Calculation of the numerical derivatives – comparison of the software

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Abstract: In the geophysical as well as other scientific practice we oftentimes need to calculate the derivatives of the measured data. Since the analytical approach cannot be used, numerical differentiation is adopted. There are many techniques to calculate the derivatives, usually as a part (or plugin) of commercial software. For 0% random noise all of the software lead to almost same results. But if noisy data are processed, the choice of the correct method (software) is far from being trivial because the differences in the outputs are surprisingly huge.

Key words: geophysics, potential fields, numerical derivatives, regularization, software

1. Introduction

In the nature, there are some situations where the classical mathematical approaches do not describe the geological (or other) situations well. This particularly holds for the calculations of the numerical derivatives. Of course, it does not mean that the mathematics used is bad. The reasons for this are in the fact that universe, nature, field, are much more complicated than we were taught at elementary courses. There is a way out, though. Throughout the years many different techniques have been developed to manage these problematic aspects. Many authors have developed their own approaches to process the data so the calculated output is acceptable (not

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too noisy, not too smooth). Usually these techniques apply filtering *(Bielik, 1982; Šefara and Bielik, 2004)* the input data and the filtered intermediate product is differentiated. Most of the used filters require the knowledge of the appropriate values of the filter parameters. These values can be estimated from the boundary conditions or by the trial and error method. On the other hand, there are some techniques that do not call for the filter parameters in advance. One of such methods is regularization, which does not need the "a priori" information about the filter parameters (regularization parameters). Potential theory in gravity and magnetics applications is very well described e.g. in *Blakely (1995), Mudretsova and Veselov (1990).* As a magnificent output of application of these methods is the structural – tectonic map *(Šefara et al., 1987).*

2. Unstable operators

To compute any type of representation from the image, information must be extracted using certain operators interacting with the image. The most common and basic questions about the operators are: Which operators to apply? Where and how to apply them? Most of the operators used in the practice somewhat involve the differentiation. It is known that differentiation is an unstable operation – small perturbations in the input lead to high perturbations in the output. The most often used derivative operators are directional derivatives, gradients, terrain aspect, curvatures, the second vertical gradient, biharmonic operator or various combinations of them.

Directional derivatives. This is a difference operator, which compares two neighboring values separated by a certain distance. In mathematics this distance can be infinitesimally small if we take the limit of the separation distance to zero. But in physics, of course, we cannot use infinitesimal distances because our measurements are always represented by the discrete data. We can never make our measurements infinitely dense (fast, small). Therefore we encounter serious problems if we deal with the differentiation of discrete data in a pure mathematical way. Because the differentiation is used in many fields, not only geophysical, this operator is one of the best known among the unstable operators.

Terrain slope (first total horizontal gradient). For a particular point on the surface, the terrain slope is based on the direction of steepest descent or ascent at that point (terrain aspect). This means that across the surface, the gradient direction can change. The slope, S, at a point P is the magnitude of the gradient at that point. From the definition of the gradient *(MapInfo, 2000)*

$$S = \sqrt{\left(\partial_x f\right)^2 + \left(\partial_y f\right)^2}.$$

Terrain aspect. This operator calculates the downhill direction of the steepest slope (i.e. dip direction). It is the direction that is perpendicular to the contour lines on the surface, and is exactly opposite to the gradient direction. The terrain aspect, A_T, is represented as an azimuth (in degrees, not radians) *(MapInfo, 2000)*:

$$A_T = \frac{180}{\pi}\mathrm{atan2}\left(\frac{\partial_y f}{\partial_x f}\right),$$

where atan2 is defined as arcus tangens for interval $\langle 0, \pi)$.

Analytical signal (total gradient). Very similar to the first total horizontal gradient and used very often in geophysics *(Berezkin, 1967; Nabighian, 1972)*:

$$A_S = \sqrt{\left(\partial_x f\right)^2 + \left(\partial_y f\right)^2 + \left(\partial_z f\right)^2}.$$

Profile curvature. This operator determines the downhill or uphill rate of change in slope in the gradient direction (opposite of slope aspect direction). It produces contour maps that show isolines of constant rate of change of steepest slope across the surface. Negative values are convex upward and indicate accelerated flow of water over the surface. Positive values are concave upward and indicate slowed flow over the surface. The profile curvature K_S is given by *(Golden Software Surfer, 2003)*

$$K_S = \frac{\left(\partial_{xx} f\right)\left(\partial_x f\right)^2 + 2\left(\partial_{xy} f\right)\left(\partial_x f\right)\left(\partial_y f\right) + \left(\partial_{yy} f\right)\left(\partial_y f\right)^2}{\left[\left(\partial_x f\right)^2 + \left(\partial_y f\right)^2\right]\left[1 + \left(\partial_x f\right)^2 + \left(\partial_y f\right)^2\right]^{3/2}}.$$

Plan curvature. This operator reflects the rate of change of the terrain aspect angle measured in the horizontal plane, and is a measure of the curvature of contours. Negative values indicate divergent water flow over the surface, and positive values indicate convergent flow. The plan curvature K_H is given by *(Golden Software Surfer, 2003)*

$$K_H = \frac{(\partial_{xx} f)(\partial_y f)^2 - 2(\partial_{xy} f)(\partial_x f)(\partial_y f) + (\partial_{yy} f)(\partial_x f)^2}{\left[(\partial_x f)^2 + (\partial_y f)^2\right]^{3/2}}.$$

Tangential curvature. This operator measures curvature in relation to a vertical plane perpendicular to the gradient direction, or tangential to the contour. The negative and positive areas are the same as for plan curvature, but the curvature values are different. Tangential curvature is related to the plan curvature by the sine of the slope φ: $K_H = K_T / \sin\varphi$. Tangential curvature K_T is given by *(Golden Software Surfer, 2003)*

$$K_T = \frac{(\partial_{xx} f)(\partial_y f)^2 - 2(\partial_{xy} f)(\partial_x f)(\partial_y f) + (\partial_{yy} f)(\partial_x f)^2}{\left[(\partial_x f)^2 + (\partial_y f)^2\right]\left[1 + (\partial_x f)^2 + (\partial_y f)^2\right]^{1/2}}.$$

2. vertical gradient. Second vertical gradient of the gravity field is an important tool in the frame of the transformation of potential fields – it suppresses the effect of regional components in the interpreted field and its local maxima are connected with the centres of isolated bodies and edges of contacts and steps. The second vertical gradient is given by

$$V_{zz} = -\left(\partial_{xx} f + \partial_{yy} f\right).$$

Biharmonic operator. Bending of thin plates and shells, viscous flow in porous media, and stress functions in linear elasticity are three examples of physical quantities that can be mathematically described using the biharmonic operator. The biharmonic operator is defined by

$$\nabla^4 f = \partial_{xxxx} f + 2\partial_{xxyy} f + \partial_{yyyy} f.$$

3. Comparison of the software

Naturally, many authors have developed formulae or algorithms for calculation of the derivatives or other unstable operators. Some of these methods are a part of some commercially available software packages. Now the question is which of these products is the best in evaluating the unstable operators. We are presenting here the comparison of results obtained by six independent software packages, namely, *GeoSoft (1997), Golden Software Surfer 8 (2003), MapInfo Professional Version 6.0 (2000), MathSoft MathCAD Professional (2000)*, the regularization method developed by Pašteka *(Pašteka and Richter, 2002)*, and the regularization method developed by Richter *(Richter and Pašteka, 2003)*.

Geosoft (1997) and *Surfer (2003)* have implemented also the low-pass filters. But these filters need their own input parameters. However, assessing the appropriate values of the filter parameters is difficult and requires a skilled user. Compared with this the regularization approach has shown to be more convenient. Based on this Surfer as well as Geosoft were used in the basic mode (without filters) as many users often use it.

Two signals are under the inspection, namely the theoretical V_z of the sphere and the V_z of the sphere influenced by the 2% white noise (Fig. 1), which is generally considered to be low. The synthetic study area will be on the grid $\{x_i = i, y_j = j\}$, where $i, j \in Z \cap \langle -25, 25 \rangle$. The spherical body is located in the point [0 m, 0 m, - 5 m], radius r = 1 m, density $\rho_{\mathrm{s}} =$ 19270 kg.m^{-3} (gold spherical nugget). The quality of the eight unstable operators was compared, namely the first horizontal gradient (V_{zx}), the first total horizontal gradient (terrain slope, S), terrain aspect (A_T), profile

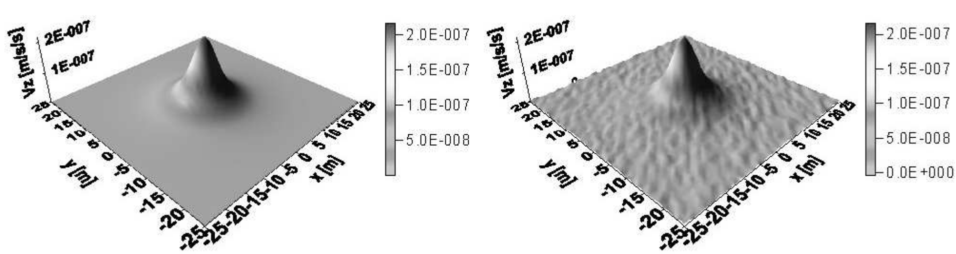

Fig. 1. The theoretical V_z of the above-mentioned sphere (left) and the signal influenced by the 2% white noise (right).

curvature (K_S), plan curvature (K_H), tangential curvature (K_T), 2. vertical gradient (V_{zz}) and biharmonic operator (B).

For the 0% white noise all of the compared commercial software leads to the more or less same results. The maximal differences are below 0.5%. Because of this we concentrated on the noisy data. All the figures of the calculated operators refer to the 2% white noise in the input. Despite this low value the differences among the results are significant.

The first horizontal gradient. Five independent software packages were applied and the results were compared with the theoretical solution (Fig. 2). The regularization methods are clearly the best and very close to the theoretical solution. The solutions by Surfer and Geosoft are so noisy that the anomaly is almost invisible. MathCAD worked in a very strange manner. Such a result is not only bad, but also confusing and misleading.

Terrain slope. Six independent software packages were applied and the results were compared with the theoretical solution (Fig. 3). The regularization methods are clearly the best again and very close to the theoretical solution. The solutions by Surfer and Geosoft are so noisy that the anomaly is almost invisible, although an experienced geophysicist might distinguish the Geosoft's result. *MapInfo* is too steep although the central parts of the anomaly could be interpretable. *MathCAD* worked in a very strange way again. Such a result is not only incorrect and noisy, but also confusing and misleading. It makes a feeling of strictly concave function which is an absolute nonsense.

Terrain aspect. Six independent software packages were applied and the results were compared with the theoretical solution (Fig. 4). The regularization methods have proven to be good again (the method of Pašteka looks worse, though), although small distortions at the borders and near the discontinuity can be seen. The solutions by *Surfer, Geosoft* and *MapInfo* are so noisy that the anomalies are absolutely invisible. They resemble a very slightly centrally correlated noise. *MathCAD* would be quite close to the theoretical solution but it is rotated and small distortions at the borders and near the discontinuity can be seen. Compared with the regularization, the part near the discontinuity is better reconstructed by the regularization.

Profile curvature. Five independent software packages were applied and the results were compared with the theoretical solution (Fig. 5). Again, the only legible result was obtained by the regularization (both methods comparable), although a banded or circular pattern is seen. *Surfer's* and *Geosoft's* results are similar in the way that the results look like pure white noise. The result of *MathCAD* resembles the Dirac delta function. Such a result is even worse than the extremely noisy ones because it can mislead the interpreter.

Tangential curvature. Five independent software packages were applied

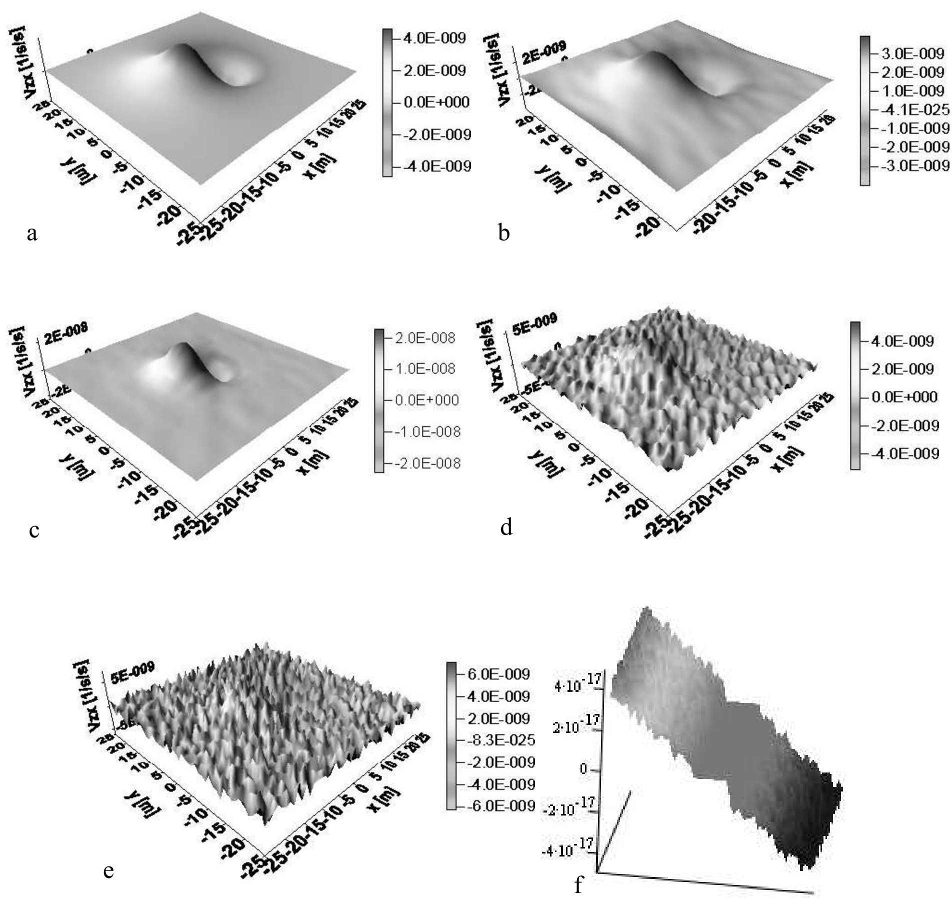

Fig. 2. The theoretical first horizontal gradient (a) and the one calculated by the method developed by *Richter (2003)* (b), the method developed by *Pašteka (2002)* (c), *Golden Software Surfer 8 (2003)* (d), *Geosoft (1997)* (e) and *MathSoft MathCAD Professional (2000)* (f).

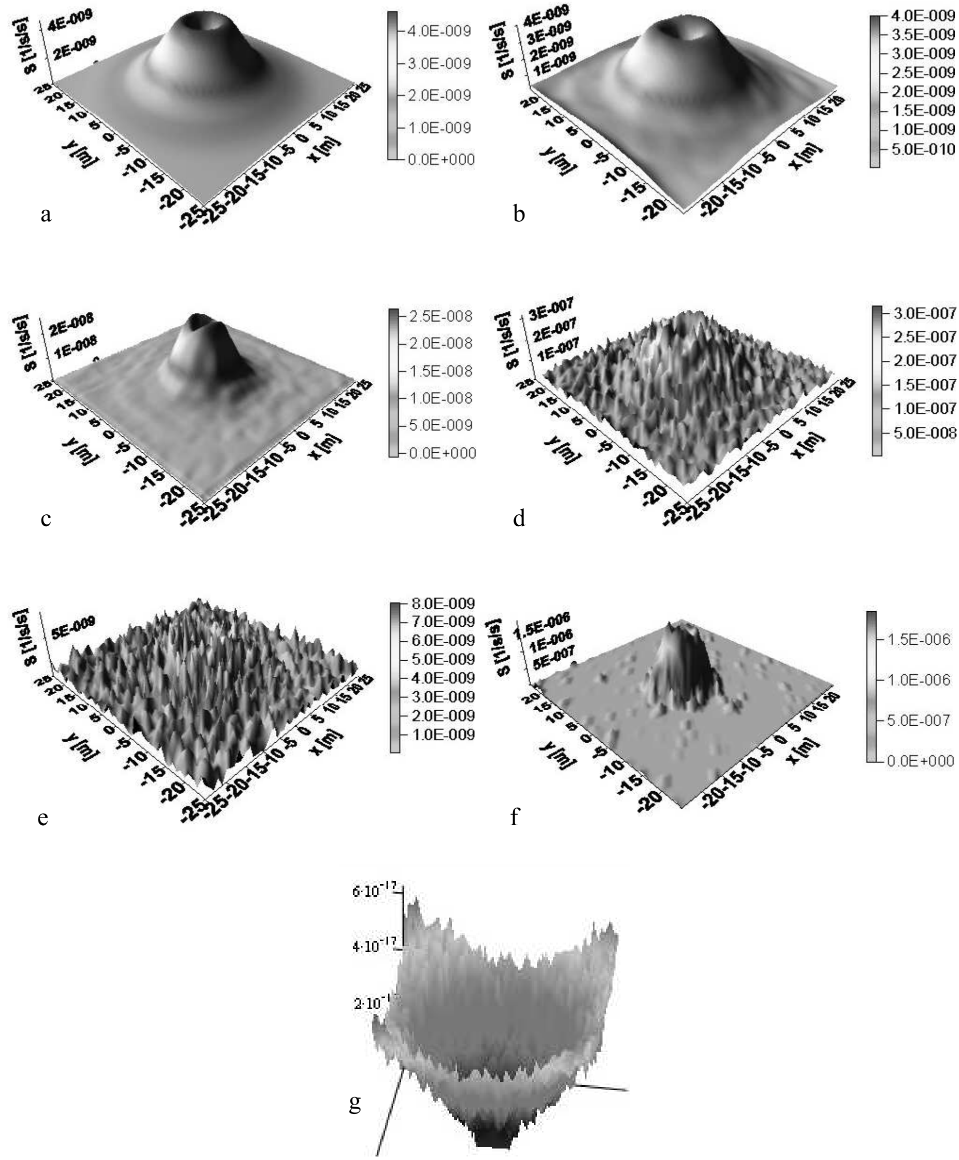

Fig. 3. The theoretical first total horizontal gradient (terrain slope) (a) and the one calculated by the method developed by *Richter (2003)* (b), the method developed by *Pašteka (2002)* (c), *Golden Software Surfer 8 (2003)* (d), *Geosoft (1997)* (e), *MapInfo Professional 6.0 (2000)* (f) and *MathSoft MathCAD Professional (2000)* (g).

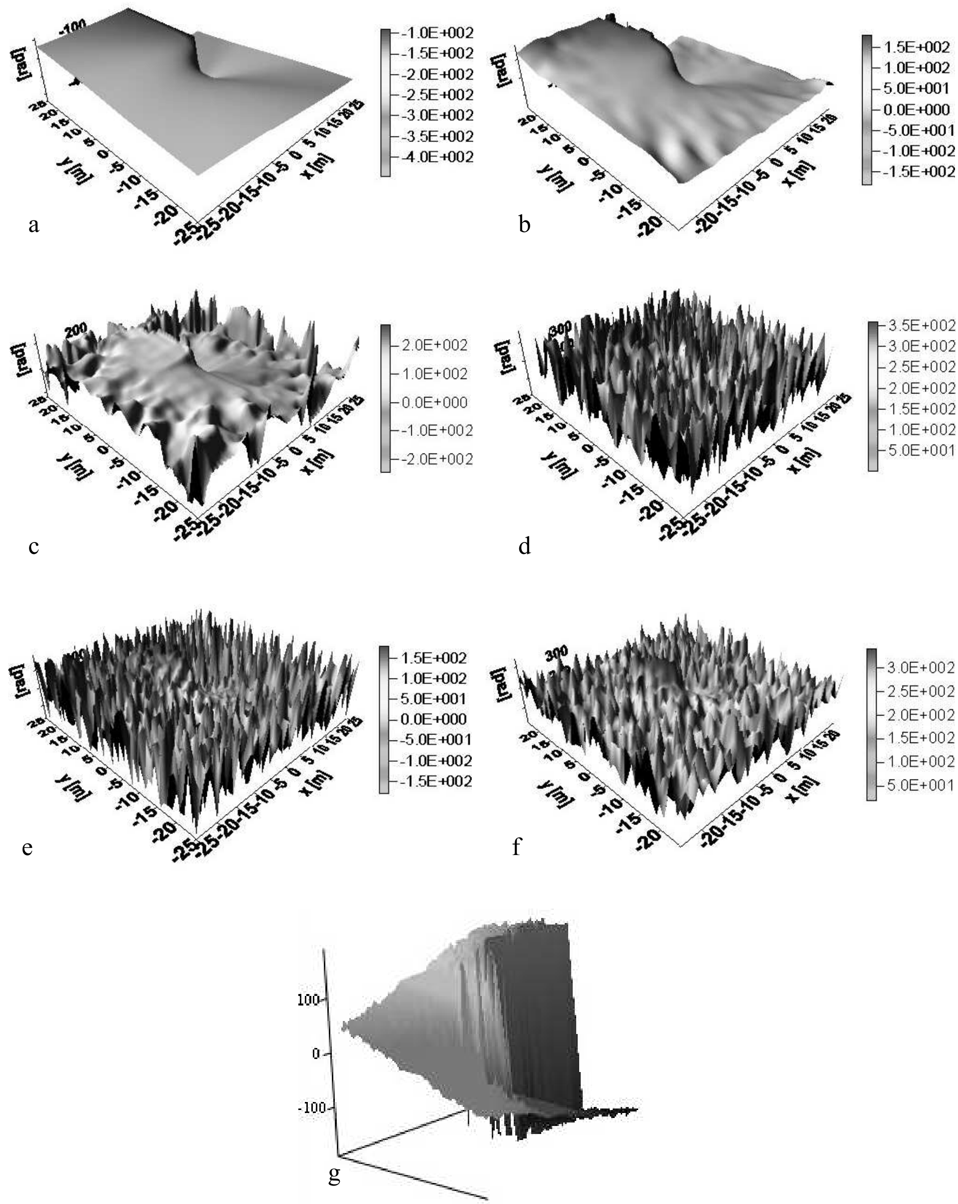

Fig. 4. The theoretical terrain aspect (a) and the one calculated by the method developed by *Richter (2003)* (b), the method developed by *Pašteka (2002)* (c), *Golden Software Surfer 8 (2003)* (d), *Geosoft (1997)* (e), *MapInfo Professional 6.0 (2000)* (f) and *MathSoft MathCAD Professional (2000)* (g).

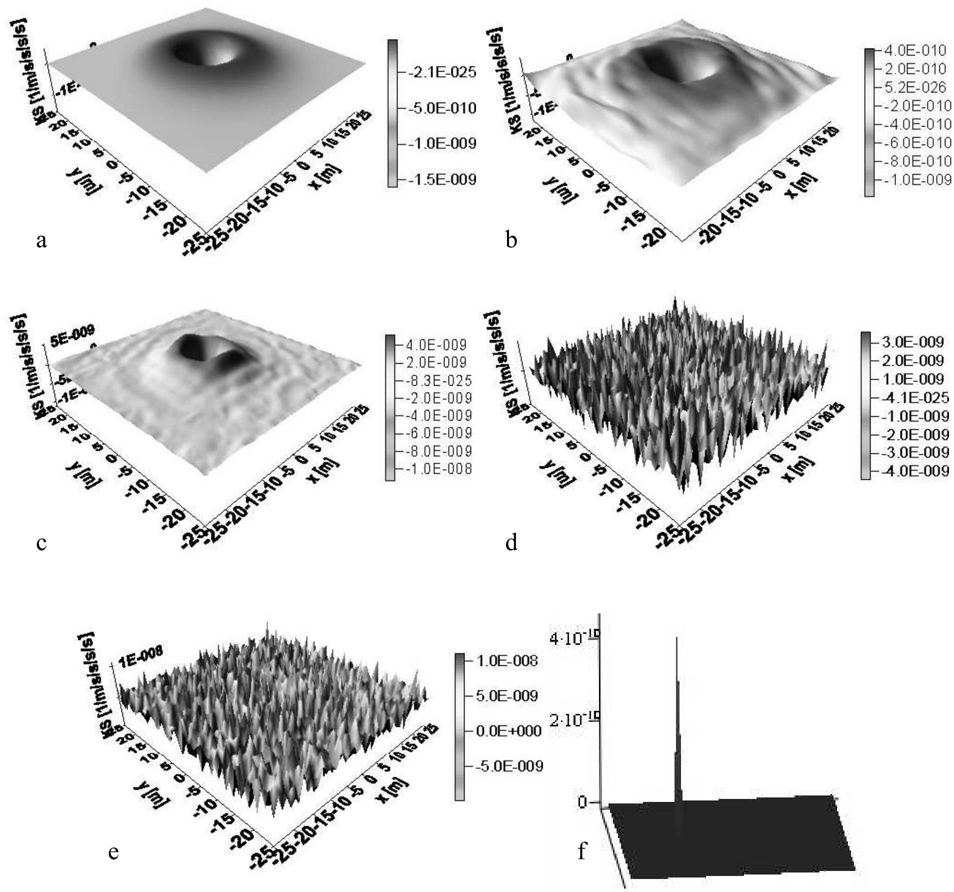

Fig. 5. The theoretical profile curvature (a) and the one calculated by the method developed by *Richter (2003)* (b), the method developed by *Pašteka (2002)* (c), *Golden Software Surfer 8 (2003)* (d), *Geosoft (1997)* (e) and *MathSoft MathCAD Professional (2000)* (f).

and the results were compared with the theoretical solution (Fig. 6). Again the regularization methods are superior to the others, although the undulated patterns are seen (both methods comparable). Geosoft looks like pure white noise. Surfer is even worse because it makes the feeling of an empty space with two spikes. Similarly, confusing work of MathCAD makes the feeling of the negative Dirac delta function.

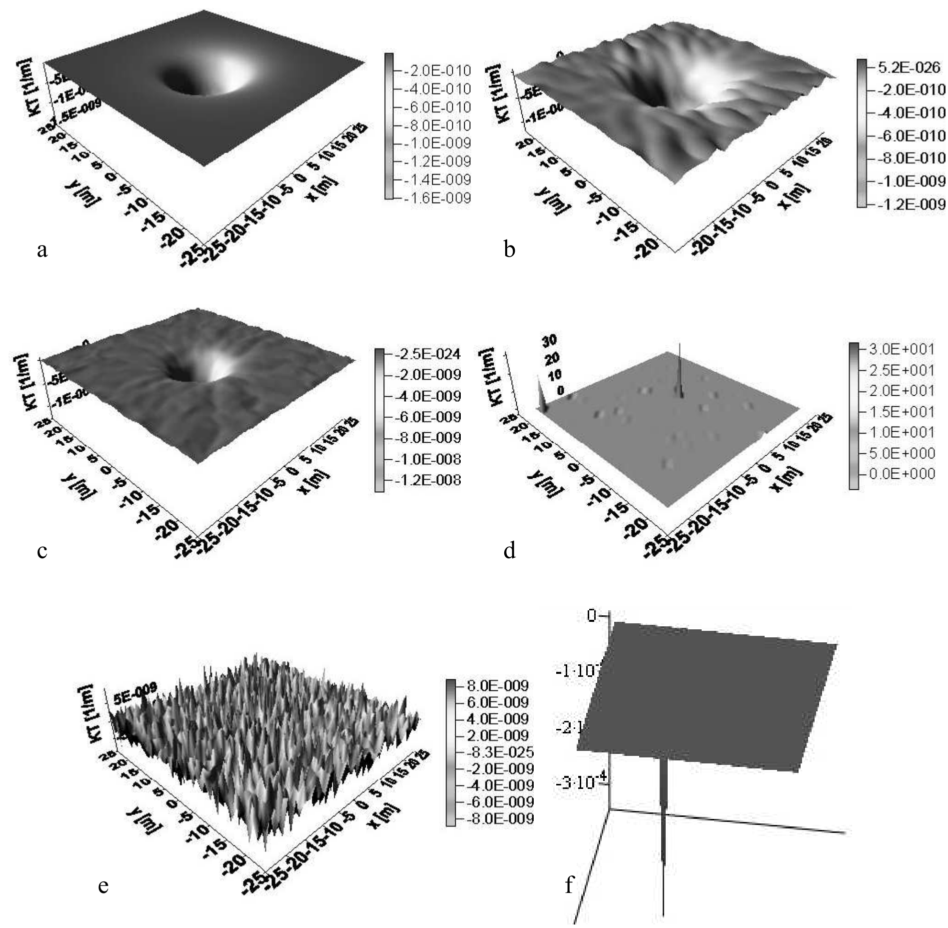

Fig. 6. The theoretical tangential curvature (a) and the one calculated by the method developed by *Richter (2003)* (b), the method developed by *Pašteka (2002)* (c), *Golden Software Surfer 8 (2000)* (d), *Geosoft (1997)* (e) and *MathSoft MathCAD Professional (2000)* (f).

To be more objective, the statistical analysis was performed. The distributions of the relative deviation of the calculated operator from the theoretical one were calculated. The graphs can be found in *Richter (2004)*. The qualitative results are presented in Tab. 1 for the 0% noise and in the Tab. 2 for the 2% white noise. A very simple criterion is used – the closest

Tab. 1. The grades assigned to the particular software packages that were used for applying the operators to the V_z of the above-mentioned sphere for 0% noise. The column "Mean" represents the average resulting grade of a particular software.
[1] *Richter and Pašteka (2003)*
[2] *Pašteka and Richter (2002)*

	V_{zx}	S	A_T	K_S	K_H	K_T	V_{zz}	B	***Mean***
Richter[1]	1	2	2	2	1	1	2	2	**1,63**
Pašteka[2]	2	1	1	1	2	2	3	3	**1,88**
Surfer 8	3	3	3	3	3	3	1	1	**2,5**
Geosoft	5	5	6	5	5	5	5	5	**5,13**
MapInfo 6.0		6	5						**5,5**
MathCAD 2000	4	4	4	4	4	4	4	4	**4**

Tab. 2. The grades assigned to the particular software packages that were used for applying the operators to the V_z of the above-mentioned sphere for 2% noise. The column "Mean" represents the average resulting grade of a particular software.
[1] *Richter and Pašteka (2003)*
[2] *Pašteka and Richter (2002)*

	V_{zx}	S	A_T	K_S	K_H	K_T	V_{zz}	B	***Mean***
Richter[1]	1	2	1	2	2	1	1	1	**1,38**
Pašteka[2]	2	1	2	1	1	2	2	2	**1,63**
Surfer 8	3	3	4	4	5	3	4	4	**3,75**
Geosoft	4	5	6	3	4	5	5	5	**4,63**
MapInfo 6.0		4	5						**4,5**
MathCAD 2000	5	6	3	5	3	4	3	3	**4**

solution to the theoretical one wins the first place and so on. In this way each software gets a grade and after all, the resulting grade is the mean of the particular grades.

Tables 1 and 2 belong to the most important results of the paper. They prove that the research in the field of regularization is important. The same way they show that the usual commercial software use non-regularization methods for the calculation of derivatives, which is not suitable for noisy data. Of course, there are various software packages calculating the derivatives by the means of regularization. The problem is, however, that such programs are usually too expensive (*Zhdanov, 2002;* e-mail communication).

5. Conclusions

Comparing the software packages it was shown that for the synthetic data (without noise) the results are in most cases comparable *(Richter, 2004)*. If it were not for the regularization methods, *Surfer* would produce the closest results to the theory in most cases. Regularization showed a tiny side effect in some cases. *Geosoft* develops clear artifacts, banded patterns in the results. *MapInfo* slightly distorts the results. *MathCAD* produces artifacts.

For data influenced by 2% random noise the regularization methods were the only that produced reasonable results. In absolutely most cases none of the other software packages calculated any interpretable solution. Their solutions are either extremely noisy, or perfectly smooth. Interpretable results are exceptions even in cases of very small noise content.

From the previous it results that the regularization is not necessary if the signal is without noise or the noise content is very low. Such data can be acquired, for example, with the highly accurate TM-4 magnetometer of the Australian company G-Tek. It has been observed that in such cases the regularization can even create some artifacts, or strange shapes, in the resulting output. By this way the regularization can be used as an independent marker of the data quality (whether it is or is not necessary to regularize). From these results it implies that in such cases whatever software can process the data without noise.

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