

VISUALISATION AND ANIMATION IN MATHEMATICS AND PHYSICS

UDC 531.012+501+518.12(045)

Eberhard Malkowsky

Department of Mathematics, University of Giessen, Arndtstrasse 2, D- 35392 Giessen, Germany

Dept. of Mathematics, Faculty of Science and Mathematics,

University of Niš, Višegradska 33, 18000 Niš, Serbia and Montenegro

E-mail address: Eberhard.Malkowsky@Math.uni-giessen.de, ema@BankerInter.net

Abstract. *In this paper, we give a survey of our own software for differential geometry and its extensions [4, 3, 2, 5]. Furthermore we deal with a few applications to represent some interesting classical results in mathematics and physics. Originally it was the aim of the software to support teaching by visualising the results from differential geometry. But it also has applications in research and in physics and the engineering sciences. The software is open, that is, its source files are available to its users. Hence it can be extended. It uses OOP, and its programming language is PASCAL.*

Key words: *computer graphics, visualisation, animation.*

1. INTRODUCTION

Visualisation and animation are of vital importance for the modern methods in mathematics and physics. They strongly support the understanding of mathematical concepts that are needed in the engineering sciences. Of course, this applies most of all to geometry and differential geometry.

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. The academic mathematical education should not be confined to teaching students the use of 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.

Students should also be encouraged to write their own programmes for the visualisation of the solution of problems. A successful completion of this task will not only give prove of the students' correct understanding of the matter, but will also add to their motivation. Moreover the students will considerably improve their command of a programming language and their techniques.

Received September 10, 2003

1991 *Mathematics Subject Classification.* Primary: 53A05, Secondary: 68N05.

Work supported by the research grant #1646 of the Serbian Ministry of Research, Technology and Development, and by the German DAAD foundation, grant number 911 103 102.

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 originally was 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 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.

The advantages of PASCAL are the *hierarchy of objects* and the *polymorphy* which is not available in some *OOP languages*. In the hierarchy of objects, a successor inherits all the data, in particular the methods and procedures, of its predecessors. Polymorphy means that virtual methods can be declared, a virtual method can be rewritten with the same name in a successor, and one may have more methods than one with the same name. The development of our software could not have been achieved without OOP.

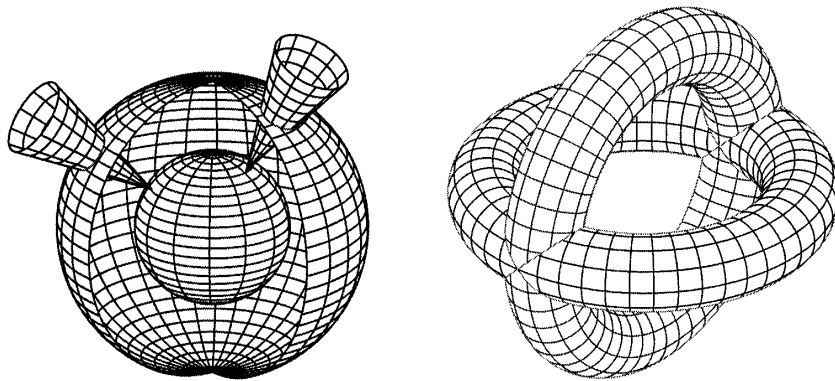


FIGURE 1. Two spheres and two cones, and two tori and their lines of intersection

2. WULFF'S CRYSTALS AND POTENTIAL SURFACES

Here we deal with the graphical representation of crystals and their *potential surfaces*.

According to *Wulff's principle* [6], the shape of a crystal is uniquely determined by its surface energy function. A surface energy function is a real valued function depending on a direction in space.

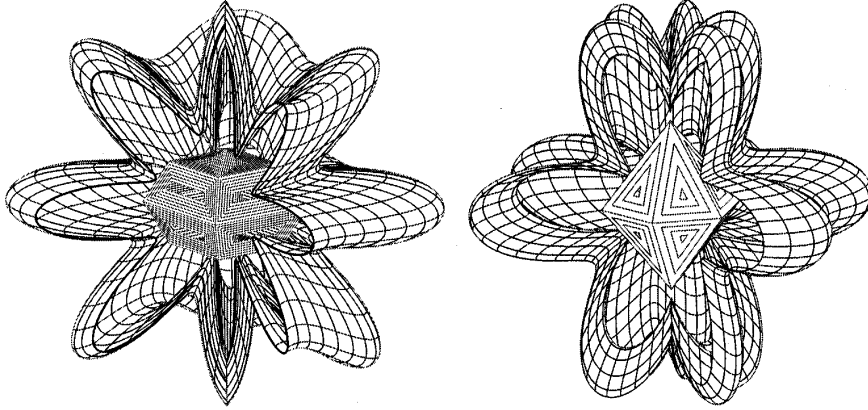


FIGURE 2. Potential surfaces and corresponding Wulff's crystals

Let ∂B^n denote the unit sphere in \mathbb{R}^{n+1} and $F : \partial B^n \rightarrow \mathbb{R}$ 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 .

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

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

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

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

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*.

Wulff gave a geometric principle of construction for crystals [6].

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

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

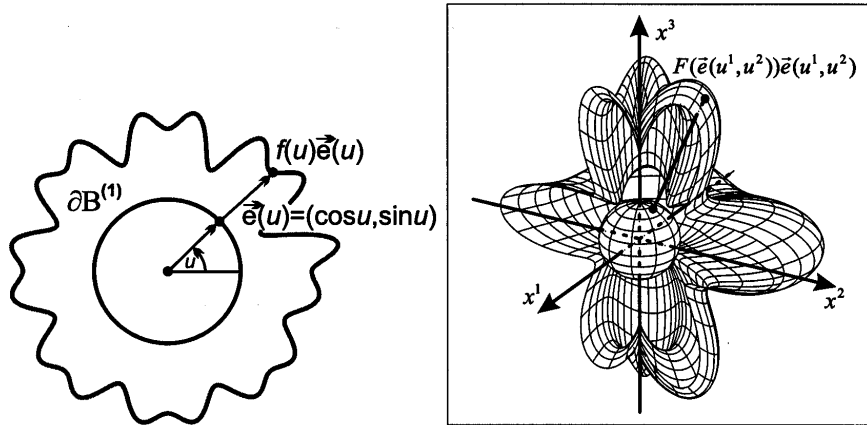


FIGURE 3. A potential curve and a potential surface

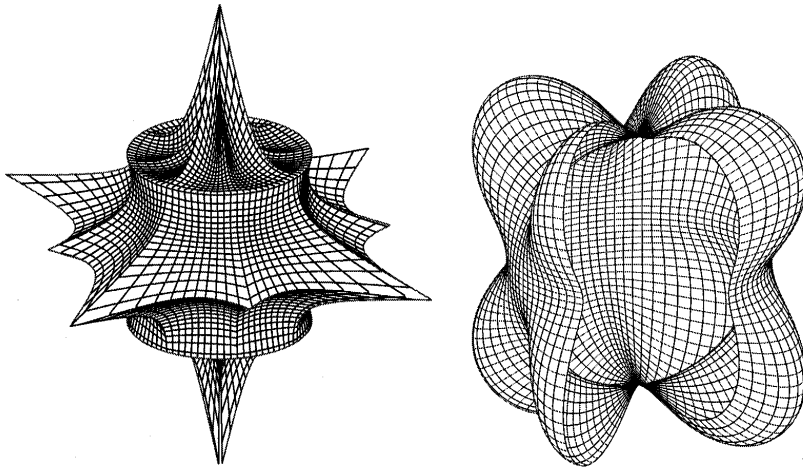


FIGURE 4. Potential surfaces

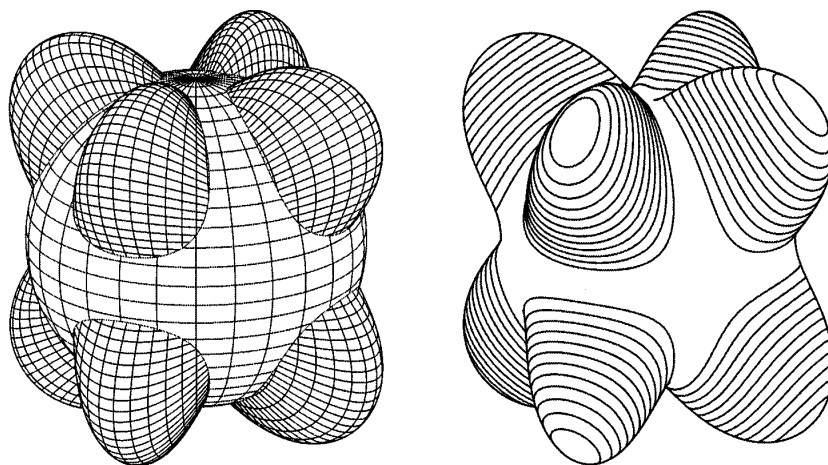


FIGURE 5. A potential surface and its intersection with a sphere and equipotential lines on a potential surface

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

Theorem 2. ([1, Satz 6.1]) *Let $F : \partial B^n \rightarrow \mathbb{R}^+$ 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*

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

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

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

Then a parametric representation for the boundary ∂C_F of Wulff's crystal corresponding to F is

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

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. If $F = \|\cdot\|$, then 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

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

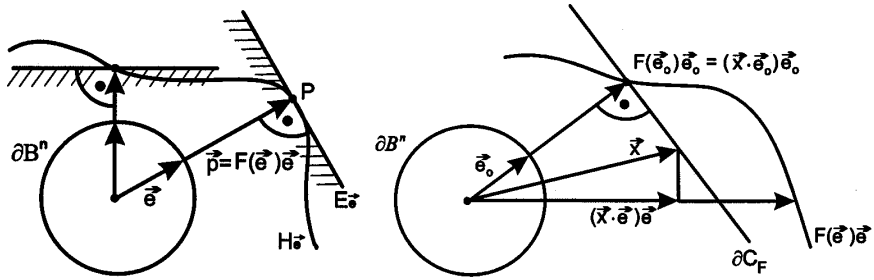


FIGURE 6. Wulff's constructions according to Theorems 1 and 2

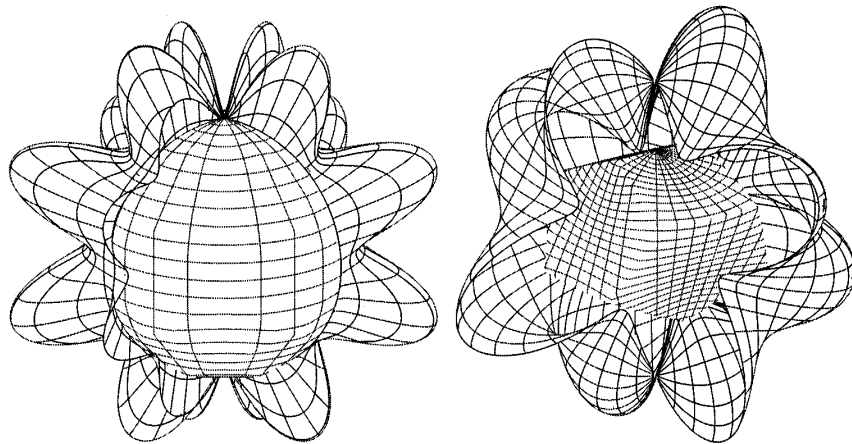


FIGURE 7. Wulff's crystals constructed by Theorems 2 and 3

The two pictures are dual to one another.

3. COORDINATE SYSTEMS AND ORTHOGONAL SYSTEMS

The choice of a suitable coordinate system is important in the solution of many problems.

Let $S = \{(x_1, \dots, x_n) : x_k \in \mathbb{R} \ (k = 1, \dots, n)\} \subset \mathbb{R}^n$. Then new coordinates $\tilde{x}_1, \dots, \tilde{x}_n$ are introduced for S by means of a function $g : \mathbb{R}^n \rightarrow \mathbb{R}^n$ if

- (1) the set $\tilde{S} = D(g)$, the domain of g , is open and $g : \tilde{S} \rightarrow S$ is one-to-one and onto;
- (2) $g \in C^1(\tilde{S})$ and its Jacobian satisfies

$$\det \frac{dg}{d\tilde{x}}(\tilde{x}) \neq 0 \text{ for all } \tilde{x} \in \tilde{S}.$$

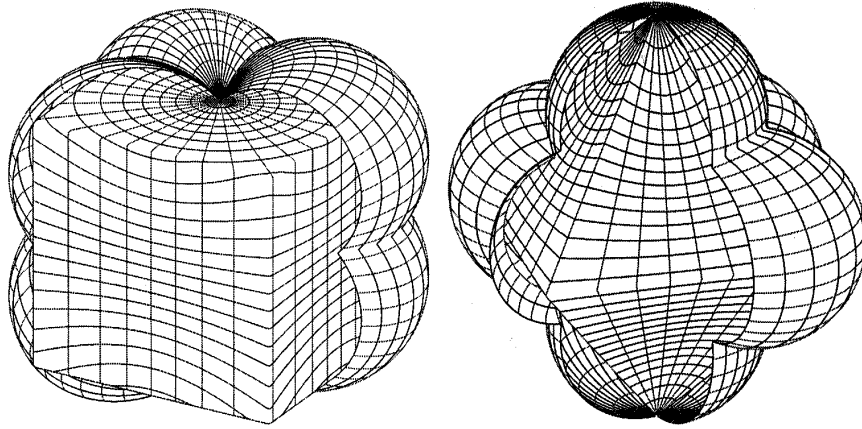


FIGURE 8. Wulff's crystals corresponding to the l_1 and l_∞ norms

Example 4. Some coordinates for the right half plane.

Let $S = \mathbb{R}^2 \setminus \{(y, z) \in \mathbb{R}^2 : y \leq 0\}$, $\tilde{S} = \{(r, \theta) \in \mathbb{R}^2 : r > 0, \theta \in (-\pi, \pi)\}$, where we write $r = \tilde{y}$ and $\theta = \tilde{z}$, and the map $g : \tilde{S} \rightarrow S$ be defined by

$$g((r, \theta)) = (r(1 + \cos \theta), r \sin \theta) \text{ (cf. Figure 9).}$$

The restriction of the familiar polar coordinates ρ and Θ given by $f : S' = \{(\rho, \Theta) \in \mathbb{R}^2 : \rho > 0, \Theta \in (-\pi/2, \pi/2)\} \rightarrow S$ with $f((\rho, \Theta)) = (\rho \cos \Theta, \rho \sin \Theta)$ defines coordinates for S . Obviously the function $h : \tilde{S} \rightarrow S'$ defined by $h(r, \theta) = (2r \cos \theta/2, \theta/2) = (\rho, \Theta)$ is one-to-one and onto with non-vanishing Jacobian. Thus $g = f \circ h : \tilde{S} \rightarrow S$ is one-to-one and onto with non-vanishing Jacobian.

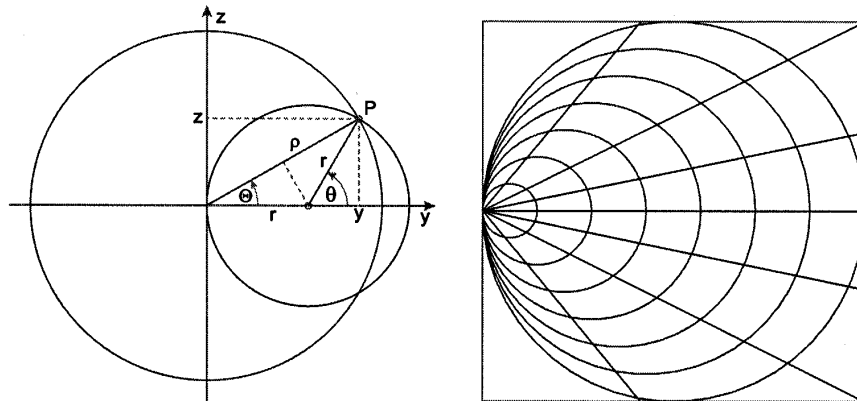


FIGURE 9. Construction of the coordinates of Example 1 and their coordinate lines

Example 5. Toroidal Coordinates for \mathbb{R}^3 .

Let

$$\tilde{S} = \{(r, \phi, \theta) \in \mathbb{R}^3 : r \in (0, \infty), \phi \in (0, 2\pi), \theta \in (-\pi, \pi)\},$$

$$S = \mathbb{R}^3 \setminus \{(x, y, z) : x \geq 0, y = 0\}$$

and the map $g = (g_1, g_2, g_3) : \tilde{S} \rightarrow S$ with $(r, \phi, \theta) \mapsto (x, y, z)$ be defined by

$$x = g_1(r, \phi, \theta) = r \cos \phi (1 + \cos \theta),$$

$$y = g_2(r, \phi, \theta) = r \cos \phi (1 + \cos \theta),$$

$$z = g_3(r, \phi, \theta) = r \sin \theta.$$

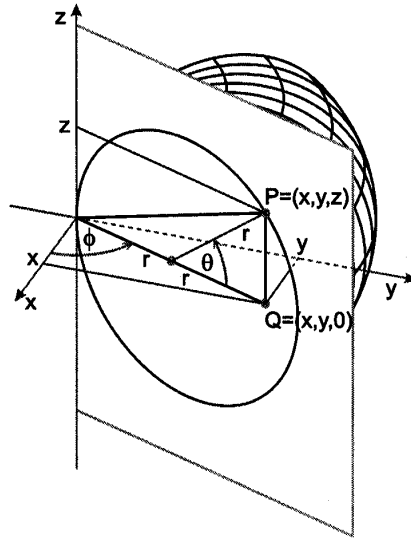


FIGURE 10. Toroidal coordinates

If ρ, φ and Θ denote the familiar spherical coordinates defined on $S' = (0, \infty) \times (0, 2\pi) \times (-\pi/2, \pi/2)$ by

$$x = \rho \cos \varphi \cos \Theta, \quad y = \rho \sin \varphi \cos \Theta \quad \text{and} \quad z = \rho \sin \Theta,$$

then the following transformation formulae hold

$$\rho = 2r \cos \frac{\theta}{2}, \quad \varphi = \phi, \quad \Theta = \theta/2,$$

$$r = \frac{\rho}{2 \cos \Theta} \quad \text{and} \quad \theta = 2\Theta.$$

The transformations from Cartesian coordinates x, y and z to toroidal coordinates are given by

$$r = \frac{x^2 + y^2 + z^2}{2\sqrt{x^2 + y^2}},$$

$$\phi = \begin{cases} \pi/2 & (x = 0, y > 0) \\ 3\pi/2 & (x = 0, y < 0) \\ \arctan \frac{y}{x} & (x > 0) \\ \arctan \frac{y}{x} + \pi & (x < 0, y \geq 0) \\ \arctan \frac{y}{x} + 2\pi & (x < 0, y < 0) \end{cases}$$

and

$$\theta = 2 \arctan \frac{z}{\sqrt{x^2 + y^2}}.$$

If \tilde{x} , \tilde{y} and \tilde{z} are coordinates for a subset S of \mathbb{R}^3 defined by a map $g : \tilde{S} \rightarrow S$, then the choice of one coordinate to be constant yields a so-called coordinate surface.

Example 6. Coordinate surfaces of the toroidal coordinates.

The choices $r = \text{const}$, $\phi = \text{const}$ and $\theta = \text{const}$ yield a torus, a half plane and half a cone, respectively, as coordinate surfaces of the toroidal coordinates.

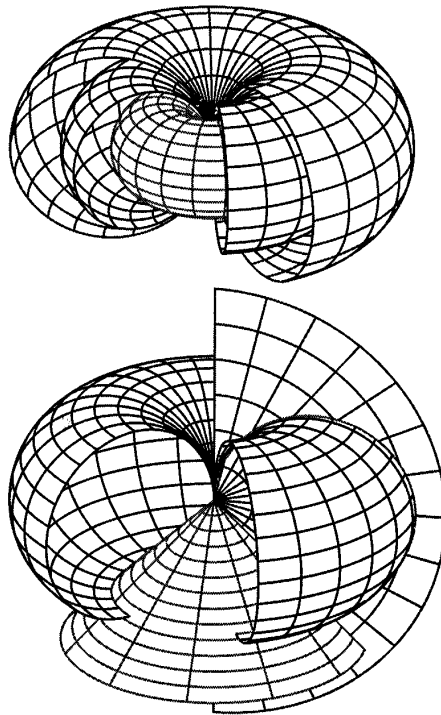


FIGURE 11. Some (ϕ, θ) coordinate surfaces and coordinate surfaces of toroidal coordinates

Triple systems of surfaces can be used to represent the coordinate surfaces of a coordinate system. They also play an important role in differential geometry to find the lines of curvature on certain surfaces.

Let $S \subset \mathbb{R}^3$ be a domain, $\vec{y}(u^1, u^2, u^3)$ be of class $C^2(D)$ and

$$\vec{y}_i \cdot \vec{y}_k = 0 \text{ for } i \neq k.$$

Then the surfaces given by $u^j = \text{const}$ determine three families of orthogonal surfaces, a so-called *triple orthogonal system*.

By *Dupin's theorem*, the surfaces of a triple orthogonal system mutually intersect in the lines of curvature.

Example 7. The triple orthogonal system of ellipsoids and hyperboloids of one and two sheets.

Let $a, b, c \in \mathbb{R}$ be given such that $0 < a^2 < b^2 < c^2$. For each $\lambda \in D_g = \mathbb{R} \setminus \{a^2, b^2, c^2\}$, a surface is given by the equation

$$(1) \quad \frac{(x^1)^2}{a^2 - \lambda} + \frac{(x^2)^2}{b^2 - \lambda} + \frac{(x^3)^2}{c^2 - \lambda} - 1 = 0.$$

If $\lambda < a^2$ then we obtain an ellipsoid. If $a^2 < \lambda < b^2$ then we obtain a hyperboloid of one sheet. If $b^2 < \lambda < c^2$ then we obtain a hyperboloid of two sheets. It can be shown that this is a triple orthogonal system. It is used to determine the lines of curvature on its surfaces.

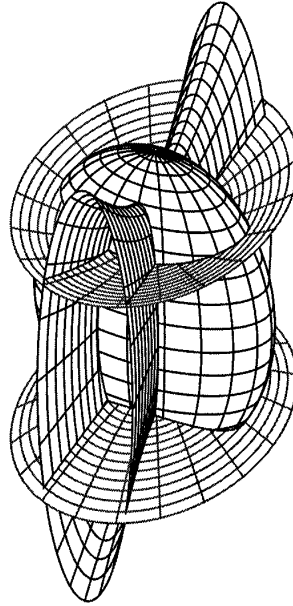


FIGURE 12. The triple orthogonal system of ellipsoids and hyperboloids

Animations for the topics of the paper are available.

REFERENCES

1. Failing M., Entwicklung numerischer ALgorithmen zur computergrafischen Darstellung spezieller Probleme der Differentialgeometrie und Kristallographie, Ph.D. Thesis, Giessen, 1996, Shaker Verlag, Aachen, 1996
2. M. Failing, E. Malkowsky, Ein effizienter Nullstellenalgorithmus zur computergrafischen Darstellung spezieller Kurven und Flächen, *Mitt. Math. Sem. Giessen* 229, 1996, (11-25)
3. E. Malkowsky, An open software in OOP for computer graphics and some applications in differential geometry, *Proceedings of the 20th South African Symposium on Numerical Mathematics*, 1994, (51-80)
4. E. Malkowsky, W. Nickel, *Computergrafik in der Differentialgeometrie*, Vieweg Verlag, Wiesbaden, Braunschweig, 1993
5. E. Malkowsky, V. Veličkovic, Visualisation of Differential Geometry, *Facta Universitatis Niš* 11(3), 2001, (127-134)
6. Wulff G., Der Curie-Wulffsche Satz über Combinationsformen von Krystallen, *Zeitschrift für Kristallographie*, 1901, V 53

VIZUALIZACIJA I ANIMACIJA U MATEMATICI I FIZICI**Eberhard Malkowsky**

U ovom radu dajemo kratak pregled svog sopstvenog softvera za diferencijalnu geometriju i njegovih proširivanja [4,3,2,5]. Nadalje obadjujemo nekoliko primena da bi predstavili neke interesantne klasične rezultate iz matematike i fizike. Početni cilj softvera bio je podrška predavanjima pomoću vizualizacije rezultata iz Diferencijalne geometrije. Ali on takodje ima primene u istraživanjima, a takodje i u fizici i inženjerskim naukama. Softver je otvoren, što znači da su njegovi izvorni fajlovi dostupni korisnicima. Zbog toga se može proširivati. Koristi OOP, a radjen je u pogramskom jeziku Pascal.