Proceedings of Institute of Mathematics of NAS of Ukraine 2004, Vol. 50, Part 3, 1415–1422

Visualisation and Animation in Mathematics and Physics

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We give some applications of our own software for geometry and differential geometry and its extensions [5, 1, 2, 4, 6–9] to the visualisation and animation of certain topics in mathematics and physics such as the graphical representation of potential surfaces, the growth of crystals, neighbourhoods in weak topologies and the study of isometric maps.

1 Introduction

Visualisation and animation are of vital importance for the modern methods in mathematical education. They strongly support the understanding of concepts in mathematics and physics. We think that the application of a commercial graphics software package is neither a satisfactory approach for the illustration of the theoretical concepts, nor can it be used as their substitute. It should not be the aim of education to teach students to use some software package by instructing them which keys to press, and how to move the mouse, regardless of how convenient this may seem. The emphasis should be put on teaching the fundamental theoretical facts.

In view of this, we developed an *open software* in PASCAL on programme level which provides the basic tools for computer graphics, in order to offer an alternative to existing graphics software packages.

The main purpose of our software is to visualise the classical results in differential geometry on PC screens, plotters, printers or any other postscript device, but it also has extensions to physics, chemistry, crystallography and the engineering sciences. To the best of our knowledge, no other comparable, comprehensive software of this kind is available.

The software is *open* which means that its source files are accessible to the users, thus enabling them to apply it in the solutions of their own problems. This makes it extendable and flexible, and applicable to both teaching and research in many fields. In contrast to this, almost all other available graphics packages are *closed*; in general, the area below the user interface is inaccessible and consequently the software cannot be extended beyond the scope of the solutions it offers.

The software uses *OOP*, *object oriented programming*, and its programming language is *PASCAL*. The software is self-contained in the sense that no graphics package is needed other than PASCAL.

2 Wulff's crystals and potential surfaces

Here we deal with the graphical representation of crystals and their *potential surfaces*[1]. According to *Wulff's principle* [10], the shape of a crystal is uniquely defined by its surface energy function. A surface energy function is a real-valued function depending on a direction in space.

Let ∂B^n denote the unit sphere in $\mathbb{R}^{n+1}$ and $F : \partial B^n \to \mathbb{R}$ be a surface energy function then

$$PM = \{\vec{x} = F(\vec{e})\vec{e} \in \mathbb{R}^{n+1} : \vec{e} \in \partial B^n\}$$

is an n-dimensional manifold which represents F.

[1]Figures in colour will be available only in electronic version.

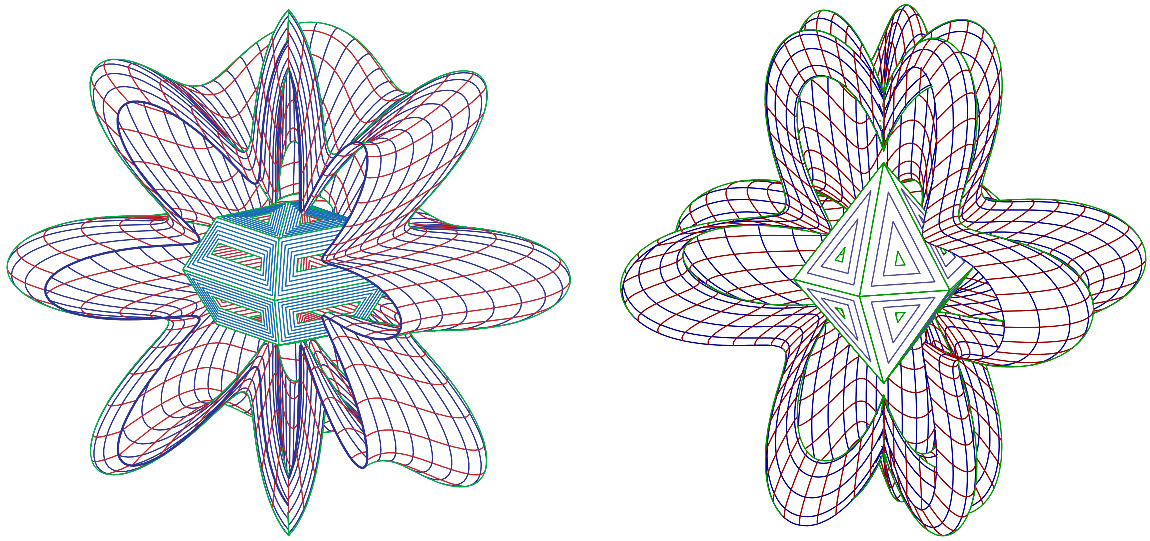

Figure 1. Potential surface and corresponding Wulff's crystals.

If $n = 1$, then $\vec{e} = \vec{e}(u) = \{\cos u, \sin u\}$ for $u \in (0, 2\pi)$ and we obtain a *potential curve* with a parametric representation

$$PC = \{\vec{x} = f(u)(\cos u, \sin u) : u \in (0, 2\pi)\}, \quad \text{where} \quad f(u) = F(\vec{e}(u)).$$

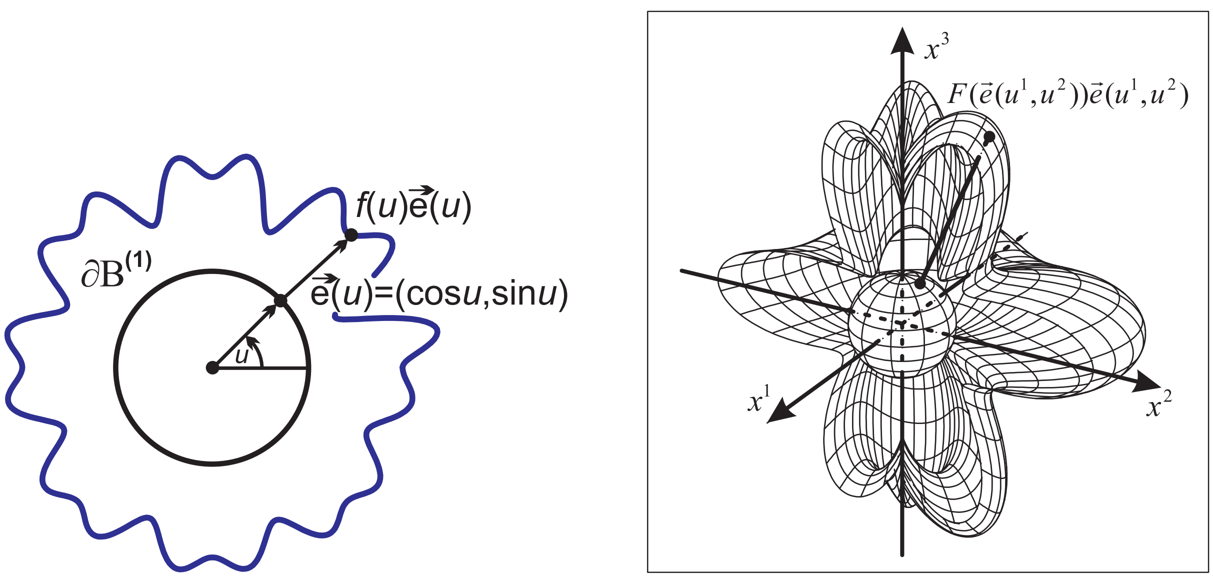

Figure 2. A potential curve and a potential surface.

If $n = 2$, then $\vec{e} = \vec{e}(u^1, u^2) = \{\cos u^1 \cos u^2, \cos u^1 \sin u^2, \sin u^1\}$ for $(u^1, u^2) \in R = (-\pi/2, \pi/2) \times (0, 2\pi)$ and we obtain a *potential surface* with a parametric representation

$$PS = \left\{\vec{x} = f\left(u^1, u^2\right)\left(\cos u^1 \cos u^2, \cos u^1 \sin u^2, \sin u^1\right) : \left(u^1, u^2\right) \in R\right\}$$

where $f(u^1, u^2) = F(\vec{e}(u^1, u^2))$.

The intersection of a potential surface and a sphere with radius r and centre in the origin is a curve which represents the constant values r of the function F; it is a so-called *equipotential line*.

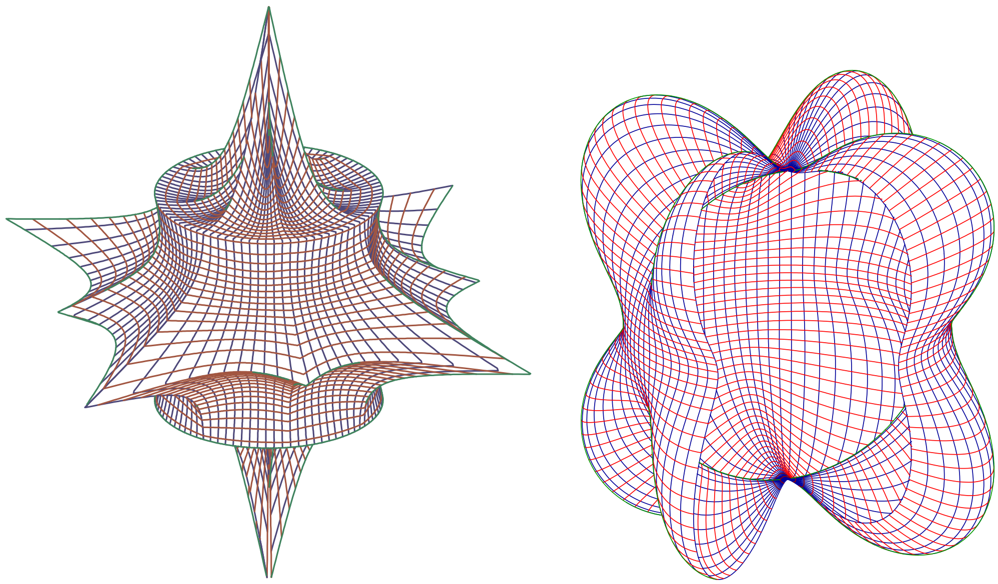

Figure 3. Potential surfaces.

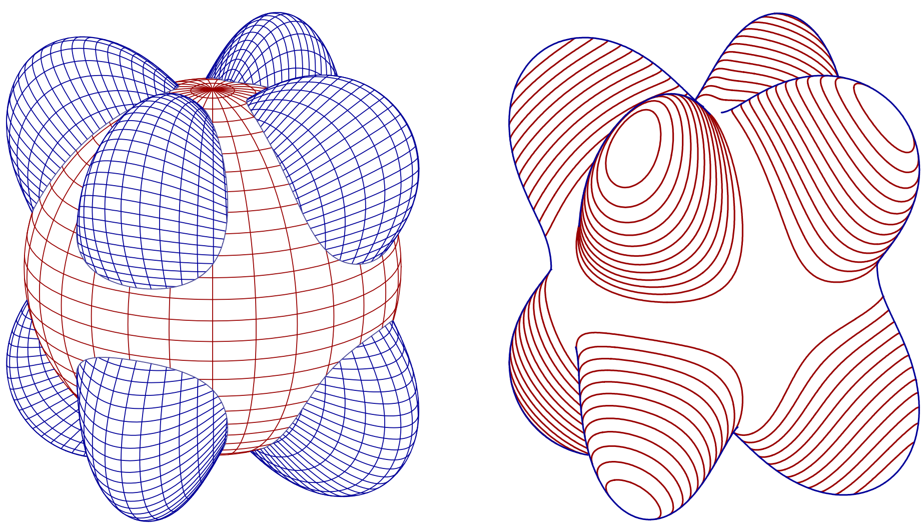

Figure 4. A potential surface and its intersection with a sphere and equipotential lines.

Wulff gave the following geometric principle of construction for crystals [10].

Theorem 1. Wulff's principle *For every* $\vec{e} \in \partial B^n$, *let* $E_{\vec{e}}$ *denote the hyperplane orthogonal to* $\vec{e}$ *and through the point* P *with position vector* $\vec{p} = F(\vec{e})\vec{e}$, *and* $H_{\vec{e}}$ *be the half space which contains the origin* 0 *and has the boundary* $E_{\vec{e}} = \partial H_{\vec{e}}$. *Then the crystal* C_F *which has* F *as its surface energy function is uniquely determined and given by*

$$C_F = \bigcap_{\vec{e} \in \partial B^n} H_{\vec{e}} = \bigcap_{\vec{e} \in \partial B^n} \{\vec{x} : \vec{x} \bullet \vec{e} \leq F(\vec{e})\}.$$

Since Wulff's construction in Theorem 1 is far from applicable for the graphical representation of crystals, we give two more useful results.

Theorem 2 ([1, Satz 6.1]). *Let* $F : \partial B^n \to \mathbb{R}^+$ *be a continuous function. Then a point* X *is on the boundary* ∂C_F *of Wulff's crystal* C_F *corresponding to* F *if and only if*

$$F(\vec{e}) \geq \vec{x} \bullet \vec{e} \text{ for all } \vec{e} \in \partial B^n \quad \text{and} \quad F(\vec{e}_0) = \vec{x} \bullet \vec{e}_0 \text{ for some } \vec{e}_0 \in \partial B^n.$$

Theorem 3 ([1, Satz 6.2]). *Let $F : \partial B^n \to \mathbb{R}^+$ be a continuous function and $CF : \partial B^n \to \mathbb{R}^+$ be defined by*

$$CF(\vec{e}) = \inf \left\{ F(\vec{u})(\vec{e} \bullet \vec{u})^{-1} : \vec{u} \in \partial B^n \text{ and } \vec{e} \bullet \vec{u} > 0 \right\}.$$

Then a parametric representation for ∂C_F is

$$\vec{x}(u^1, u^2) = CF(\vec{e}(u^1, u^2))\vec{e}(u^1, u^2) \text{ for } (u^1, u^2) \in (-\pi/2, \pi/2) \times (0, 2\pi).$$

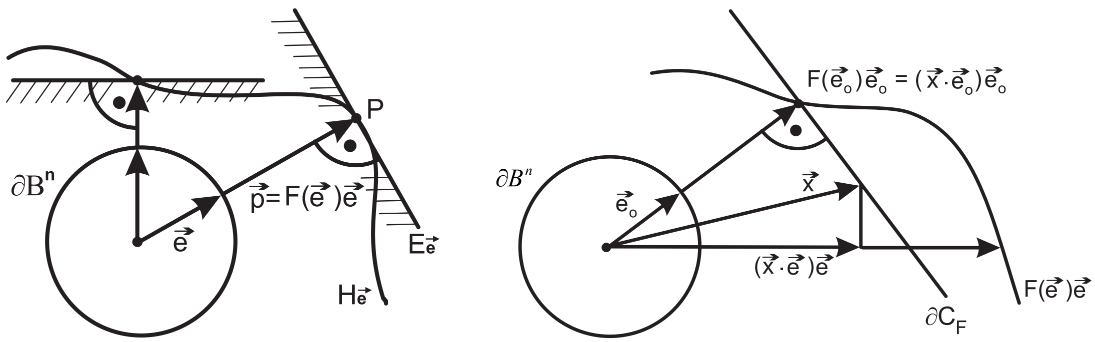

Figure 5. Wulff's constructions according to Theorems 1 and 2.

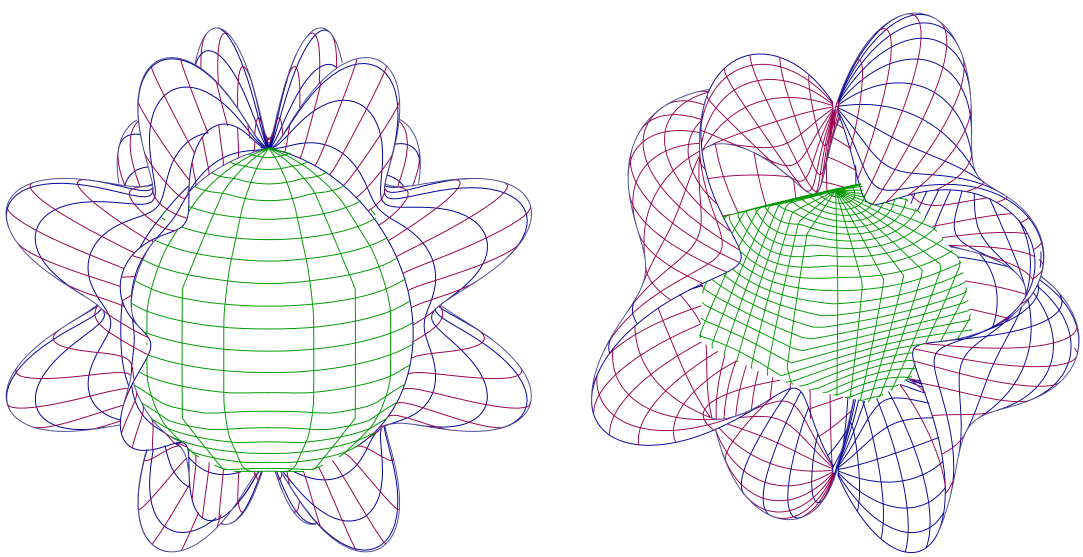

Figure 6. Wulff's crystals constructed by Theorems 2 and 3.

Although we have used both Theorems 2 and 3 to develop algorithms and programmes for the graphic representation of Wulff's crystals, in some cases a parametric representation can explicitly be given for the boundary of a Wulff's crystal, that is for the function CF.

One such case is when the function F is equal to a norm in three-dimensional space. Then if $F = \|\cdot\|$, the boundary of Wulff's crystal corresponding to F is a sphere with respect to the dual norm of $\|\cdot\|$. Here we represent the potential surfaces and corresponding Wulff's crystals for the ℓ_1 and ℓ_∞ norms $\|\cdot\|_1$ and $\|\cdot\|_\infty$ given by

$$\|\vec{x}\|_1 = |x_1| + |x_2| + |x_3| \quad \text{and} \quad \|\vec{x}\|_\infty = \max_{1 \le k \le 3} |x_k| \quad \text{for } \vec{x} = \{x_1, x_2, x_3\}.$$

The two pictures are dual to one another.

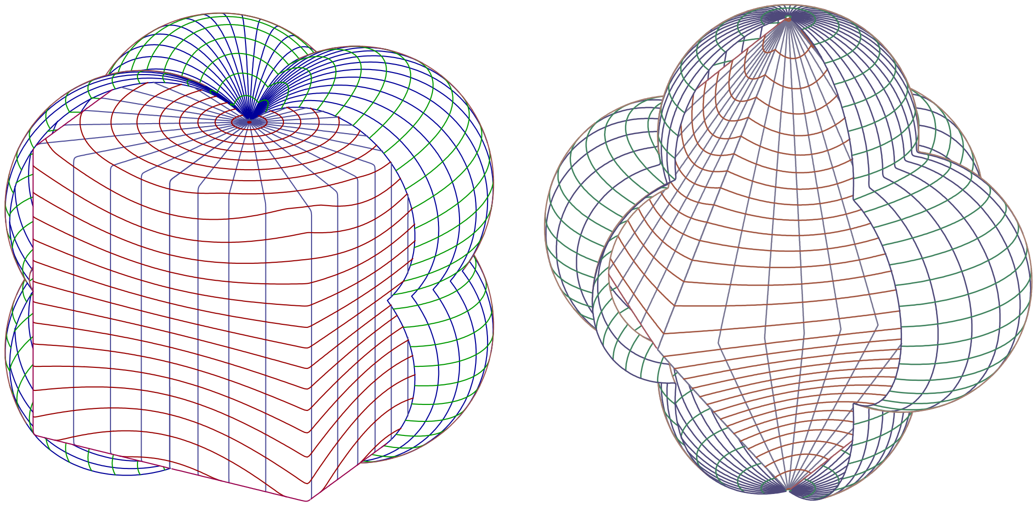

Figure 7. Wulff's crystals corresponding to the ℓ_1 and ℓ_∞ norms.

3 Weak topologies

Let $(X,\mathcal{T})$ be a topological space. A subbase for the topology $\mathcal{T}$ is a collection $\Sigma \subset \mathcal{T}$ such that given any point $x \in X$ and a neighbourhood N of x there exists a finite collection $\{N_1,\dots,N_n\}$ of members of Σ with $x \in \bigcap_{k=1}^n N_k \subset N$. It is well known that if $X \neq \varnothing$ and Σ is a collection of sets with $\bigcup \Sigma = X$ then there is a unique topology $\mathcal{T}$ such that Σ is a subbase for $\mathcal{T}$; $\mathcal{T}$ is the weakest topology with $\Sigma \subset \mathcal{T}$, it is called the topology generated by Σ and consists of $\varnothing$, X and all unions of finite intersections of members of Σ.

Let X be a set, $(Y,\mathcal{T})$ be a topological space and $f : X \to Y$ be a map. Then the topology on X generated by the collection $\{f^{-1}(O) : O \in \mathcal{T}\}$ is called the weak topology by f, written $w(X,f)$; then f is continuous as a map from $(X, w(X,f))$ to $(Y,\mathcal{T})$ and $w(X,f)$ is the weakest topology on X such that this is true. If $\Sigma(Y)$ is a subbase for $\mathcal{T}$ then $\Sigma = \{f^{-1}(G) : G \in \Sigma(Y)\}$ is a subbase for $w(X,f)$.

If the topology of Y is metrizable and given by the metric d, we may use the concept of the weak topology by f to define a metric ρ on X by $\rho = d \circ f$.

Example 1. Here we consider $Y = \mathbb{R}^n$ with

$$d_p(y,\tilde{y}) = \begin{cases} \sum_{k=1}^{n} |y_k - \tilde{y}_k|^p & (0 < p < 1), \\ \left(\sum_{k=1}^{n} |y_k - \tilde{y}_k|^p\right)^{1/p} & (1 \le p < \infty), \end{cases}$$

and $d_\infty(y,\tilde{y}) = \max_{1\le k\le n} |y_k - \tilde{y}_k|$, that is the limit case $d_\infty(y,\tilde{y}) = \lim_{p\to\infty} d_p(y,\tilde{y})$. If we put $\|y\|_p = d_p(y,0)$, then $\|\cdot\|_p$ is a norm for $1 \le p \le \infty$; the linear topology given by d_p for $0 < p < 1$ is not locally convex. We use the concept of the weak topology to introduce metrics on certain subsets of $S \subset \mathbb{R}^2$ and $\mathbb{R}^3$ and represent neighbourhoods of zero with respect to these metrics. The functions $f : S \to \mathbb{R}^2$ or $f : S \to \mathbb{R}^3$ have the special form

$$f(x_1,x_2) = (f_1(x_1), f_2(x_2)) \quad \text{or} \quad f(x_1,x_2,x_3) = (f_1(x_1), f_2(x_2), f_3(x_3)).$$

Fig. 9 shows the images under the function $f = (\tan \pi/2, \tan \pi/2, \tan \pi/2)$ of the spheres $S_{p,r}(0) = \{x \in \mathbb{R}^3 : d_p(x) = r\}$ for $p = 1.7$ and $r = .55$ and $r = .85$. An animation for this is available.

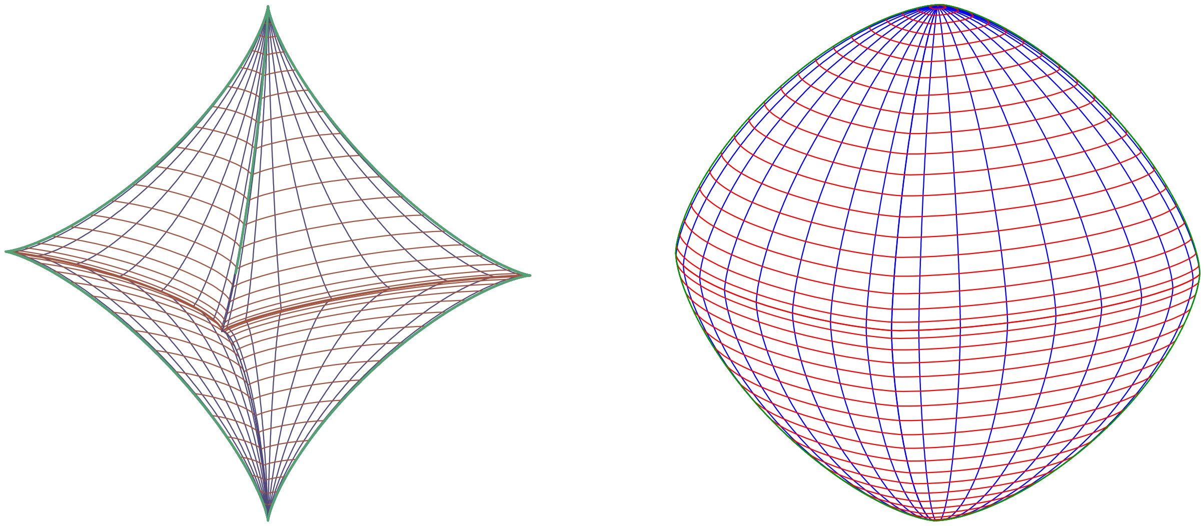

Figure 8. Spheres with respect to the metrics $d_{3/4}$ and $d_{3/2}$.

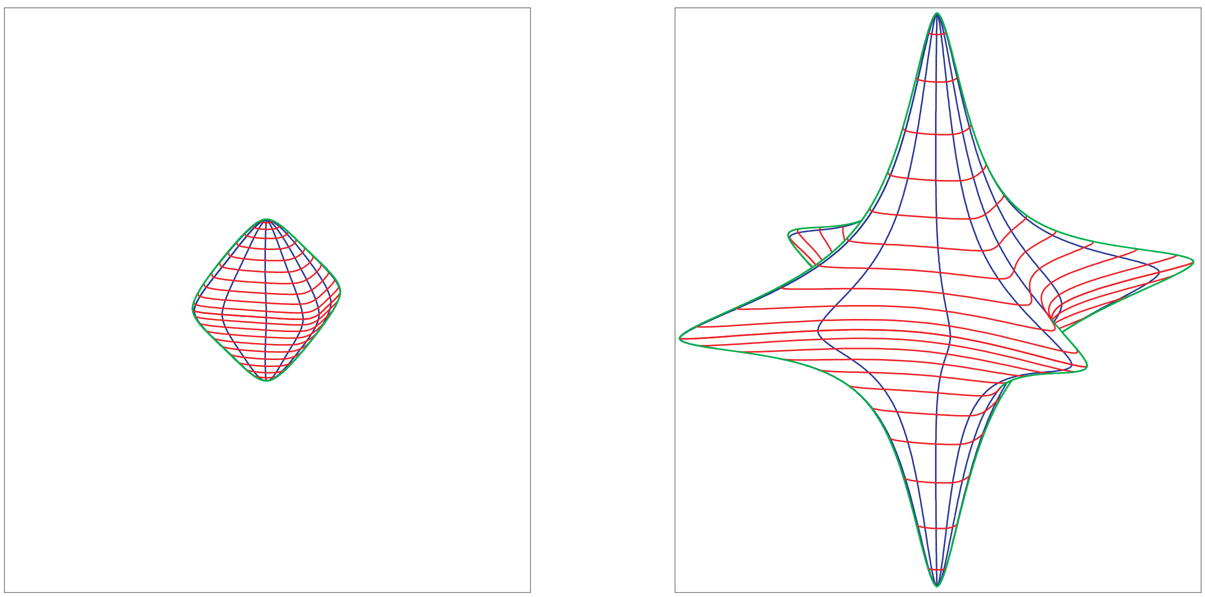

Figure 9. Images of spheres under the function f.

We use the functions $f : S_f = \mathbb{R} \times (0,\infty) \times \mathbb{R} \to \mathbb{R}^3$ and $g : S_g = \mathbb{R} \times \mathbb{R} \times (-1,1) \to \mathbb{R}^3$ with $f(x_1,x_2,x_3) = (x_1, \log x_2, x_3)$ and $g(x_1,x_2,x_3) = (x_1,x_2,\tan(x_3\pi/2))$ to introduce metrics on S_f and S_g, and write $\rho_f = d_2 \circ f$ and $\rho_g = d_1 \circ g$.

4 Isometric maps of surfaces

Let $D \subset \mathbb{R}^2$ be a domain and S be a surface given by a parametric representation

$$\vec{x}(u^i) = \left(x^1(u^1,u^2), x^2(u^1,u^2), x^3(u^1,u^2)\right) \quad \text{for } (u^i) = (u^1,u^2) \in D$$

with coordinate functions $x^k \in C^r(D)$ $(r \geq 1)$ and $\vec{x}_1 \times \vec{x}_2 \neq \vec{0}$ on D, where $\vec{x}_k = \partial\vec{x}/\partial u^k$ for $k = 1,2$. The functions $g_{ik} : D \to \mathbb{R}$ with $g_{ik} = \vec{x}_i \bullet \vec{x}_k$ for $i,k = 1,2$ are called the first fundamental coefficients of S.

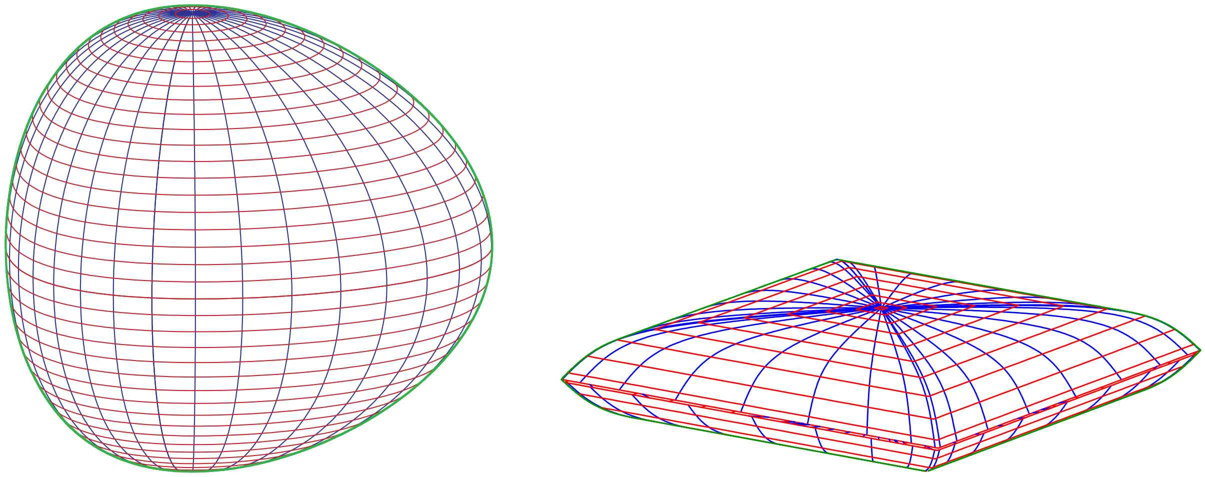

Figure 10. Spheres centred in the origin of S_f and S_g with respect to ρ_f and ρ_g.

Let S and S^* be surfaces with parametric representations $\vec{x}(u^i)$ and $\vec{x}^*(\tilde{u}^i)$ and $F : S \to S^*$ a map onto S^* given by the functions $h^i \in C^r(D)$ with $\tilde{u}^i = h^i(u^1, u^2)$ $(i = 1, 2)$ and non-vanishing Jacobian. We may introduce new parameters u^{*i} for S^* by putting $\tilde{u}^i = h^i(u^{*1}, u^{*2})$ $(i = 1, 2)$. Then the map F is given by $u^{*i} = u^i$ $(i = 1, 2)$, and S and S^* are said to have the same parameters.

A map $F : S \to S^*$ is called *isometric* if the length of every arc on S is the same as that of its corresponding image. It is well known that a map $F : S \to S^*$ is isometric if and only if the first fundamental coefficients g_{ik} and g^*_{ik} of S and $S^*$with respect to the same parameters (u^j) and (u^{*j}) satisfy $g_{ik}(u^j) = g^*_{ik}(u^{*j})$ for $i, k = 1, 2$ ([3, Satz 57.1, p. 213]).

We consider surfaces of revolution and screw surfaces given by parametric representations

$$\vec{x}(u^i) = (u^1 \cos u^2, u^1 \sin u^2, h(u^1)) \quad \text{and} \quad \tilde{\vec{x}}(\tilde{u}^i) = (\tilde{u}^1 \cos \tilde{u}^2, \tilde{u}^1 \sin \tilde{u}^2, c\tilde{u}^2 + f(\tilde{u}^1)),$$

where c is a constant.

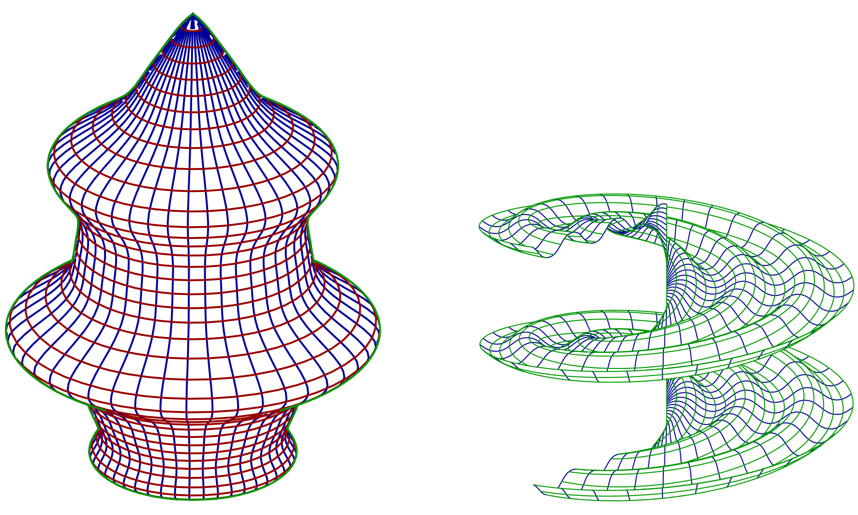

Figure 11. A surface of revolution and a screw surface.

It is well known that every screw surface S can be mapped isometrically onto a surface of revolution (cf. [3, Satz 57.4 (Bour), p. 217]).

Example 2. We consider the catenoid with a parametric representation

$$\vec{x}(u^i) = \big(u^1 \cos u^2, u^1 \sin u^2, a \operatorname{arcosh}(u^1/a)\big), \quad \text{where } a > 0 \text{ is a constant.}$$

We put $k^2 = a^2 - c^2$ for $0 \le c \le a$. Then the catenoid is isometric with any of the screw surfaces given by the function f with

$$f(u^{*1}) = k \log\left(\sqrt{(u^{*1})^2 + c^2} + \sqrt{(u^{*1})^2 - k^2}\right) - c \arctan\left(\frac{k}{c}\sqrt{\frac{(u^{*1})^2 + c^2}{(u^{*1})^2 - k^2}}\right).$$

The special cases $c = 0$ and $c = a$ yield the catenoid and the helikoid.

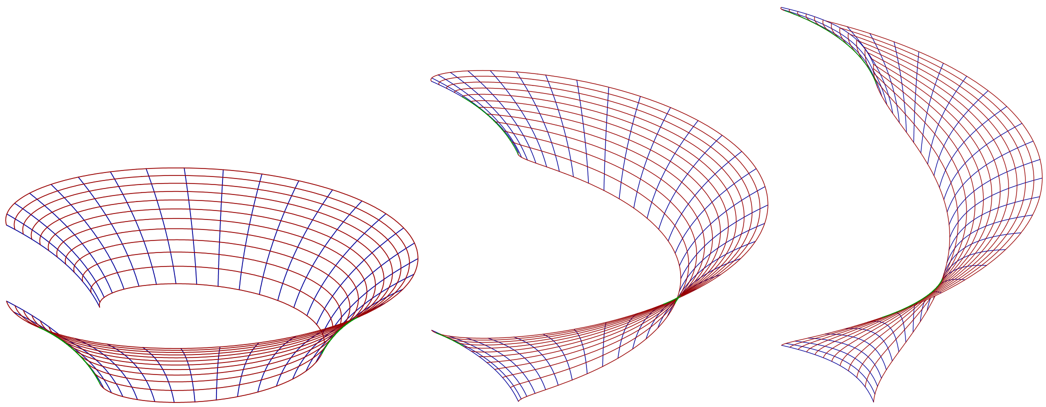

Figure 12. Surfaces of revolution with $c = a/8, a/2, 7a/8$, isometric with a catenoid and a helikoid.

Animations are available for Figs. 8, 9 and Example 2.

Acknowledgements

Research supported by the German DAAD foundation (German Academic Exchange Service), grant No. 911 103 102 8 and the research grant # 1646 of the Serbian Ministry of Science, Technology and Development.

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