High-accuracy practical spline-based 3D and 2D integral transformations in potential-field geophysics

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ABSTRACT
Potential, potential field and potential-field gradient data are supplemental to each other for resolving sources of interest in both exploration and solid Earth studies. We propose flexible high-accuracy practical techniques to perform 3D and 2D integral transformations from potential field components to potential and from potential-field gradient components to potential field components in the space domain using cubic B-splines. The spline techniques are applicable to either uniform or non-uniform rectangular grids for the 3D case, and applicable to either regular or irregular grids for the 2D case. The spline-based indefinite integrations can be computed at any point in the computational domain. In our synthetic 3D gravity and magnetic transformation examples, we show that the spline techniques are substantially more accurate than the Fourier transform techniques, and demonstrate that harmonicity is confirmed substantially better for the spline method than the Fourier transform method and that spline-based integration and differentiation are invertible. The cost of the increase in accuracy is an increase in computing time. Our real data examples of 3D transformations show that the spline-based results agree substantially better or better with the observed data than do the Fourier-based results. The spline techniques would therefore be very useful for data quality control through comparisons of the computed and observed components. If certain desired components of the potential field or gradient data are not measured, they can be obtained using the spline-based transformations as alternatives to the Fourier transform techniques.

Key words: Integral transformations, Cubic B-splines, Gravity, Magnetic, Gravity gradients

INTRODUCTION
The vertical components of the gravity acceleration field and the total-field magnetic data are traditionally measured and the potential-field gradients are increasingly observed for a wide scope of studies in exploration (Nabighian et al. 2005a, b). Horizontal derivatives are used for detecting edges of source bodies (Blakely and Simpson 1986; Grauch and Cordell 1987). Both horizontal and vertical derivatives are needed for determining the lateral location and depth of single or multiple simple sources with Euler deconvolution (Thompson 1982; Reid et al. 1990; Ravat 1996; Nabighian and Hansen 2001; Hansen and Suciu 2002; Ravat et al. 2002; FitzGerald, Reid and McInerney 2004), the 2D analytic signal (Nabighian 1972, 1974) and the 3D total gradient techniques.

Gravity, magnetic field and gradient data are also applied to solid Earth studies, such as crustal structure (Behrendt, Meister and Henderson 1966; Thomas, Grieve and Sharpton 1988; Allen and Hinze 1992; Bosum et al. 1997; Cochran et al. 1999; Berrino, Corrado and Riccardi 2008), the
Potential, Potential Field (PF) and Potential-field Gradient (PG) data are supplemental to each other for resolving sources. Transformations facilitate data comparison and provide more means for interpretation by transforming the measured data into other forms of data. The fast Fourier transform (FT) is used widely in potential-field geophysics (e.g., Blakely 1996; Sandwell and Smith 1997; Mickus and Hinojosa 2001; Carbó et al. 2003). In theory, the Fourier transform techniques could be applied to perform potential-field transformations. However, the results of the Fourier transform techniques are often less accurate than one might like, and the Fourier transform techniques are only applied to regular grid points (e.g., Ricard and Blakely 1988; Wang 2006).

High-accuracy spline-based techniques of 3D and 2D potential-field upward continuation (Wang 2006) and potential field and gradient component transformations and derivative computations (Wang, Krebes and Ravat 2008) have been developed. In this paper, we propose flexible high-accuracy computations (Wang, Krebes and Ravat 2008) have been developed. In this paper, we propose flexible high-accuracy techniques of 3D and 2D integral transformations from PF components to potential and from PG components to PF components in the space domain with cubic B-splines. Using synthetic 3D gravity and magnetic transformation examples, we find that the spline techniques are substantially more accurate than the Fourier transform techniques, and demonstrate that harmonicity is confirmed substantially better for the spline method than the Fourier transform method and that spline-based integration and differentiation are invertible. Real data examples of 3D transformations show that the spline-based results agree substantially better (from gravity-gradient components to gravity) or better (between gravity-gradient components) with the observed data than do the Fourier-based results. For synthetic or real-data examples, relative root mean square errors between the computed values and the corresponding exact or observed values are taken to measure the accuracy.

POSSIBLE, POTENTIAL FIELD AND POTENTIAL-FIELD GRADIENT

Let \( U(x, y, z) \) be the potential, \( f(x, y, z) \) be the potential field, and \( D(x, y, z) \) be the potential-field gradient tensor. For convenience, we use a uniform notation with \( U(x, y, z) \) and its derivatives in this paper.

A potential field component equals to the corresponding partial derivative of the potential:

\[
f_i(x, y, z) = U_i(x, y, z) = \frac{\partial U}{\partial x}, \quad i = x, y, z.
\]  

(1)

Analogously, a potential-field gradient component equals to the corresponding second-order partial derivative of the potential:

\[
D_{ij}(x, y, z) = f_{ij}(x, y, z) = \frac{\partial f_i}{\partial y} = U_{ij}(x, y, z) = \frac{\partial^2 U}{\partial x \partial y}.
\]  

(2)

Any potential field \( f(x, y, z) \) is conservative and curl free, i.e. \( \nabla \times f(x, y, z) = 0 \), so that \( U_{ij}(x, y, z) = U_{ij}(x, y, z) \), \( i, j = x, y, z \), \( i \neq j \).

(3)

In the region outside the sources any potential field \( f(x, y, z) \) is divergence free, i.e. \( \nabla \cdot f(x, y, z) = 0 \). Therefore Laplace’s equation holds

\[
U_{zz}(x, y, z) = -[U_{xx}(x, y, z) + U_{yy}(x, y, z)].
\]  

(4)

Considering equations (3) and (4), for the 3D case only five (e.g., \( U_{xx}, U_{yy}, U_{zz}, U_{xy}, U_{yz} \)) of the nine components of the gradient tensor \( D(x, y, z) \) are independent. Analogously, for the 2D case only two (e.g., \( U_{xx}, U_{xy} \)) of the four components of the gradient tensor \( D(x, x) \) are independent.

CALCULATING HORIZONTAL INDEFINITE INTEGRALS WITH CUBIC B-SPLINES

The 2D case

Approximate \( V(x) = U_{xk}, k = x, z \) or \( V(x) = U_x \) with splines, satisfying conditions (A7) and (A8). The interpolation coefficients \( \{C_i\} \) can be determined (Appendix A). We then have

\[
\int V(x)dx = \sum_{i=1}^{N+1} C_i N_i^{-1}(x),
\]  

(5)

where \( N_i^{-1}(x) \) is given by equation (A3) in Appendix A.

The 3D case

Approximate \( V(x, y) = U_{xk}, k = x, y, z \) or \( V(x, y) = U_x \) with splines, satisfying conditions (B3) through (B6). The interpolation coefficients \( \{C_{i,j}\} \) can be determined (Appendix B). We
then have
\[ \int V(x, y) dx = \sum_{i=1}^{N_x+1} \sum_{j=1}^{N_y+1} N_i(x) C_{ij} N_j(y). \] (6)

Similarly, approximating \( V(x, y) = U_{ik}, k = x, y, z \) or \( V(x, y) = U_y \) with splines, satisfying conditions (B3) through (B6). We then have
\[ \int V(x, y) dy = \sum_{i=1}^{N_x+1} \sum_{j=1}^{N_y+1} N(x) C_{ij} N_j(y), \] (7)

where \( N(x), N^{-1}(x) \) are given by equation (A3) in Appendix A, and \( N(y), N^{-1}(y) \) are similarly obtained for subscript \( j \).

**TRANSFORMATIONS FROM PF COMPONENTS TO POTENTIAL**

**2D transformations from \( U_x \) to \( U \)**

Let \( V(x) \) be \( U_x(x) \) and use equation (5) to obtain \( U(x) \).

**3D transformations from \( U_x \) or \( U_y \) to \( U \)**

Let \( V(x, y) \) be \( U_{x}(x, y) \) or \( U_{y}(x, y) \) and use equation (6) or (7) to obtain \( U(x, y) \).

**TRANSFORMATIONS FROM PG COMPONENTS TO PF COMPONENTS**

**2D transformations from \( U_{xx} \) to \( U_x, U_z \)**

Let \( V(x) \) be \( U_{xx}(x) \) and use equation (5) to obtain \( U_{x}(x) \).

Knowing \( U_{x}(x) \), calculate \( U_{x}(\xi) \) (Wang et al. 2008) from
\[ U_{x}(\xi) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{U_{x}(x)}{\xi - x} dx. \] (8)

**2D transformations from \( U_{xx} \) to \( U_x, U_z \)**

Let \( V(x) \) be \( U_{xx}(x) \) and use equations (5) to obtain \( U_{x}(x) \).

Knowing \( U_{x}(x) \), \( U_{x}(\xi) \) can be calculated (Wang et al. 2008) from
\[ U_{x}(\xi) = -\frac{1}{\pi} \int_{-\infty}^{\infty} \frac{U_{x}(x)}{\xi - x} dx. \] (9)

**3D transformations from \( U_{xy} \) to \( U_x, U_y, U_z \)**

Consider equations (6) and (7). Let \( V(x, y) \) be \( U_{xy}(x, y) \), then \( U_{x}(x, y) \) and \( U_{y}(x, y) \) can be calculated. Knowing \( U_{x}(x, y) \) and \( U_{y}(x, y) \), calculate \( U_{x}(\xi, \eta) \) (Wang et al. 2008) from
\[ U_{x}(\xi, \eta) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{(\xi - x)U_{x}(x, y) + (\eta - y)U_{y}(x, y)}{[(x - \xi)^2 + (y - \eta)^2]^{3/2}} dxdy. \] (10)

3D transformations from \( U_{xz} \) or \( U_{yz} \) to \( (U_x, U_y, U_z) \)

Let \( V(x, y) \) be \( U_{xz}(x, y) \) or \( U_{yz}(x, y) \) and use equation (6) or (7) to obtain \( U_{x}(x, y) \). Knowing \( U_{x}(\xi, \eta) \), calculate \( U_{x}(\xi, \eta) \) and \( U_{y}(\xi, \eta) \) (Wang et al. 2008) from
\[ U_{x}(\xi, \eta) = -\frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{(\xi - x)U_{x}(x, y)}{[(x - \xi)^2 + (y - \eta)^2]^{3/2}} dxdy, \] (11)
\[ U_{y}(\xi, \eta) = -\frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{(\eta - y)U_{y}(x, y)}{[(x - \xi)^2 + (y - \eta)^2]^{3/2}} dxdy. \] (12)

**EVALUATION OF INFINITE INTEGRALS AND DOUBLE INTEGRALS**

Equations (8 and 9) are similar infinite integral relations. When the computational domain \( D_1 = \{a \leq x \leq b \} \) is well beyond the lateral extent of all sources of interest, approximate each infinite integral with a definite integral and evaluate it using the spline technique. To avoid a singularity, the sampling point \( (\xi, \eta) \) must not coincide with a spline knot \( (x, y) \). The centre of each interval of the spline grid is an ideal location for a sampling point. For a given point \( (\xi, \eta) \), approximate the whole of the integrand in equation (8), e.g., with splines, the interpolation coefficients \{ \( C_i \) \} can be determined (Appendix A). Thus, we have
\[ U_{x}(\xi) = \frac{1}{\pi} \sum_{i=1}^{N_x+1} C_i(\xi)[N^{-1}_i(b) - N^{-1}_i(a)]. \] (13)

where \( N^{-1}(\cdot) \) is given by equation (A3) in Appendix A.

Equations (10 and 12) are similar infinite double integral relations. When the computational domain \( D_2 = \{(a \leq x \leq b, c \leq y \leq d) \} \) is well beyond the lateral extent of all sources of interest, approximate each infinite double integral with a definite double integral and evaluate it using the spline technique. To avoid a singularity, the sampling point \( (\xi, \eta) \) must not coincide with a spline knot \( (x, y) \). The centre of each rectangular unit of the spline grid is an ideal location for a sampling point. For a given point \( (\xi, \eta) \), approximate the whole of the integrand in equation (10), e.g., with splines, the interpolation coefficients \{ \( C_{ij} \) \} can be determined (Appendix A).
B. Thus, we have

\[ U_i(\xi, \eta) = \frac{1}{2\pi} \sum_{j=1}^{N_x+1} \sum_{j=1}^{N_y+1} \left[ N^{-1}(b) - N^{-1}(a) \right] C_{ij}(\xi, \eta) \times \left[ N^{-1}(d) - N^{-1}(c) \right], \]

(14)

where \( N^{-1}(\cdot) \) is given by equation (A3) in Appendix A, and \( N^{-1}(\cdot) \) is similarly obtained for subscript \( j \).

SYNTHETIC EXAMPLES

3D gravity example of \( U_z \) obtained from noisy \( U_{xz} \) with the spline technique and comparison with the Fourier transform technique

In equation (6), let \( V(x, y) = U_{xz} \), calculate \( U_z \). The 3D sources are four solid spheres with densities and geometrical parameters listed in Table 1. Figure 1 shows the effectiveness of computing \( U_z \) from \( U_{xz} \) in the noisy situation. Figure 1(f) shows the \( U_{xz} \) data contaminated by random noise with a zero mean and a standard deviation of 0.65 mGal/km. Figure 1a shows the exact theoretical \( U_z \) map. The \( U_z \) map obtained using the spline technique is shown in Fig. 1(b). In order to improve the performance of both the spline technique and the Fourier transform technique, expand the original grids with 32 data points on each side of the computational domain and taper the expanded parts, but just keep the computed \( U_z \) values on the original grids. The \( U_z \) map obtained using the spline technique from the expanded \( U_{xz} \) data is shown in Fig. 1(c). The \( U_z \) map obtained using the Fourier transform technique is shown in Fig. 1(d). Fig. 1(e) shows the \( U_z \) map obtained using the Fourier transform technique from the expanded \( U_{xz} \) data.

In order to measure the difference between the computed values \( V_z \) and the corresponding exact or observed values \( V_{0z} \), define the RE (relative root mean square error) as

\[ \text{RE} = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (V_{0z} - V_z)^2} \]

(15)

Table 1 Source parameters of the four solid spheres in Fig. 1.
The centre of a sphere is at \((x_0, y_0, z_0)\). The radius of the sphere is \( a \) and its density is \( \rho \).

<table>
<thead>
<tr>
<th>Sphere</th>
<th>( x_0 )(km)</th>
<th>( y_0 )(km)</th>
<th>( z_0 )(km)</th>
<th>( a )(km)</th>
<th>( \rho )(kg/m(^3))</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.0</td>
<td>0.0</td>
<td>6.0</td>
<td>3.8</td>
<td>1200</td>
</tr>
<tr>
<td>2</td>
<td>10.0</td>
<td>0.0</td>
<td>1.6</td>
<td>1.5</td>
<td>1500</td>
</tr>
<tr>
<td>3</td>
<td>-5.0</td>
<td>8.7</td>
<td>1.6</td>
<td>1.5</td>
<td>1500</td>
</tr>
<tr>
<td>4</td>
<td>-5.0</td>
<td>-8.7</td>
<td>1.6</td>
<td>1.5</td>
<td>1500</td>
</tr>
</tbody>
</table>

Compared with Fig. 1(b), Fig. 1(d) is significantly less accurate. Compared with Fig. 1(c), Fig. 1(e) is significantly less accurate and based on Fig. 1(e) one can hardly identify the large source located at the centre. So, the results computed with the spline technique agree substantially better with the exact data than do the results computed with the Fourier transform technique. This statement is verified by comparing the REs shown in Table 2.

The pertinent computation times of this example with a 2.80 GHz laptop computer for different grid sizes and different methods are listed in Table 3. The extra time overhead of the spline method is the penalty for its increased accuracy.

Let the grid dimension be \( N \), and the computation time be \( Y \). For the spline method, \( Y(N) = C_Y(N)N^{2.9} \). For the Fourier transform method, \( Y(N) = C_Y(N)N^{2} \log_{10}N \). The boundedness of \( C_Y(N) \) and \( C_Y(N) \) (Table 3) suggests the polynomial \( O(N^{2.9}) \) growth for the spline method and the usual \( O(N^{2} \log_{10}N) \) growth for the Fourier transform method.

3D example of magnetic potential computed from a noisy \( x \)-component of magnetic induction with the spline technique and comparison with the Fourier transform technique

The 3D source is a solid sphere, whose magnetic and geometrical parameters are the following: inclination, declination and intensity of magnetization of the sphere are 60 degree, 20 degree and 1 A/m, respectively; the centre of the sphere is at \((0, 0, 1.2 \text{ km})\) and the radius of the sphere is 0.5 km. Analytical magnetic potential \( (U_m) \) and \( x \)-component of magnetic induction \( (B_x) \) can be calculated (Blakey 1996). \( U_m = -\mu_0 \int_{B_x} dx \)

where \( \mu_0 \) is permeability of free space. In equation (6), let \( V(x,y) = B_y(x,y) \) and calculate \( U_m \). Figure 2 shows the effectiveness of computing \( U_m \) from \( B_x \) in the noisy situation. The \( B_x \) data contaminated by random noise with a zero mean and a standard deviation of 0.5 nT are shown in Fig. 2(f). Figure 2(a) shows the exact theoretical \( U_m \) map. The \( U_m \) map obtained using the spline technique is shown in Fig. 2(b). In order to improve the performance of both the spline technique and the Fourier transform technique, expand the original grids with 32 data points on each side of the computational domain and taper the expanded parts, but only keep the computed \( U_m \) values on the original grids. The \( U_m \) map obtained using the spline technique from the expanded \( B_x \) data is shown in Fig. 2(c). Figure 2(d) shows the \( U_m \) map obtained using the Fourier transform technique. The \( U_m \) map obtained using the Fourier transform technique from the expanded \( B_x \) data is shown in Fig. 2(e). Compared with Fig. 2(b), Fig. 2(d) is significantly less accurate. So is Fig. 2(e), compared with
Figure 1 The 3D gravity example of $U_z$ obtained from noisy $U_{xz}$ data using the spline technique and the Fourier transform technique. The sources are four solid spheres with densities and geometrical parameters listed in Table 1. Data spacing is 0.5 km in both the x and y directions. (a) $U_z$ (analytical). (b) $U_z$ from $U_{xz}$ (spline). (c) $U_z$ from expanded $U_{xz}$ (spline). (d) $U_z$ from $U_{xz}$ (FT). (e) $U_z$ from expanded $U_{xz}$ (FT). (f) Noisy $U_{xz}$ (contaminated by random noise with a zero mean and a standard deviation of 0.65 mGal/km).

Fig. 2(c). Therefore, the results computed with the spline technique agree substantially better with the exact data than do the results computed with the Fourier transform technique. The REs shown in Table 4 strongly support this statement.

3D gravity example of $U_{xz}$ obtained from rectangular-gridded $U_{zz}$ with the spline technique

This is a 3D gravity example of $U_{xz}$ recovered from exact and noisy rectangular-gridded $U_{zz}$ data using the spline technique (Wang et al. 2008). The 3D sources are five solid spheres with densities and geometrical parameters listed in Table 5. The data spacing is 0.15 km in the x direction and 0.10 km in the y direction. Figure 3(d) shows the exact theoretical $U_{zz}$ data. The $U_{xz}$ map obtained using the spline technique from the exact $U_{zz}$ data is shown in Fig. 3(b). Figure 3(e) shows the $U_{zz}$ data contaminated by random noise with a zero mean and a standard deviation of 0.41 mGal/km. The $U_{xz}$ map obtained using the spline technique from the noisy $U_{zz}$ data is shown in Fig. 3(c). Compared with the exact $U_{xz}$ (Fig. 3a), the REs are 0.37% and 0.62% for the exact and noisy cases in Fig. 3(b, c), respectively.

<table>
<thead>
<tr>
<th>Panel</th>
<th>(b)</th>
<th>(c)</th>
<th>(d)</th>
<th>(e)</th>
</tr>
</thead>
<tbody>
<tr>
<td>RE (%)</td>
<td>8.72</td>
<td>7.29</td>
<td>19.13</td>
<td>10.29</td>
</tr>
</tbody>
</table>

REAL DATA EXAMPLES

The real data are the free air gravity and full tensor gravity gradient dataset ($U_z$ and $U_{xx}$, $U_{xy}$, $U_{xz}$, $U_{yy}$, $U_{yz}$, $U_{zz}$).
collected in the Gulf of Mexico. The dataset satisfies equation (4) (Laplace’s equation) well. Using the spline-based techniques, the following transformations are performed.

3D gravity-gradient component transformations

Examples of these are shown in Fig. 4. The computed $U_{zz}$ recovered from the observed $U_{xz}$ and $U_{yz}$ (Fig. 5b) data using the spline technique (Wang et al. 2008) and the Fourier transform technique are shown in Fig. 4(b) and 4(c), respectively. Compared with the observed $U_{zz}$ data (Fig. 4a), the RE is 6.89% for the spline technique and 14.86% for the Fourier transform technique.

Figures 4(e,f) show the computed $U_{xz}$ recovered from the observed $U_{zz}$ data using the spline technique and the Fourier transform technique, respectively. Compared with the
Spline-based potential-field integral transformations

Table 4 REs between panels I, I = (b), (c), (d), (e) and panel (a) in Fig. 2

<table>
<thead>
<tr>
<th>Panel</th>
<th>(b)</th>
<th>(c)</th>
<th>(d)</th>
<th>(e)</th>
</tr>
</thead>
<tbody>
<tr>
<td>RE (%)</td>
<td>1.43</td>
<td>1.37</td>
<td>17.34</td>
<td>10.23</td>
</tr>
</tbody>
</table>

Table 5 Source parameters of the five solid spheres in Figs. 3, 6, 7, 8 and 9. The centre of a sphere is at \((x_0, y_0, z_0)\). The radius of the sphere is \(a\), and its density is \(\rho\)

<table>
<thead>
<tr>
<th>Sphere</th>
<th>(x_0)(km)</th>
<th>(y_0)(km)</th>
<th>(z_0)(km)</th>
<th>(a)(km)</th>
<th>(\rho)(kg/m(^3))</th>
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</thead>
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<td>5</td>
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<td>-1.5</td>
<td>0.6</td>
<td>0.5</td>
<td>1000</td>
</tr>
</tbody>
</table>

observed \(U_{xz}\) data (Fig. 4d), the RE is 10.45% for the spline technique and 10.57% for the Fourier transform technique.

The computed \(U_{xy}\) recovered from the observed \(U_{xz}\) data with the spline technique and the Fourier transform technique are shown in Figs. 4(h, i), respectively. Compared with the observed \(U_{xy}\) data (Fig. 4g), the RE is 9.41% for the spline technique and 12.40% for the Fourier transform technique.

The results computed with the spline technique agree better with the observed data than do the results computed with the Fourier transform technique, although the differences in this example are not as pronounced as in other cases, e.g., between Figs. 2(c) and 2(e), or Figs. 5(g) and 5(h).

3D gravity \(U_z\) obtained from gravity-gradient components \(U_{xz}\) and \(U_{yz}\)

An example is shown in Fig. 5. Figure 5(b) shows the observed \(U_{yz}\) data. The observed \(U_{xz}\) data are shown in Fig. 4(d).

Figure 3 The 3D gravity example of \(U_{xz}\) obtained from exact and noisy rectangular-gridded \(U_{zz}\) data using the spline technique. The sources are five solid spheres with densities and geometrical parameters listed in Table 5. Data spacing is 0.15 km in the x direction and 0.10 km in the y direction. (a) \(U_{xz}\) (analytical). (b) \(U_{xz}\) from exact \(U_{zz}\). (c) \(U_{xz}\) from noisy \(U_{zz}\). (d) \(U_{zz}\) (analytical). (e) Noisy \(U_{zz}\) (contaminated by random noise with a zero mean and a standard deviation of 0.41 mGal/km).
In equation (6), let $V(x,y) = U_{xz}$ and calculate gravity $U_z$. In equation (7), let $V(x,y) = U_{yz}$ and calculate $U_z$ again. Figures 5(c, d) are the computed $U_z$ obtained from $U_{yz}$ with the spline technique and the Fourier transform technique, respectively. Figures 5(e, f) are the computed $U_z$ obtained from $U_{xz}$ with the spline technique and the Fourier transform technique, respectively. Figure 5(g) shows the computed $U_z$ with the spline technique averaged from panels (c) and (e). The computed $U_z$ with the Fourier transform technique averaged from panels (d) and (f) is shown in Fig. 5(h). Compared with the observed $U_z$ data (Fig. 5a), the REs are: (c) 15.07%, (d) 63.51%, (e) 23.25%, (f) 79.27%, (g) 12.01%, (h) 65.34%.

 Apparently, the results computed with the spline technique agree substantially better with the observed $U_z$ data than do the results computed with the Fourier transform technique.

**HARMONICITY AND INVERTIBILITY TESTS**

**Harmonicity test using computed $U_{xx}$, $U_{yy}$, and analytical $U_{xz}$**

This is a 3D gravity example of harmonicity confirmation for the spline technique. The sources are five solid spheres with densities and geometrical parameters listed in Table 5. Data spacing is 0.05 km in both the x and y directions. There are three steps:

(I) compute potential $U$ from the forwarded potential field $U_{xz}$; compute the first-order partial derivative $\tilde{U}_x$ from the potential $U$; then compute the second-order partial derivative $U_{xx}$ from the $\tilde{U}_x$.

(II) compute potential $U$ from the forwarded potential field $U_{yz}$; compute the first-order partial derivative $\tilde{U}_y$ from the potential $U$; then compute the second-order partial derivative $U_{yy}$ from the $\tilde{U}_y$.

(III) sum up the exact theoretical $U_{xz}$ and the $U_{xx}$ and $U_{yy}$ calculated in (I) and (II).

Define the norm of an array of values $V_i$:

$$\text{Norm} = \frac{1}{N} \sum_{i=1}^{N} (V_i)^2.$$  \hspace{1cm} (16)

Steps (I), (II) and (III) apply to both the spline technique and the Fourier transform technique. Figures 6(a) and 6(d) are analytical $U_{xx}$ and $U_{yy}$, respectively. The spline-based $U_{xx}$ (Fig. 6b) and $U_{yy}$ (Fig. 6e) agree substantially better with the
analytical results than do the Fourier transform-based $U_{xx}$ (Fig. 6c) and $U_{yy}$ (Fig. 6f).

The sum of Figs. 6(a), 6(d) and 6(g) (analytical $U_{zz}$), the exact theoretical second-order derivatives, is exactly zero everywhere, perfectly satisfying Laplace’s equation. The sum of Figs. 6(b), 6(e) and 6(g), shown in Fig. 6(h) (Norm 0.002 mGal/km), is nearly zero, almost perfectly satisfying Laplace’s equation, which confirms harmonicity for the spline technique. The $U_{xx}$ and $U_{yy}$ are so accurately calculated with the spline technique, $U_{zz}$ can be reliably obtained using the Laplace’s equation (equation 4). Interestingly, one can identify the four shallow sources shown as distinct anomalies on Fig. 6(h).

The sum of Figs. 6(c), 6(f) and 6(g), shown in Fig. 6(i) (norm 0.302 mGal/km), is not nearly as close to zero as the sum in Fig. 6(h). i.e., harmonicity is substantially less well confirmed.
for the Fourier transform method than the spline method. Both methods have some edge effects. However, the edge problem is significantly less severe for the spline technique than the Fourier transform technique.

Harmonicity tests using computed $U_{xx}$, $U_{yy}$, $U_{zz}$

These are further harmonicity tests for the spline technique and the Fourier transform technique. The sources are five solid spheres with densities and geometrical parameters listed in Table 5. Data spacing is 0.05 km in both the x and y directions. (a) $U_{xx}$ (analytical). (b) $U_{xx}$ (spline). (c) $U_{xx}$ (FT). (d) $U_{yy}$ (analytical). (e) $U_{yy}$ (spline). (f) $U_{yy}$ (FT). (g) $U_{zz}$ (analytical). (h) $U_{xx}$(spline) + $U_{yy}$(spline) + $U_{zz}$(analytical). (i) $U_{xx}$(FT) + $U_{yy}$(FT) + $U_{zz}$(analytical).

Figure 6 3D gravity example of harmonicity confirmation for the spline technique and comparison with the Fourier transform technique. $U_{xx}$ and $U_{yy}$ are computed, $U_{zz}$ is analytical. The sources are five solid spheres with densities and geometrical parameters listed in Table 5. Data spacing is 0.05 km in both the x and y directions. (a) $U_{xx}$ (analytical). (b) $U_{xx}$ (spline). (c) $U_{xx}$ (FT). (d) $U_{yy}$ (analytical). (e) $U_{yy}$ (spline). (f) $U_{yy}$ (FT). (g) $U_{zz}$ (analytical). (h) $U_{xx}$(spline) + $U_{yy}$(spline) + $U_{zz}$(analytical). (i) $U_{xx}$(FT) + $U_{yy}$(FT) + $U_{zz}$(analytical).

(I) Compute potential $U$ from the forwarded potential field $U_\iota$; compute the first-order partial derivative $\tilde{U}_x$ from the potential $U$; then compute the second-order partial derivative $U_{xx}$ from the $\tilde{U}_x$.

(II) Compute potential $U$ from the forwarded potential field $U_\iota$; compute the first-order partial derivative $\tilde{U}_y$ from the potential $U$; then compute the second-order partial derivative $U_{yy}$ from the $\tilde{U}_y$.

(III) It takes the following steps to compute $U_{zz}$: Compute $U_{xy}$ from the $\tilde{U}_x$ obtained in (I), and compute $U_{yx}$ from the $\tilde{U}_y$ obtained in (II); compute $U_{xz}$ from $U_{xy}$ and $U_{xx}$ obtained in (I); compute $U_{yz}$ from $U_{yx}$ and $U_{yy}$ obtained in (II); compute $U_{zz}$ from $U_{xz}$ and $U_{yz}$.

(IV) Sum up the $U_{xx}$, $U_{yy}$ and $U_{zz}$ calculated in (I), (II) and (III).

(I), (II), (III) and (IV) apply to both the spline technique and the Fourier transform technique. Figures 7(h, i) are the $U_{xy}$ maps computed with the spline technique and the Fourier transform technique, respectively. Both are very close to
analytical $U_{xy}$ as shown in Fig. 7(g). However, comparing with analytical $U_{xz}$ (Fig. 7a) and $U_{yz}$ (Fig. 7d), the spline-based $U_{xz}$ (Fig. 7b) and $U_{yz}$ (Fig. 7e) are obviously substantially better than the Fourier transform-based $U_{xz}$ (Fig. 7c) and $U_{yz}$ (Fig. 7f). Figures 8(a, b) are the $U_{zz}$ maps and Figures 8(d, e) are the $U_{xx} + U_{yy} + U_{zz}$ maps obtained using the spline technique and the Fourier transform technique, respectively.

(V) There is another alternative way to compute $U_{zz}$ using the Fourier transform technique: compute $U_z$ from the $U$ obtained in (I); then compute $U_{zz}$ from $U_z$. Figure 8f is the Fourier transform-based $U_{xx} + U_{yy} + U_{zz}$ map, where $U_{zz}$ (Fig. 8c) is the $U_{zz}$ map computed through the alternative way using the Fourier transform technique. Apparently, this alternative approach is impractical to compute $U_{zz}$ using the Fourier transform technique.

The norms (equation 16) for Figs. 8(d, e, f) are 0.144, 0.507, 165.232 mGal/km, respectively. i.e., harmonicity is again substantially less well confirmed for the Fourier transform method than the spline method.

Invertibility test

This is a 3D gravity example to test the invertibility of spline-based integration and differentiation. The sources are five solid spheres with densities and geometrical parameters listed in Table 5. Data spacing is 0.1 km in both the x and y directions. Figure 9(d) shows the exact theoretical $U_x$ data. The $U$ map obtained from the exact $U_x$ data using the spline-based integration is shown in Fig. 9(b); compared with the exact $U$ (Fig. 9a), the RE is 5.99%. Figure 9(c) shows the $U_y$ map
Figure 8 3D gravity example to test harmonicity of the spline technique and comparison with the FT technique. $U_{xx}$ (Fig. 6), $U_{yy}$ (Fig. 6), $U_{zz}$ are all computed. The sources are five solid spheres with densities and geometrical parameters listed in Table 5. Data spacing is 0.1 km in both the x and y directions. (a) $U_{zz}$ (spline). (b) $U_{zz}$ (FT). (c) $U_{zz}$ (alternative FT). (d) $U_{xx} + U_{yy} + U_{zz}$ (spline). (e) $U_{xx} + U_{yy} + U_{zz}$ (FT; $U_{zz}$ panel b). (f) $U_{xx} + U_{yy} + U_{zz}$ (FT; $U_{zz}$ panel c).

Figure 9. 3D gravity example to test whether spline-based integration and differentiation are invertible. The sources are five solid spheres with densities and geometrical parameters listed in Table 5. Data spacing is 0.1 km in both the x and y directions. (a) $U$ (analytical). (b) $U$ obtained from analytical $U_x$ using spline-based integration. (c) $U_x$ obtained from $U$ in panel (b) using spline-based differentiation. (d) $U_x$ (analytical).
obtained from the $U$ as shown in Fig. 9(b) using the spline-based differentiation; compared with the exact $U$, the RE is only 0.01%.

We have obtained the potential from the field and recovered the field from the computed potential nicely, so that spline-based integration and differentiation are invertible.

CONCLUSIONS

Potential, potential field and potential-field gradient data are supplemental to each other for resolving sources of interest. We advanced spline-based techniques for 3D and 2D potential-field upward continuation and potential field and gradient component transformations and derivative computations in the previous studies. In this paper, we propose flexible high-accuracy practical techniques to perform 3D and 2D integral transformations from PF components to potential and from PG components to PF components in the space domain using cubic B-splines. The spline techniques are applicable to either uniform or non-uniform rectangular grids for the 3D case, and applicable to either regular or irregular grids for the 2D case. The spline-based indefinite integrations can be computed at any point in the computational domain, as can the horizontal derivatives.

In our synthetic 3D gravity examples ($U_z$ obtained from noisy $U_{xz}$, $U_{xz}$ obtained from rectangular-gridded $U_{zz}$, and the demonstration that harmonicity is confirmed substantially better for the spline technique than the Fourier transform technique and spline-based integration and differentiation are invertible) and magnetic examples ($U_m$ obtained from noisy $B_z$), we have shown that the spline techniques are substantially more accurate and hence may provide better insights into understanding the sources than the Fourier transform techniques, and $U_{zz}$ can be reliably obtained using the Laplace’s equation since the $U_{xz}$ and $U_{zy}$ are very accurately calculated with the spline technique. The cost of the increase in accuracy is some increase in computing time compared to the Fourier transform technique. However, the speed is still fast, e.g., the spline-based computation of $U_z$ from $U_{xz}$ on a 128 by 128 grid was performed within 5 seconds with a 2.80 GHz laptop computer. For the 3D gravity $U_z$ obtained from $U_{xz}$ example, the complexities of the computational time growth are polynomial $O(N^2)$ growth for the spline method and the usual $O(N^2 \log(N))$ growth for the Fourier transform method.

Our real data examples of 3D transformations show that the spline-based results agree substantially better (from gravity-gradient components to gravity) or better (between gravity-gradient components) with the observed data than do the Fourier-based results.

The spline techniques would therefore be very useful for data quality control through comparisons of the computed and observed components. If certain desired components of the potential field or gradient data are not measured, they can be obtained using the spline-based transformations as alternatives to the Fourier transform techniques.

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**APPENDIX A: UNIVARIATE CUBIC B-SPLINE INTERPOLATION**

In the domain \( D_t = \{ x | a \leq x \leq b \} \), make a partition

\[
x_{-3} < x_{-2} < x_{-1} < x_0 = a < x_1 < \ldots < x_N = b < x_{N+1} < x_{N+2} < x_{N+3}.
\]
The univariate cubic B-splines, whose interior knots are \( \{ x_i, i = 0, 1, \ldots, N \} \), can then be expressed as

\[
S(x) = \sum_{j=1}^{N+1} C_j N_i(x),
\]

(A1)

where \( C_j \) are interpolation coefficients. The unified formula for interpolation, differentiation and integration is

\[
S^n(x) = \sum_{j=1}^{N+1} C_j N_i^n(x),
\]

(A2)

where

\[
N_i^n(x) = (x_{i+2} - x_{i-2})B_i^n(x),
\]

(A3)

and

\[
B_i^n(x) = \frac{3!}{(3-n)!} \sum_{k=-n+2}^{i+n-2} (-1)^{i-k} W_k (x_k - x)^{3-n},
\]

(A4)

\[
W_k = \prod_{m=k+1}^{i+n-2} \frac{1}{x_k - x_m},
\]

(A5)

\[
(x_k - x)^{3-n} = \begin{cases} (x_k - x)^{3-n}, & \text{for } x \leq x_k \\ 0, & \text{for } x > x_k \end{cases}
\]

(A6)

The \( n \) in equation (A2) has the following meaning: when \( n \) is a positive integer, calculate the \( n \)th-order derivative; when \( n \) is a negative integer, calculate the \(|n|\)th-order integral; when \( n = 0 \), do not calculate either derivative or integral, i.e. \( N_i^0(x) = N_i(x) \).

\( V(x) \) is a function defined in the domain \( D_1 = \{ V(i), i = 0, 1, \ldots, N \} \) are known values of \( V(x) \) at the interior knots. Use the univariate cubic B-splines (A1) to approximate \( V(x) \) while satisfying the following conditions

\[
S(x_i) = V(i), \quad i = 0, 1, \ldots, N.
\]

(A7)

\[
\frac{\partial S(x)}{\partial x} = \frac{\partial V(x)}{\partial x}, \quad \text{at } x_0, \ x_N.
\]

(A8)

Substituting equation (A2) into equations (A7) and (A8), using a difference quotient to replace \( \frac{\partial V(x)}{\partial x} \), and considering the localized nonzero characteristics of the cubic B-splines

\[
N_i(x_k) = 0, \quad \text{for } |i - k| > 1,
\]

(A9)
yields

\[
YC = V.
\]

(A10)

where the dimensions are \( Y(N+3, N+3), C(N+3, 1) \) and \( V(N+3, 1) \).

From equation (A10) one obtains

\[
C = Y^{-1}V.
\]

(A11)

i.e., the interpolation coefficients are determined.

**APPENDIX B: BIVARIATE CUBIC B-SPLINE INTERPOLATION**

In the domain \( D_2 = [(x, y) | a \leq x \leq b, c \leq y \leq d] \), make a partition

\[
x_{-1} < x_{-2} < x_{-1} < x_0 = a < x_1 < \ldots < x_{N_x} = b
\]

\[
< x_{N_x+1} < x_{N_x+2} < x_{N_x+3}.\]

\[
y_{-1} < y_{-2} < y_{-1} < y_0 = c < y_1 < \ldots < y_{N_y} = d
\]

\[
< y_{N_y+1} < y_{N_y+2} < y_{N_y+3}
\]

The bivariate cubic B-splines, whose interior knots are \( \{(x_i, y_j), i = 0, 1, \ldots, N_x, \ j = 0, 1, \ldots, N_y \} \), can be expressed as

\[
S(x, y) = \sum_{i=1}^{N_x+1} \sum_{j=1}^{N_y+1} N_i(x) C_{i,j} N_j(y),
\]

(B1)

where \( C_{i,j} \) are interpolation coefficients. The unified formula for interpolation, differentiation and integration is

\[
S^n(x, y) = \sum_{i=1}^{N_x+1} \sum_{j=1}^{N_y+1} N_i^n(x) C_{i,j} N_j^n(y),
\]

(B2)

where \( N_i^n(x) \) is shown in equation (A3), and \( N_j^n(y) \) is similarly obtained for subscript \( j \).

\( V(x, y) \) is a function defined in the domain \( D_2 \). \( \{ V(i, j), i = 0, 1, \ldots, N_x, \ j = 0, 1, \ldots, N_y \} \) are known values of \( V(x, y) \) at the interior knots. Use the bivariate cubic B-splines (B1) to approximate \( V(x, y) \) while satisfying the following conditions

\[
S(x_i, y_j) = V(i, j), \quad i = 0, 1, \ldots, N_x, \ j = 0, 1, \ldots, N_y.
\]

(B3)

\[
\frac{\partial S(x, y)}{\partial x} = \frac{\partial V(x, y)}{\partial x}, \quad \text{at } (x_0, y_j), \ (x_{N_x}, y_j), \ j = 0, 1, \ldots, N_y.
\]

(B4)

\[
\frac{\partial S(x, y)}{\partial y} = \frac{\partial V(x, y)}{\partial y}, \quad \text{at } (x_i, y_0), \ (x_i, y_{N_y}), \ i = 0, 1, \ldots, N_x.
\]

(B5)

\[
\frac{\partial^2 S(x, y)}{\partial x \partial y} = \frac{\partial^2 V(x, y)}{\partial x \partial y}, \quad \text{at } (x_0, y_0), \ (x_0, y_{N_y}), \ (x_{N_x}, y_0), \ (x_{N_x}, y_{N_y}).
\]

(B6)
Substituting equation (B2) into equation (B3–B6), using difference quotients to replace \( \frac{\partial V(x,y)}{\partial x}, \frac{\partial V(x,y)}{\partial y} \) and \( \frac{\partial^2 V(x,y)}{\partial x\partial y} \), and considering the localized nonzero characteristics of the cubic B-splines (A9), yields

\[
XCY = V. \tag{B7}
\]

where the dimensions are \( X(Nx+3, Nx+3), C(Nx+3, Ny+3), Y(Ny+3, Ny+3) \) and \( V(Nx+3, Ny+3) \).

From equation (B7) one obtains

\[
C = X^{-1}Vy^{-1}. \tag{B8}
\]

i.e., the interpolation coefficients are determined. Because of the localized feature of the cubic B-splines, a large matrix is decomposed into two much smaller matrixes. The computations are fast.