Visualization of gridded scalar data with uncertainty in geosciences

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Abstract
Characterization of the earth’s subsurface involves the construction of 3D models from sparse data and so leads to simulation results that involve some degree of uncertainty. This uncertainty is often neglected in the subsequent visualization, due to the fact that no established methods or available software exist. We describe a visualization method to render scalar fields with a probability density function at each data point. We render these data as isosurfaces and make use of a colour scheme, which intuitively gives the viewer an idea of which parts of the surface are more reliable than others. We further show how to extract an envelope that indicates within which volume the isosurface will lie with a certain confidence, and augment the isosurfaces with additional geometry in order to show this information. The resulting visualization is easy and intuitive to understand and is suitable for rendering multiple distinguishable isosurfaces at a time. It can moreover be easily used together with other visualized objects, such as the geological context. Finally we show how we have integrated this into a visualization pipeline that is based on the Visualization Toolkit (VTK) and the open source scenegraph OpenSG, allowing us to render the results on a desktop and in different kinds of virtual environments.

Key words: Visualization, Visualisation, 3D, Uncertainty, Scalar Fields, Monte Carlo Simulation

1. Introduction
The major problem with the characterization of the subsurface of the earth and with the construction of corresponding models is the uncertainty of the data. Direct borehole measurements are very limited due to technical issues and costs. Normally, data are available along boreholes from core samples and geophysical well logging. On a larger scale the data have to be estimated, using geophysical measurements like seismics and the interpreted structural model as support. Thus the subsurface models are derived from limited information and include uncertainties. Using these subsurface models as a basis for the prognosis of hydrogeological, geothermal, reservoir or geotechnical processes generates results with uncertainties as well. One common method to quantify parameter uncertainty and the corresponding system evolution is Monte-Carlo analysis (e.g. Deutsch, 2002). Using geostatistical techniques, for example sequential Gaussian simulation and indicator simulation, multiple stochastically equivalent realizations of the input model are generated, which are independently simulated (Rouhani et al, 1996). Simulation results of a scalar type can then be summarized to a probability density function with mean and standard deviation at each vertex. As parallel computing becomes increasingly available, the assessment of uncertainty using Monte-Carlo simulation becomes a more and more attractive method, in particular for scarce data situations such as deep geological systems. The dataset we use as an example is a geothermal reservoir analysis for the Urach Spa site (Germany, Swabian Alb) and has been described in more detail in Watanabe et al (2010).

An important problem with these gridded scalar fields that involve uncertainty is that the data values at all points of a certain grid-cell do not uniquely define where the isosurface will lie, because this location depends on the data values and their standard deviation of all the points in the near field (see Figure 1 for an example). In order to properly assess in detail the data and the uncertainty, a good visualization needs to outline the regions where the uncertainty is high and also indicate within which envelope an isosurface will lie with a certain confidence.

Preprint submitted to Computers and Geosciences September 13, 2010
Our initial idea was to render the scalar data (pressure, temperature) as isosurfaces and map the standard deviation to the colour as has been described, for example, by Rhodes et al (2003). This approach works well for a single isosurface, as is shown in the medical applications that Rhodes et al (2003) describe. However, as we want to show the spatial contiguity of the scalar field, we have to render multiple isosurfaces. Using this colour scheme with our data revealed that the viewers need the colour on the isosurfaces to understand which isosurfaces they are looking at. For two-dimensional maps, Hengl (2003) suggests the use of the HSI (Hue, Saturation, Intensity) colour model. Hue is used to visualize the scalar data values and the saturation is used to visualize the uncertainty as paleness. This results in maps, which become whiter or paler in regions where the data is more uncertain, and for which the data is clearly shown with stronger colours where it is certain.

Djurcilov et al (2002) use a similar colour scheme together with volume rendering for visualizing 3D ocean data. They use a 2D transfer function for the colour mapping to show both data value and its uncertainty. The data value is mapped to the colour and the corresponding uncertainty to the alpha channel. This results in a volume visualization where the data are solidly shown when the uncertainty is low and become translucent where it is high. Both aforementioned methods only provide information on where the uncertainty is high but do not give an idea of the different shapes isoslines or isosurfaces could have, due to the uncertainty.

Osporio and Brodlie (2008) describe a raster-based approach to generate ‘thick contours’ for two dimensional maps that show the uncertainty involved and apply it to an example data set from oceanography. Their approach could be extended to 3D applications by using volume rendering and showing ‘thick isosurfaces’. Johnson and Sanderson (2003) have shown such a similar approach for 3D data by representing the average value with an isosurface and then rendering the uncertainty of the scalar field as a semi-transparent envelope around it, using volume rendering. Grigoryan and Rheingans (2004) use a point based rendering approach to create fuzzy-looking ‘thick surfaces’, which are represented by fewer and fewer points at the outer areas where the probability of the surfaces lying there is lower. What both these methods have in common is that they show a ‘thick’ isosurface that looks solid at the locations where it is likely for the isosurface to be located and that fades into translucency and haziness where its positions become more and more unlikely. However, if the uncertainty is high, the isosurfaces that have been generated in this way might fill in the space between them and clutter the display. Further, it will be difficult for the viewers to estimate how thick the isosurfaces are and to estimate how far they can look into this semi-transparent volume. As a consequence it will be hard for the viewer to recognize if the isosurface intersects a certain feature, such as a borehole, with a given confidence.

Many authors, e.g. Lodha et al (1996), Pang et al (1997) or Newman and Lee (2004) describe approaches where the uncertainty is displayed by glyphs placed along the surface. Some of these approaches could be easily implemented using the Visualization Toolkit (Schroeder et al, 1996), for example by using the vtkGlyph3D class to place a sphere at every vertex of an isosurface, the size of the sphere corresponding to the local magnitude of the standard deviation. The problem with most of the glyph-based techniques is that the user’s perception of the size of the glyphs often depends
on view direction and that they can easily clutter the display, which is not the case with colour-based techniques. Further the perception of a glyph’s size can be influenced by the surrounding scene that might create some effect of size illusion (for an example see Sterzer and Rees, 2006).

In our work we combine colour-based and glyph-based techniques. We use a colour scheme that is similar to the one from Hengl (2003), making use of a two-dimensional transfer function. One dimension maps the average data value to the colour, while the other dimension maps the uncertainty of the data value to a combination of saturation and brightness. While the overall colour stays the same, the surface becomes greyish and dark in regions of high uncertainty and looks dirty, which is a pattern intuitively understandable. One problem with such a bivariate colour scheme is, as Hengl (2003) has already pointed out, that the colours are harder to distinguish in regions of high uncertainty. However, this would be no problem for isosurface rendering, if only some regions of a surface showed high uncertainty, so that the user, with the help of the spatial coherency, can still identify the different isosurfaces. In order to show the volume in which the isosurface will lie with a given confidence, we augment the representation of the standard deviation’s magnitude by colour mapping with glyphs (lines) that indicate the possible locations of the isosurface. The rest of this article will first describe the two dimensional colour map, the extraction and generation of lines indicating the envelope in which the isosurface will lie with a certain confidence, then explain the implementation and finally show an example of the application of our visualization.

2. Methodology

We developed two methods for the visualization of uncertainty, which are complementary and show different features of the data set. One uses colour mapping and is suitable to indicate to the viewer in which regions of the isosurface the standard deviation is high but does not show the possible displacement of the isosurface that is due to this uncertainty. The other one is glyph based and renders within which volume each isosurface will lie with a certain confidence even if it is not possible to infer the actual standard deviation from this point of the visualization. Both together provide a good assessment of both the data and its uncertainty in 3D space and allow the simultaneous visualization of multiple isosurfaces without confusing the viewer.

2.1. Showing uncertainty via colour mapping

The colour model most commonly used in computer graphics is the hardware-oriented RGB model, which is used, for example, in CRT monitors. It can be represented by a cube with red, green and blue values on the axis (see top of Figure 2). The resulting colour is generated by adding the individual contributions of the primary colours red, green and blue. If all primaries have the same value, different grey shades are produced with (1,1,1) representing white and (0,0,0) black.

![Figure 2: The RGB (top) and HSV (bottom) colour models.](image)

For our task, which involves using the colour of the isosurface to represent the data value while simultaneously giving the viewer an idea of the data’s uncertainty, it is advantageous to use the HSV (Hue - Saturation - Value) model, proposed by Smith (1978). This model can be represented as an upside down hexcone and is shown at the bottom of Figure 2. The top of the cone corresponds to a Value of 1 (maximum brightness). The fully saturated colours lie on the fringe and Hue is measured as the angle around the vertical axis, starting with red. In the centre of the top Saturation is zero and Value (brightness) is one (white). Along the vertical axis, different grey shades are produced with (1,1,1) representing white and (0,0,0) black.

For easier distinction the words Hue–Saturation–Value will be used in upper case throughout this article when they refer to the HSV model.
Figure 3: Four different two dimensional colour maps and corresponding isosurface visualizations. Vertical axis: variation of standard deviation, ranging from lowest value in the whole data set (bottom) to highest value (top). Horizontal axis: colour mapped data value (mean), again from its lowest value (left) to highest (right). A: Standard deviation is not shown and all isosurfaces are rendered with full colour saturation. B: Standard deviation is mapped to a combination of Value and Saturation. While the isosurface in dark blue is still rendered with full colour intensity, indicating low standard deviation, the light blue isosurface behind it becomes greyish, indicating its higher uncertainty. However, due to the smooth transition in colour saturation and value, regions of different uncertainty on isosurfaces are still hard to see. C: Using a steeper gradient for Saturation and Value for a window in the middle of standard deviation’s range emphasises regions of high uncertainty. D: Nearly the same as in C, but using a high value for Value. In regions of very high uncertainty isosurfaces’ colour fade into white. Our impression is that a colour map with a low value for Value representing high uncertainty, such as in C, supports recognition of the uncertain regions better.

axis Value is changed. The figure also shows the correspondence between the two models. The top plane of the HSV model shows the projected view from the top along the diagonal axis of the RGB model’s cube.

In our application the data value is mapped to a colour with Saturation and Value of one. In order to show the corresponding standard deviation, both Saturation and Value are varied depending on it. This is done using a linear ramp for which the start and end values in terms of standard deviation can be adjusted, so that the regions representing data with some (but low) standard deviation are still rendered with full colour saturation and the regions representing data with high standard deviation become more evident. The values for Saturation and Value that are used for regions with high standard deviation can be chosen interactively, so that the user can adjust the visualization to fit the environment and the surfaces can not become completely colourless and black. The resulting visualisation shows the isosurfaces in their normal colour where the standard deviation is low, appearing greyish and dark or dirty in regions where it is high. Figure 3 provides four different examples showing different colour maps and the corresponding visualisation of some isosurfaces.

The suggested colour scheme interferes slightly with the lighting and shading common in 3D visualization as these also vary the brightness of the objects, dependent on light direction and surface normal. As we also vary the Saturation to a large extent and because the user can interactively change viewing direction (lighting in our scene is usually done by a headlight) and the applied colour map, the regions of high uncertainty still remain visible.

2.2. Showing uncertainty using geometry

The colour mapping shown in Figure 3 indicates in which parts of the isosurfaces the data used have a high standard deviation and so are more unreliable compared to other parts. However, due to the mean and the uncertainty of the data in the whole neighborhood, the iso-
surface can have many different shapes and can be dislocated within a certain range. In order to obtain the envelope that will contain the isosurface with a certain confidence and to indicate this envelope, we have chosen the following approach. For each of the data points we calculate the upper and lower boundary of the confidence interval. This can be done using the scaled variable (Z) of the normal distribution of the scalar field function (i.e. pressure, temperature). According to, for example, Swan and Sandilands (1995):

\[ Z = \frac{\text{value} - \text{Mean(Data)}}{\text{StandardDeviation(Data)}}. \]

Z is then used to look up the probability that some data is below this value in tables. Based on the inverse process we look up Z for a given probability and then calculate:

\[ \text{LowerValue} = \text{Mean} - Z \times \text{StandardDeviation} \]
\[ \text{UpperValue} = \text{Mean} + Z \times \text{StandardDeviation} \]

Doing this for every grid point, we can extract three isosurfaces: one from the mean of the data, and one from the lower and the upper end of the confidence interval. Subsequently a ray is ‘shot’ from the mean isosurface along the surface normal until it intersects the upper and lower confidence isosurfaces. These rays are then visualized as lines, emanating from the mean surface and indicating the envelope corresponding to the confidence interval. It is important to be aware that the thickness of the envelope does not only depend on the standard deviation but on the overall setting. If, for example, neighbouring isosurfaces diverge, the envelopes will become thicker (the lines become longer), even if the standard deviation is the same all over the isosurface. When visualizing additional structures, such as boreholes, it becomes easily visible if these are, for example, intersected by one of the shown surfaces or lines, and so might be intersected by the isosurface with a given confidence. Figure 4 shows an example of how this visualization for a single isosurface looks and compares it to other rendering options.

3. Implementation

Our implementation is mainly based on two open source libraries and the Qt toolkit for the implementation of the user interface. We use the Visualization Toolkit\(^2\) (VTK, Schroeder et al, 1996) for data exchange and extraction of isosurfaces and the scene graph OpenSG\(^3\) (Reiners et al, 2002) for rendering. We

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\(^2\)www.vtk.org
\(^3\)http://opensg.vrsourc.org/trac
needed to implement a two-dimensional transfer function for the colour lookup and the generation of geometry that is needed to show the possible displacements of the mean surface given a certain confidence. By writing our own CVtkOsgActor class that we derived from vtkOpenGLActor, we transfer the geometry created by the VTK pipeline into OpenSG geometry. The approach is similar to the one by Rajlich (2009). In this way we could incorporate our visualization method into the commercial software VRED from PI-VR GmbH\(^4\), so that we can use both the desktop environment and our projection-based stereoscopic visualisation centre.

The user interface for steering the visualization is shown in Figure 5. After loading the data set using one of VTK’s file formats, the users are shown which different scalar attributes are present in the VTK file for the vertices of the grid. They first have to choose which of these attributes represents the mean and which one represents the corresponding standard deviation. Then the confidence interval needs to be chosen for which the envelope is calculated that contains the isosurface (with this confidence). Two additional data arrays are then added to the data object (vtkDataSet), which contain for each vertex the value of the low end of the confidence interval and the value of the high end. Further two histograms are computed and shown in the user interface, one showing the distribution of the data value and the other the distribution of the standard deviation. Users can add, move, and remove vertical lines in the histogram for the data values and so indicate for which values isosurfaces should be generated. Two vertical lines in the histogram for the standard deviation indicate the start and endpoint for the linear ramp of the Saturation and Value mapping.

To generate the colour mapping, we have implemented a two-dimensional transfer function, the vtkLookupTable2D class, that is derived from vtkLookupTable and maps from the data value and its standard deviation to a colour. The normal mechanism within VTK is that the vtkPolyDataMapper calls the function vtkLookupTable::MapScalarsThroughTable2(), which is declared virtual, so that we can override it in our class and our function is called instead. The function in our class first uses VTK’s standard function and maps the data values to the colours using a HSV based table with Value and Saturation being one. Subsequently we retrieve the standard deviation of the data, change Saturation and Value accordingly, transfer the colour to RGB space and return it. Example code for the conversion between the HSV and RGB colour model can be found in Foley et al (1996).

\(^4\)www.pi-vr.de

![Image](image-url)
4. Application

The example data set we use for the visualization is an uncertainty analysis of thermo-hydro-mechanical (THM) coupled processes in a hot-dry-rock geothermal reservoir that is described in detail in Watanabe et al (2010). It represents a stimulated geothermal reservoir in crystalline rock based on data from the Urach Spa location in southwest Germany. The geometry of the reservoir is shown in Figure 7. The hydraulically active area allows the reservoir to be represented by an 800x300x300m large block that is situated in a depth between 3850m and 4150m. Two boreholes, one for the injection and one for the production are placed 400m away from each other. As the problem is symmetric, only one half of the reservoir has been simulated. To analyze the uncertainty of the reservoir evolution that is due to limited data availability, Monte-Carlo simulations have been conducted with a stochastic reservoir model. 100 realizations with different permeability distributions have been used to simulate the THM (thermo-hydro-mechanical) processes over the reservoir. The resulting data have been summarized, so that they describe statistical analysis (mean and standard deviation) at each vertex of the grid.

Figure 7: Model set-up of the geothermal reservoir.
Figure 8 shows the simulated hydraulic pressure after 15 years of thermal water loop and streamlines, indicating the water flow, which is directed from the injection borehole (left) to the production borehole (right). It can be clearly seen that the standard deviation is high around the injection borehole (left), because the colours there become less saturated and are greyish and dark. Around the production borehole the colours are still bright and saturated, indicating a low standard deviation.

The general pattern of high standard deviation around the injection borehole and lower standard deviation around the production borehole is due to the fact that the pressure changes mainly at the locations where the temperature changes, which is at the cooling front around the injection borehole. The cooling front in turn is mainly affected by the velocity fields in the different realizations. After 15 years the cooling front still has not reached the production borehole, so that the standard deviation is still low around it.

Figure 9 shows several visualizations of our example data set's temperature field using our new visualization method (at the top and at the bottom right) and the 2D visualizations for the temperature and its standard deviation that were used in Watanabe et al (2010), shown at the bottom left of the figure. The 2D visualizations are horizontal sections through the data set in 4000m depth (vertically the center of the reservoir). The temperature is lowest near to the injection borehole, due to the reinjection of cold water, and increases with distance. The standard deviation of the temperature is low around the injection borehole because these regions are cooled down after 15 years of water injection, regardless of the uncertainty of the permeability distribution. Further away the cooling front is reached and the standard deviation is high because the uncertainty of the permeability in turn causes uncertainty of the velocity field and so leads to differences for the advancement of the cooling front. Further outwards the cooling front has not arrived and so the temperature is high and the standard deviation low. Looking at the emphasized isoline (thick black line) in the 2D section through the temperature and overlaying its course onto the 2D section showing the standard deviation of the temperature, it can be seen that the isoline cuts through these regions at its lower end.

As can be seen, the 2D sections show the general pattern very well for the depth of 4000m. However, the viewers can not assess if and how fast this pattern changes with depth. For this they would need to look at additional sections. If the pattern changes fast, many sections are needed and a 3D visualization becomes more practical. The aforementioned features can
be seen in the 3D visualization within their 3D spatial course and coherency. The isosurface near the injection borehole has a blue saturated colour and indicates that both temperature and standard deviation are low. The green isosurface further out corresponds to the isosurface emphasized in the 2D figures. The green colour is less saturated and darker in the centre, already indicating a higher standard deviation. The isosurface’s left and right fringes pointing towards the viewer are dark and grey and so indicate a very high uncertainty. This can be better seen in the close up at the bottom right of Figure 9, where we additionally included the 2D section to show the correspondence. It is also visible from this 3D visualization that this pattern, higher uncertainty at the left and right fringes, stays further upwards and downwards. Only at the top and bottom of the reservoir does the uncertainty seem to be equally high in the horizontal middle of the isosurface. The next isosurface (yellow) further outwards shows the same pattern but much less intensely and its overall uncertainty is already much lower. Further away from the injection borehole the cooling front has not yet arrived at this time step. So red isosurfaces show a high temperature with low uncertainty and are turning, so that they are lying flat, showing the geothermal gradient of the undisturbed formation.

5. Conclusions

The visualization method presented in this article is suitable for rendering multiple isosurfaces at a time because the applied colour scheme still allows the users...
to recognize which isosurfaces they are looking at, despite the fact that it is also used for rendering the magnitude of the uncertainty. The resulting visualization is intuitive to understand and does not confuse the viewer. The augmentation of the isosurface with lines that indicate the volume within which it will lie with a certain confidence makes the user aware how far the different isosurfaces shown might move and allows the user to judge if objects, such as boreholes, might be intersected by this isosurface with this confidence. The comparison of the 3D visualization method with a method currently often used for display – taking side-by-side views of sections through the data set, which display the data value and its standard deviation – shows that all features can be seen with the new method as well, but within the 3D context, so that the new visualization provides more information.

One drawback of this visualization method is that the scheme relies on at least a certain variability within the standard deviation. If several isosurfaces lie completely in a region of very high uncertainty, these are all rendered in dark grey, becoming indistinguishable for the user. So viewers depend on recognizing which isosurfaces they are looking at by the overall spatial context and knowledge of the physical problem. One solution is to apply sufficiently high minimum values for Satura
tion and Value, so that even with very high uncertainty, the colour (Hue) indicating the data value becomes distinguishable. However, this diminishes the visual colour range that can be used for making the user aware of the uncertainty.

6. Acknowledgements

We thank Dr. Alison E. Martin for proofreading the manuscript and thus making it more readable and the two anonymous reviewers for their valuable comments. This project has been funded by the ‘Earth and Environment’ Program of the German Helmholtz Association.

References


