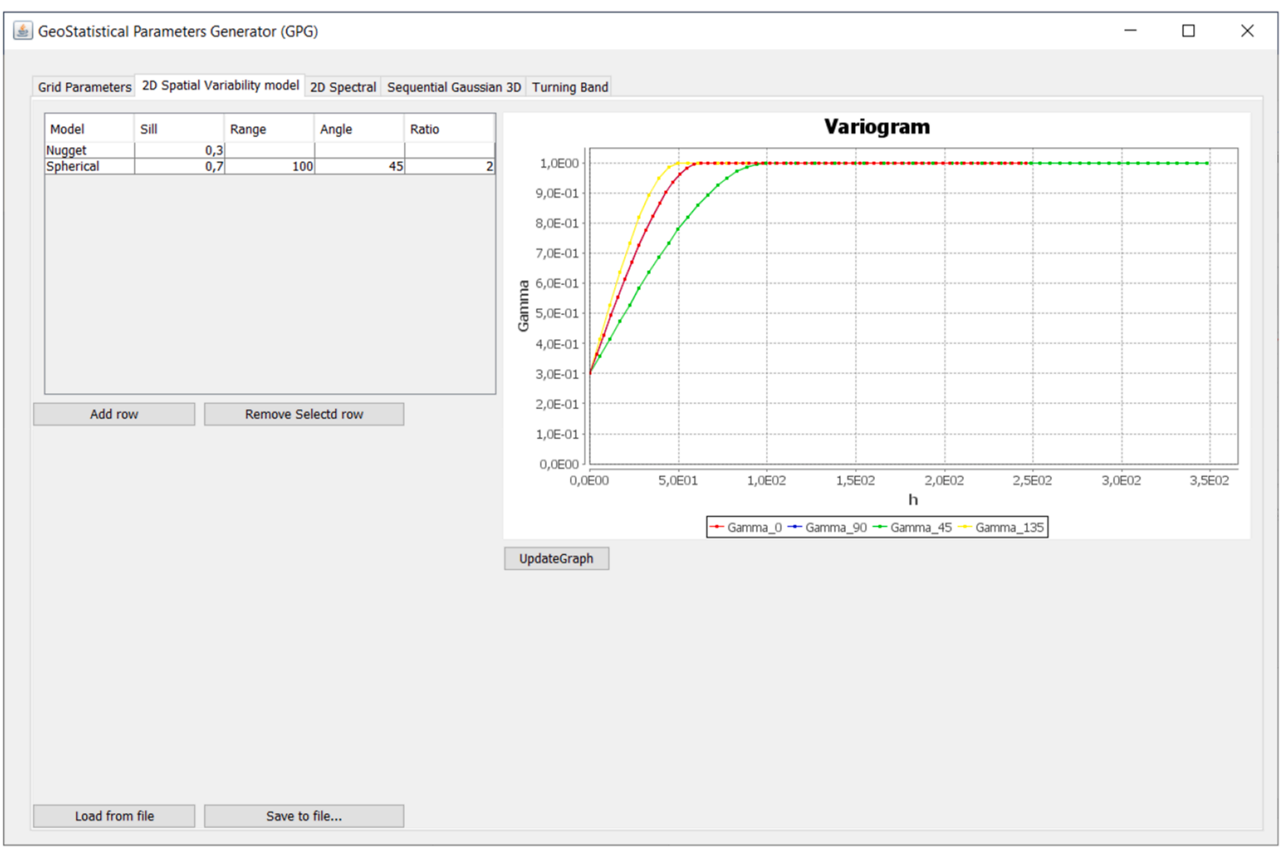


Fig. 1. Multi-tab GUI (GPG) to manage geostatistics activity. Tab named "2D Spatial variability model" to manage the variogram. The user can define the theoretical variogram among nugget, spherical, exponential and gaussian models. For each structure, it is possible to set the sill, the range, the angle of the principal axis and the range max and min ratio. A preview of the theoretical variogram is visualized in the right part of the window.

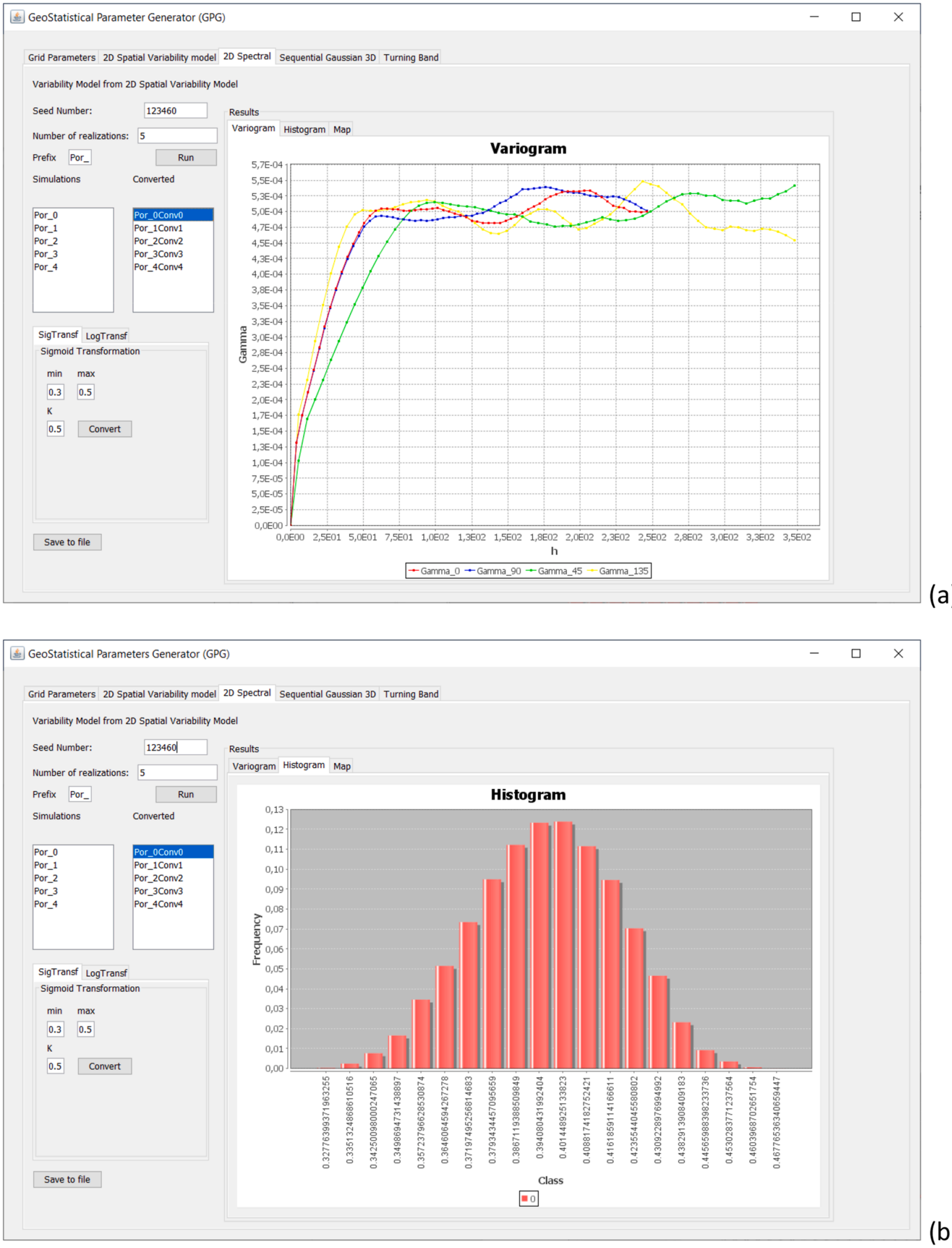


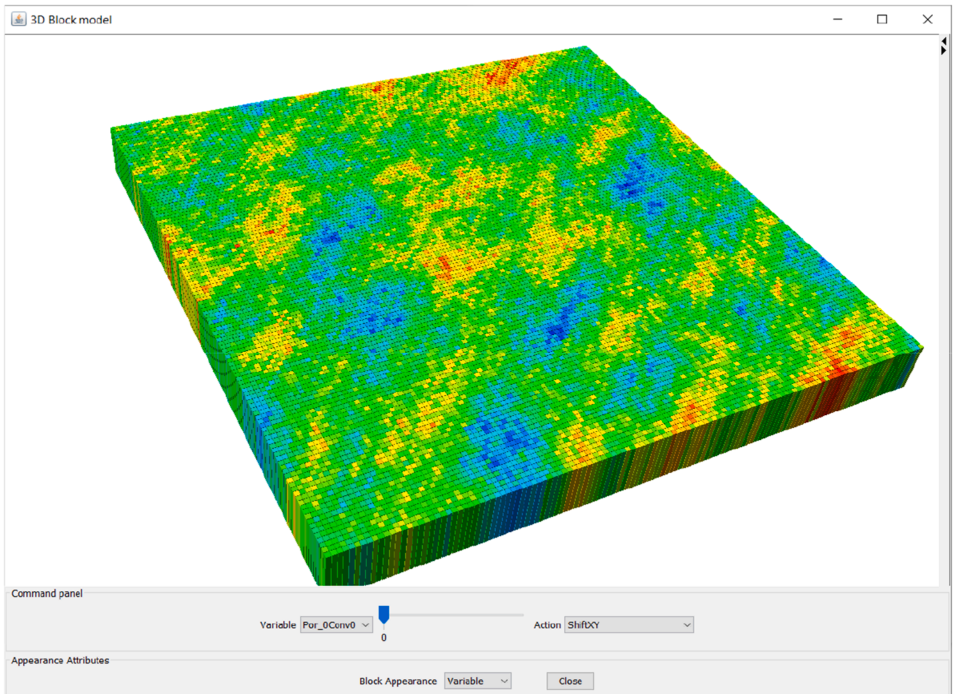
Fig. 2. GPG window output ("2D Spectral" tab): (a) GSD set can be selected in the list (top-left part of the window). Experimental variograms are displayed in the right part (Results-Variogram tab); (b) Histogram visualization of the selected variable (Results-Histogram tab).

where $s > 0$ controls steepness (smaller $s \rightarrow$ more mass near a and a). The lognormal transformation is obtained using the transformation $Z = e^X$, then rescaling Z between a and b. The geostatistics simulated fields can be exported in csv file format.

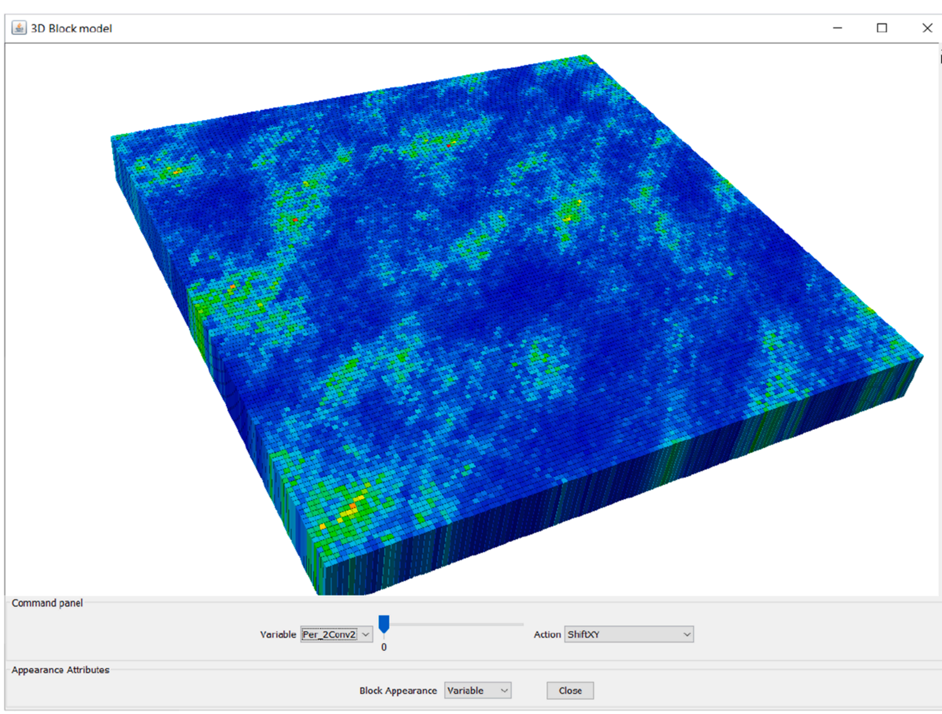
The grid of the model with the assigned GSD can be imported and visualized in TOUGH2Viewer, as shown in Fig. 3.

2.2. The sequential Gaussian method

The SGSIM code from [13] has been implemented maintaining his



(a)



(b)

Fig. 3. Visualization in Tough2Viewer of a GSD scenarios: (a) porosity (using a gaussian distribution); (b) Permeability (using lognormal distribution).

main structure and input format. Through the "GeoStatistical Parameters generator" GUI (see Fig. 4), it is possible to set the grid parameters and the geostatistical parameters (variograms structures, conditioning data, co-located variables, histogram shape and additional parameters). The GSD scenarios are generated by clicking the "run" button of the GeoStatisticalTools->Sequential Gaussian tab->Run & Results tab, then it is possible to verify, within the same tab, each GSD displaying the variograms related to the geostatistical simulated data, histograms and statistics. Depending by the input parameters used for the SGSIM simulation, the GSD follow a Gaussian distribution or follow a user-defined distribution (please refer to user manual of [13]). As with the Spectral Simulation method, it is possible to use the Gaussian distribution with a given mean and variance; it is also possible to generate a lognormal distribution. An example of a 3D simulated model generated using the Sequential Gaussian simulation method is shown in Fig. 5.

2.3. The variables assignation

Using the INCON generator function (under the "Tools" TOUGH2-Viewer's menu), the GSD can be imported into the TOUGH numerical model. In the variable list, the new generated parameters can be used for the scenario's generation, using the MultiSimulation generator window.

2.4. The scenario generation and run

The MultiSimulation generator window (see Fig. 6) is a feature for generation of scenarios. Assuming n=number of selected GSD scenarios of permeability and m=number of selected GSD scenarios of porosity, the MultiSimulation generator window can generate: (i) n x m scenarios, by combining the selected GSD scenarios; (ii) if $n = m$, it is possible optionally to generate just n scenarios without cross-combining the GSD scenarios.

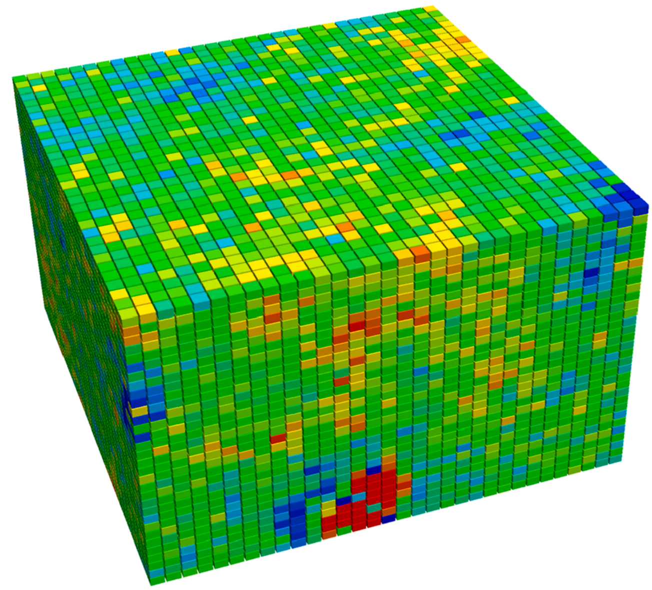


Fig. 5. 3D model visualization. Each block of the model has been assigned a value obtained by the SGSIM geostatistical simulation.

Optionally, TOUGH simulations can be run directly by TOUGH2-Viewer, by setting the appropriate name and path of the TOUGH executable. The simulation will be run in series, in each generated folder.

3. Conclusion

The uncertainty and the sensitivity analysis of numerical models are

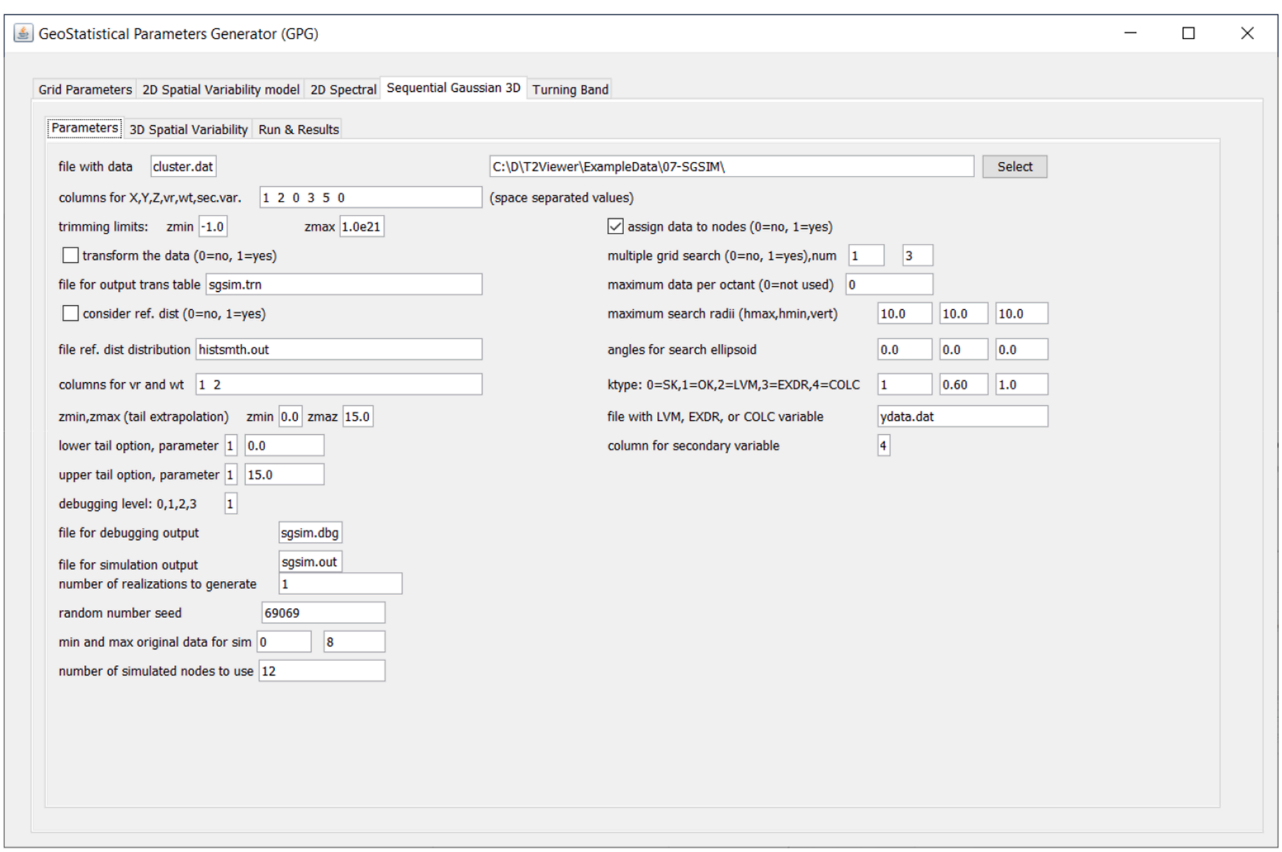


Fig. 4. GPG SGSIM GUI – for the input of the parameters.

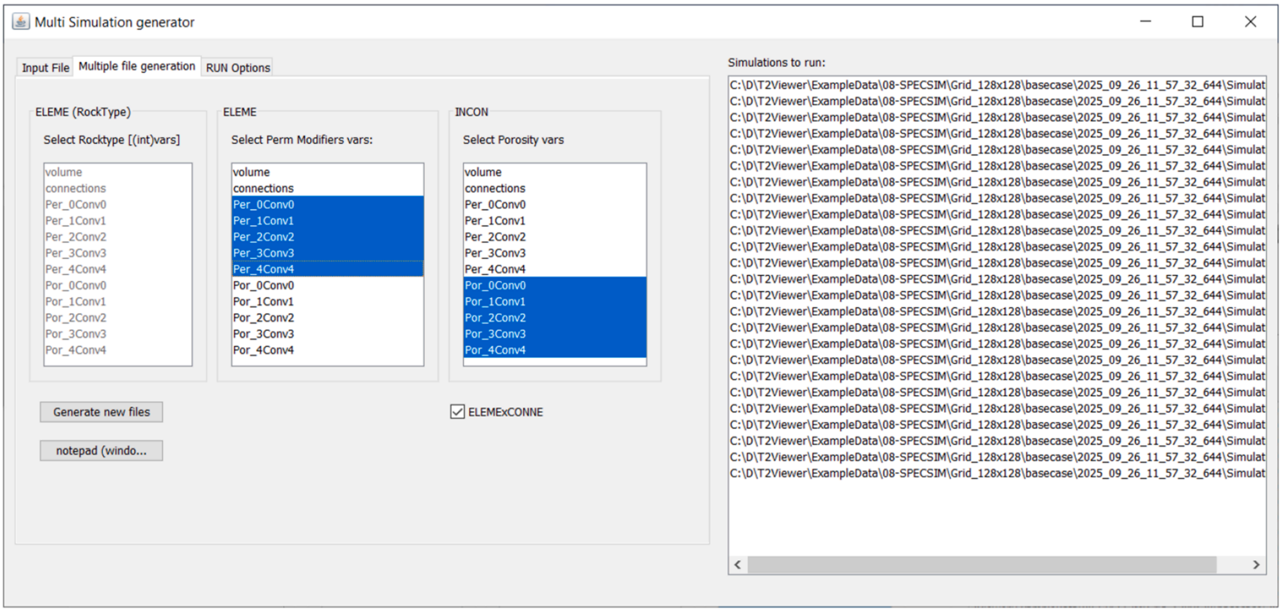


Fig. 6. The Multi Simulation generator window: (a) a set of GSD scenarios has been generated and ready for the TOUGH simulation. In the example, five generated values of permeability modifier and five generated values of porosity are used to build twenty-five scenarios. Optionally, TOUGH simulations can be run directly from TOUGH2Viewer, by setting the executable name and the binary folder (not shown here).

crucial for the validation of the results and risks assessment. The use of geostatistical simulated parameters through easy to use GUI and the automate generation of GSD scenarios, can simplify the workflow and reduce the pre and post processing time of TOUGH numerical simulations runs and analysis.

CRediT authorship contribution statement

Stefano Bonduà: Writing – review & editing, Writing – original draft, Visualization, Validation, Supervision, Software, Resources, Project administration, Methodology, Investigation, Funding acquisition, Formal analysis, Data curation, Conceptualization. **Bortolotti Villiam:** Writing – review & editing, Visualization, Validation, Supervision, Software, Resources, Project administration, Methodology, Investigation, Funding acquisition, Formal analysis, Data curation, Conceptualization.

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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