

Applications of Mathematics

Josef Ježek; Stanislav Saic; Karel Segeth

Numerical modeling of the movement of a rigid particle in viscous fluid

Applications of Mathematics, Vol. 44 (1999), No. 6, 469--479

Persistent URL: <http://dml.cz/dmlcz/134422>

Terms of use:

© Institute of Mathematics AS CR, 1999

Institute of Mathematics of the Academy of Sciences of the Czech Republic provides access to digitized documents strictly for personal use. Each copy of any part of this document must contain these *Terms of use*.



This paper has been digitized, optimized for electronic delivery and stamped with digital signature within the project *DML-CZ: The Czech Digital Mathematics Library* <http://project.dml.cz>

NUMERICAL MODELING OF THE MOVEMENT OF A RIGID PARTICLE IN VISCOUS FLUID¹

JOSEF JEŽEK, STANISLAV SAIC, KAREL SEGETH, Praha

Abstract. Modeling the movement of a rigid particle in viscous fluid is a problem physicists and mathematicians have tried to solve since the beginning of this century. A general model for an ellipsoidal particle was first published by Jeffery in the twenties. We exploit the fact that Jeffery was concerned with formulae which can be used to compute numerically the velocity field in the neighborhood of the particle during his derivation of equations of motion of the particle. This is our principal contribution to the subject. After a thorough check of Jeffery's formulae, we coded software for modeling the flow around a rigid particle based on these equations. Examples of its applications are given in conclusion. A practical example is concerned with the simulation of sigmoidal inclusion trails in porphyroblast.

Keywords: numerical modeling, rigid particle, viscous flow, equations of motion, elliptic integrals

MSC 2000: 35Q30, 76D05

1. INTRODUCTION

Modeling the movement of a rigid particle in viscous fluid was considered a fundamental problem physicists and mathematicians tried to solve as soon as at the beginning of this century. One of the first publications is Einstein's paper [1] where a spherical particle is treated. A more general model for an ellipsoidal particle was published by Jeffery [5] at the beginning of the twenties. The significance of the equations of motion Jeffery derived was mostly theoretical in his time. They could become the basis for numerical modeling only with the development of computers.

¹This research was partly supported by the Grant Agency of the Czech Republic under Grants No. 102/96/0419 and 201/97/0217.

Publications employing Jeffery's equations of motion of an ellipsoidal particle to modeling the origin of the preferred orientation of minerals in rocks began to appear in the sixties (cf., e.g., [2], [3], [8], [11]).

The fact that Jeffery was concerned with formulae which can be used to compute numerically the velocity field in the neighborhood of a particle during his derivation of the equations of motion of the particle, remained unnoticed. The reason apparently was, on the one hand, the complexity of the formulae and minor errors, possibly misprints, in them and, on the other hand, the necessity to apply an efficient procedure for repeated evaluation of elliptic integrals. Our first task, therefore, was to check the derivation published in [5]. The resulting corrected equations are presented in Sec. 2. Further, we coded software for modeling the flow around a rigid particle based on these equations. Examples of its application are given in Sec. 3. A practical example is concerned with the computer simulation of sigmoidal inclusion trails in crystallizing porphyroblast.

2. DERIVATION OF EQUATIONS OF MOTION

Let us repeat briefly the course of derivation of the equations of motion as presented in [5]. It demonstrates the enormous intuition and experience of the author who was able to guess in advance which terms have to be included in the formulae and got the coefficients of these terms through the mutual comparison of the formulae. We mostly use the original notation of Jeffery.

We asked our colleagues for help with the check in several places, e.g. when the differentiation of integrals with respect to a parameter (appearing also in the limits of integration), differentiation of implicit functions, and, in general, differentiation of complicated functions was concerned. We even used the software package Mathematica [12] in several extremely hard cases. Our thanks are due to J. Chleboun and E. Vitásek of the Mathematical Institute of the Academy of Sciences of the Czech Republic.

An ellipsoidal particle is described by the equation

$$(2.1) \quad \frac{x^2}{a^2} + \frac{y^2}{b^2} + \frac{z^2}{c^2} = 1,$$

where x , y , and z are the Cartesian coordinates referred to the axes fixed in the particle and a , b , and c are the semiaxes of the ellipsoid.

Jeffery writes the equations of motion for the fluid without any particle (or at a large distance from the particle) in the form

$$(2.2) \quad \begin{aligned} u_0 &= \mathbf{a}x + \mathbf{h}y + \mathbf{g}z + \eta z - \zeta y, \\ v_0 &= \mathbf{h}x + \mathbf{b}y + \mathbf{f}z + \zeta x - \xi z, \\ w_0 &= \mathbf{g}x + \mathbf{f}y + \mathbf{c}z + \xi y - \eta x, \end{aligned}$$

where u_0 , v_0 , and w_0 are components of the velocity that are equal to the product of the tensor of the velocity gradient and the coordinates. The symmetric and skewsymmetric parts of the tensor of the velocity gradient are

$$\begin{bmatrix} \mathbf{a} & \mathbf{h} & \mathbf{g} \\ \mathbf{h} & \mathbf{b} & \mathbf{f} \\ \mathbf{g} & \mathbf{f} & \mathbf{c} \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} 0 & \zeta & -\eta \\ -\zeta & 0 & \xi \\ \eta & -\xi & 0 \end{bmatrix}.$$

It is the appropriate choice of components of the tensor of the velocity gradient that allows us to describe various particular and practically important cases of the fluid motion.

Denote the viscosity coefficient by μ , the density by ϱ , and the spins, i.e. the angular velocities of the ellipsoid about its axes, by ω_1 , ω_2 , and ω_3 . A standard derivation that assumes a small Reynolds number and is based on neglecting small quantities in the Navier-Stokes equations

$$\begin{aligned} \mu \nabla^2 u - \frac{\partial p}{\partial x} &= \varrho \left(\frac{\partial u}{\partial t} - \omega_3 v + \omega_2 w \right), & \mu \nabla^2 v - \frac{\partial p}{\partial y} &= \varrho \left(\frac{\partial v}{\partial t} - \omega_1 w + \omega_3 u \right), \\ \mu \nabla^2 w - \frac{\partial p}{\partial z} &= \varrho \left(\frac{\partial w}{\partial t} - \omega_2 u + \omega_1 v \right) \end{aligned}$$

finally leads to equations for the steady motion of fluid with a particle, i.e. to the differential equations

$$(2.3) \quad \mu \nabla^2 u = \frac{\partial p}{\partial x}, \quad \mu \nabla^2 v = \frac{\partial p}{\partial y}, \quad \mu \nabla^2 w = \frac{\partial p}{\partial z},$$

$$(2.4) \quad \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0$$

for the velocity components u , v and w , and the pressure p . The first three equations are the Stokes equations, the fourth is the continuity equation that expresses the incompressibility of the fluid.

We then arrive at the equations

$$(2.5) \quad u = \omega_2 z - \omega_3 y, \quad v = \omega_3 x - \omega_1 z, \quad w = \omega_1 y - \omega_2 x$$

which have to be satisfied on the surface of the ellipsoid and describe the adhesion of the fluid to the particle. The particle thus does not slip in the fluid. In this way, we obtain the equations of motion of the particle from the equations of motion (2.3) of the fluid via the conditions (2.5).

In this phase, Jeffery guesses the formulae for the velocity components and writes

$$\begin{aligned}
 (2.6) \quad u &= u_0 + \frac{\partial}{\partial x}(R\chi_1 + S\chi_2 + T\chi_3) + W\frac{\partial\chi_3}{\partial y} - V\frac{\partial\chi_2}{\partial z} \\
 &\quad + A\left(x\frac{\partial^2\Omega}{\partial x^2} - \frac{\partial\Omega}{\partial x}\right) + H\left(x\frac{\partial^2\Omega}{\partial x\partial y} - \frac{\partial\Omega}{\partial y}\right) + G'\left(x\frac{\partial^2\Omega}{\partial x\partial z} - \frac{\partial\Omega}{\partial z}\right) \\
 &\quad + y\left(H'\frac{\partial^2\Omega}{\partial x^2} + B\frac{\partial^2\Omega}{\partial x\partial y} + F\frac{\partial^2\Omega}{\partial x\partial z}\right) \\
 &\quad + z\left(G\frac{\partial^2\Omega}{\partial x^2} + F'\frac{\partial^2\Omega}{\partial x\partial y} + C\frac{\partial^2\Omega}{\partial x\partial z}\right), \\
 v &= v_0 + \frac{\partial}{\partial y}(R\chi_1 + S\chi_2 + T\chi_3) + U\frac{\partial\chi_1}{\partial z} - W\frac{\partial\chi_3}{\partial x} \\
 &\quad + x\left(A\frac{\partial^2\Omega}{\partial x\partial y} + H\frac{\partial^2\Omega}{\partial y^2} + G'\frac{\partial^2\Omega}{\partial y\partial z}\right) \\
 &\quad + H'\left(y\frac{\partial^2\Omega}{\partial x\partial y} - \frac{\partial\Omega}{\partial x}\right) + B\left(y\frac{\partial^2\Omega}{\partial y^2} - \frac{\partial\Omega}{\partial y}\right) + F\left(y\frac{\partial^2\Omega}{\partial y\partial z} - \frac{\partial\Omega}{\partial z}\right) \\
 &\quad + z\left(G\frac{\partial^2\Omega}{\partial x\partial y} + F'\frac{\partial^2\Omega}{\partial y^2} + C\frac{\partial^2\Omega}{\partial y\partial z}\right), \\
 w &= w_0 + \frac{\partial}{\partial z}(R\chi_1 + S\chi_2 + T\chi_3) + V\frac{\partial\chi_2}{\partial x} - U\frac{\partial\chi_1}{\partial y} \\
 &\quad + x\left(A\frac{\partial^2\Omega}{\partial x\partial z} + H\frac{\partial^2\Omega}{\partial y\partial z} + G'\frac{\partial^2\Omega}{\partial z^2}\right) \\
 &\quad + y\left(H'\frac{\partial^2\Omega}{\partial x\partial y} + B\frac{\partial^2\Omega}{\partial y\partial z} + F\frac{\partial^2\Omega}{\partial z^2}\right) \\
 &\quad + G\left(z\frac{\partial^2\Omega}{\partial x\partial z} - \frac{\partial\Omega}{\partial x}\right) + F'\left(z\frac{\partial^2\Omega}{\partial y\partial z} - \frac{\partial\Omega}{\partial y}\right) + C\left(z\frac{\partial^2\Omega}{\partial z^2} - \frac{\partial\Omega}{\partial z}\right),
 \end{aligned}$$

where Ω , χ_1 , χ_2 and χ_3 are functions to be defined later while capital Latin letters (possibly with primes) are coefficients to be found.

Let λ be a nonnegative zero of the equation

$$(2.7) \quad \frac{x^2}{a^2 + \lambda} + \frac{y^2}{b^2 + \lambda} + \frac{z^2}{c^2 + \lambda} = 1.$$

Let us introduce the function

$$\Delta(\lambda) = \sqrt{(a^2 + \lambda)(b^2 + \lambda)(c^2 + \lambda)}.$$

Comparing (2.7) with the definition of the ellipsoid (2.1), we find easily that $\Lambda = 0$ is also a zero of the equation (2.7). Through definite integrals we further introduce several quantities that depend on Λ , namely

$$\begin{aligned} \alpha &= \int_{\Lambda}^{\infty} \frac{d\lambda}{(a^2 + \lambda)\Delta(\lambda)}, & \beta &= \int_{\Lambda}^{\infty} \frac{d\lambda}{(b^2 + \lambda)\Delta(\lambda)}, & \gamma &= \int_{\Lambda}^{\infty} \frac{d\lambda}{(c^2 + \lambda)\Delta(\lambda)}, \\ \alpha' &= \int_{\Lambda}^{\infty} \frac{d\lambda}{(b^2 + \lambda)(c^2 + \lambda)\Delta(\lambda)}, & \alpha'' &= \int_{\Lambda}^{\infty} \frac{\lambda d\lambda}{(b^2 + \lambda)(c^2 + \lambda)\Delta(\lambda)}, \\ \beta' &= \int_{\Lambda}^{\infty} \frac{d\lambda}{(a^2 + \lambda)(c^2 + \lambda)\Delta(\lambda)}, & \beta'' &= \int_{\Lambda}^{\infty} \frac{\lambda d\lambda}{(a^2 + \lambda)(c^2 + \lambda)\Delta(\lambda)}, \\ \gamma' &= \int_{\Lambda}^{\infty} \frac{d\lambda}{(a^2 + \lambda)(b^2 + \lambda)\Delta(\lambda)}, & \gamma'' &= \int_{\Lambda}^{\infty} \frac{\lambda d\lambda}{(a^2 + \lambda)(b^2 + \lambda)\Delta(\lambda)}. \end{aligned}$$

Note that

$$\begin{aligned} \alpha' &= \frac{\gamma - \beta}{b^2 - c^2}, & \alpha'' &= \frac{b^2\beta - c^2\gamma}{b^2 - c^2}, & \beta' &= \frac{\alpha - \gamma}{c^2 - a^2}, & \beta'' &= \frac{c^2\gamma - a^2\alpha}{c^2 - a^2}, \\ & & \gamma' &= \frac{\beta - \alpha}{a^2 - b^2}, & \gamma'' &= \frac{a^2\alpha - b^2\beta}{a^2 - b^2}. \end{aligned}$$

All these integrals can be expressed through Legendre elliptic integrals of the 1st and 2nd kinds

$$F(\varphi, k) = \int_0^{\varphi} \frac{d\psi}{\sqrt{1 - k^2 \sin^2 \psi}}, \quad E(\varphi, k) = \int_0^{\varphi} \sqrt{1 - k^2 \sin^2 \psi} \, d\psi.$$

The corresponding formulae valid for various cases of mutual relations among the semiaxes a , b , and c can be found in Sec. 3.13 of [4]. The evaluation of the elliptic integrals was carried out with help of EL2 subroutine of [10] that computes the general elliptic integral of the 2nd kind,

$$\text{EL2}(q, r, s, t) = \int_0^q \frac{(s + t\sigma^2) d\sigma}{(1 + \sigma^2)\sqrt{(1 + \sigma^2)(1 + r^2\sigma^2)}}.$$

Then

$$F(\varphi, k) = \text{EL2}(\tan \varphi, \sqrt{1 - k^2}, 1, 1), \quad E(\varphi, k) = \text{EL2}(\tan \varphi, \sqrt{1 - k^2}, 1, 1 - k^2).$$

Following [5], we can now define functions Ω , χ_1 , χ_2 , and χ_3 . We put

$$\begin{aligned} \Omega &= \int_{\Lambda}^{\infty} \left\{ \frac{x^2}{a^2 + \lambda} + \frac{y^2}{b^2 + \lambda} + \frac{z^2}{c^2 + \lambda} - 1 \right\} \frac{d\lambda}{\Delta(\lambda)}, \\ \chi_1 &= \alpha'yz, \quad \chi_2 = \beta'zx, \quad \chi_3 = \gamma'xy. \end{aligned}$$

The first step of the procedure consists in the verification that all these functions are harmonic. Recall that in the course of the verification we have to differentiate $\Lambda(x, y, z)$ defined implicitly as a zero of the equation (2.7). The result is

$$\frac{\partial \Lambda}{\partial x} = \frac{2xP^2}{a^2 + \Lambda}, \quad \frac{\partial \Lambda}{\partial y} = \frac{2yP^2}{b^2 + \Lambda}, \quad \frac{\partial \Lambda}{\partial z} = \frac{2zP^2}{c^2 + \Lambda},$$

where

$$\frac{1}{P^2} = \frac{x^2}{(a^2 + \Lambda)^2} + \frac{y^2}{(b^2 + \Lambda)^2} + \frac{z^2}{(c^2 + \Lambda)^2}.$$

Mathematica [12] proved to be an indispensable tool in this phase of verification of the formulae of [5].

The next step consists in the proof that the functions u , v , and w introduced in (2.6) satisfy the continuity equation (2.4). This can really be proved due to the fact that the relation

$$\mathbf{a} + \mathbf{b} + \mathbf{c} = 0$$

follows from the equations of motion (2.2).

Let us now turn to fulfilling the equations of motion (2.3). Substituting the functions u , v , and w introduced in (2.6) into (2.3), we conclude that the equations of motion will be satisfied if we put

$$p = p_0 + 2\mu \left(A \frac{\partial^2 \Omega}{\partial x^2} + B \frac{\partial^2 \Omega}{\partial y^2} + C \frac{\partial^2 \Omega}{\partial z^2} + (F + F') \frac{\partial^2 \Omega}{\partial y \partial z} + (G + G') \frac{\partial^2 \Omega}{\partial z \partial x} + (H + H') \frac{\partial^2 \Omega}{\partial x \partial y} \right),$$

where p_0 is a constant mean pressure at a large distance from the ellipsoid. In addition, we use the fact that the functions u_0 , v_0 , and w_0 defined by (2.2) satisfy the Stokes equations with the pressure p replaced by the constant pressure p_0 . These functions are, therefore, harmonic.

Before proceeding further, we explicitly substitute for the functions Ω , χ_1 , χ_2 , and χ_3 , and their derivatives into (2.6). The result is

$$\begin{aligned}
 (2.8) \quad u &= x\{\mathbf{a} + \gamma'W - \beta'V - 2(\alpha + \beta + \gamma)A\} \\
 &+ y\{\mathbf{h} - \zeta + \gamma'T - 2\beta H + 2\alpha H'\} \\
 &+ z\{\mathbf{g} + \eta + \beta'S - 2\gamma G' + 2\alpha G\} \\
 &- \frac{2xP^2}{(a^2 + \Lambda)\Delta(\Lambda)} \left[\{R + 2(b^2 + \Lambda)F + 2(c^2 + \Lambda)F'\}yz/\{(b^2 + \Lambda)(c^2 + \Lambda)\} \right. \\
 &\quad + \{S + 2(c^2 + \Lambda)G + 2(a^2 + \Lambda)G'\}zx/\{(c^2 + \Lambda)(a^2 + \Lambda)\} \\
 &\quad + \{T + 2(a^2 + \Lambda)H + 2(b^2 + \Lambda)H'\}xy/\{(a^2 + \Lambda)(b^2 + \Lambda)\} \\
 &\quad - \{V - 2(c^2 + \Lambda)C + 2(a^2 + \Lambda)A\}z^2/(c^2 + \Lambda)^2 \\
 &\quad \left. + \{W - 2(a^2 + \Lambda)A + 2(b^2 + \Lambda)B\}y^2/(b^2 + \Lambda)^2 \right], \\
 v &= x\{\mathbf{h} + \zeta + \gamma'T + 2\beta H - 2\alpha H'\} \\
 &+ y\{\mathbf{b} + \alpha'U - \gamma'W - 2(\alpha + \beta + \gamma)B\} \\
 &+ z\{\mathbf{f} - \xi + \alpha'R - 2\gamma F + 2\beta F'\} \\
 &- \frac{2yP^2}{(b^2 + \Lambda)\Delta(\Lambda)} \left[\{R + 2(b^2 + \Lambda)F + 2(c^2 + \Lambda)F'\}yz/\{(b^2 + \Lambda)(c^2 + \Lambda)\} \right. \\
 &\quad + \{S + 2(c^2 + \Lambda)G + 2(a^2 + \Lambda)G'\}zx/\{(c^2 + \Lambda)(a^2 + \Lambda)\} \\
 &\quad + \{T + 2(a^2 + \Lambda)H + 2(b^2 + \Lambda)H'\}xy/\{(a^2 + \Lambda)(b^2 + \Lambda)\} \\
 &\quad + \{U - 2(b^2 + \Lambda)B + 2(c^2 + \Lambda)C\}z^2/(c^2 + \Lambda)^2 \\
 &\quad \left. - \{W - 2(a^2 + \Lambda)A + 2(b^2 + \Lambda)B\}x^2/(a^2 + \Lambda)^2 \right], \\
 w &= x\{\mathbf{g} - \eta + \beta'S - 2\alpha G + 2\gamma G'\} \\
 &+ y\{\mathbf{f} + \xi + \alpha'R + 2\gamma F - 2\beta F'\} \\
 &+ z\{\mathbf{c} + \beta'V - \alpha'U - 2(a + \beta + \gamma)C\} \\
 &- \frac{2zP^2}{(c^2 + \Lambda)\Delta(\Lambda)} \left[\{R + 2(b^2 + \Lambda)F + 2(c^2 + \Lambda)F'\}yz/\{(b^2 + \Lambda)(c^2 + \Lambda)\} \right. \\
 &\quad + \{S + 2(c^2 + \Lambda)G + 2(a^2 + \Lambda)G'\}zx/\{(c^2 + \Lambda)(a^2 + \Lambda)\} \\
 &\quad + \{T + 2(a^2 + \Lambda)H + 2(b^2 + \Lambda)H'\}xy/\{(a^2 + \Lambda)(b^2 + \Lambda)\} \\
 &\quad - \{U - 2(b^2 + \Lambda)B + 2(c^2 + \Lambda)C\}y^2/(b^2 + \Lambda)^2 \\
 &\quad \left. + \{V - 2(c^2 + \Lambda)C + 2(a^2 + \Lambda)A\}x^2/(a^2 + \Lambda)^2 \right].
 \end{aligned}$$

It now remains to fulfil the conditions (2.5) on the ellipsoid surface, i.e. for $\Lambda = 0$. To this aim, we put $\Lambda = 0$ in these equations as well as in the definition of the functions α , β , γ and the derived functions denoted by one prime or two primes. Therefore, the lower limit of integration in the integrals defining the functions α , β ,

γ , etc. will equal 0. These functions will be denoted by α_0 , β_0 , γ_0 , etc. Finally, we arrive at the formulae for the sought coefficients in (2.8) that read

$$\begin{aligned}
 A &= \frac{1}{6}\{2\alpha_0''\mathbf{a} - \beta_0''\mathbf{b} - \gamma_0''\mathbf{c}\}/(\beta_0''\gamma_0'' + \gamma_0''\alpha_0'' + \alpha_0''\beta_0''), \\
 B &= \frac{1}{6}\{2\beta_0''\mathbf{b} - \gamma_0''\mathbf{c} - \alpha_0''\mathbf{a}\}/(\beta_0''\gamma_0'' + \gamma_0''\alpha_0'' + \alpha_0''\beta_0''), \\
 C &= \frac{1}{6}\{2\gamma_0''\mathbf{c} - \alpha_0''\mathbf{a} - \beta_0''\mathbf{b}\}/(\beta_0''\gamma_0'' + \gamma_0''\alpha_0'' + \alpha_0''\beta_0''), \\
 F &= \frac{\beta_0\mathbf{f} - c^2\alpha_0'(\xi - \omega_1)}{2\alpha_0'(b^2\beta_0 + c^2\gamma_0)}, & F' &= \frac{\gamma_0\mathbf{f} + b^2\alpha_0'(\xi - \omega_1)}{2\alpha_0'(b^2\beta_0 + c^2\gamma_0)}, \\
 G &= \frac{\gamma_0\mathbf{g} - a^2\beta_0'(\eta - \omega_2)}{2\beta_0'(c^2\gamma_0 + a^2\alpha_0)}, & G' &= \frac{\alpha_0\mathbf{g} + c^2\beta_0'(\eta - \omega_2)}{2\beta_0'(c^2\gamma_0 + a^2\alpha_0)}, \\
 H &= \frac{\alpha_0\mathbf{h} - b^2\gamma_0'(\zeta - \omega_3)}{2\gamma_0'(a^2\alpha_0 + b^2\beta_0)}, & H' &= \frac{\beta_0\mathbf{h} + a^2\gamma_0'(\zeta - \omega_3)}{2\gamma_0'(a^2\alpha_0 + b^2\beta_0)}, \\
 R &= -\frac{\mathbf{f}}{\alpha_0'}, & S &= -\frac{\mathbf{g}}{\beta_0'}, & T &= -\frac{\mathbf{h}}{\gamma_0'}, \\
 U &= 2b^2B - 2c^2C, \\
 V &= 2c^2C - 2a^2A, \\
 W &= 2a^2A - 2b^2B.
 \end{aligned}$$

Mathematica [12] was again used in this phase of the verification. Our conclusion now is that the formulae (2.6) and (2.8) have been checked and the coefficients appearing in them have been uniquely determined. We have corrected several errors (obviously misprints) in the formulae (26) of Jeffery's paper [5] that define the coefficients F , F' , G , G' , H , and H' .

According to [5], expressing now the moment of forces acting on the ellipsoid and taking into account that the resulting moment vanishes if there are no external forces, we arrive at the equations of motion of the ellipsoid in the form

$$\begin{aligned}
 (2.9) \quad (b^2 + c^2)\omega_1 &= b^2(\xi + \mathbf{f}) + c^2(\xi - \mathbf{f}), \\
 (c^2 + a^2)\omega_2 &= c^2(\eta + \mathbf{g}) + a^2(\eta - \mathbf{g}), \\
 (a^2 + b^2)\omega_3 &= a^2(\zeta + \mathbf{h}) + b^2(\zeta - \mathbf{h}).
 \end{aligned}$$

3. COMPUTER IMPLEMENTATION AND EXAMPLES OF THE RESULTS OF MODELING

The flow around a rotating ellipsoidal particle can be modeled in such a way that we solve the equations of rotation of the particle (2.9) and evaluate the velocity field (2.8) simultaneously. For this purpose, we coded the VIFLAP program in Fortran (see [7]) that extends the published software [6]. The user of VIFLAP specifies the form of the rigid particle (the size of semiaxes), its initial position (Euler angles), and the tensor of the velocity gradient. The user further gives the initial coordinates of a chosen number of points (called *markers*) and the information whether the markers are fixed in space during the computation or move together with the fluid flowing around the particle.

After the program is initiated, the position of the rigid particle and the markers, as well as the components of velocity of the fluid at marker positions are output in time intervals given. These results are then visualized by a module coded in the MATLAB language. An example of computation of the velocity field in the vicinity of a rotating particle is shown in Fig. 1. It is a prolate ellipsoid with the axis ratio 1 : 1.5 : 3 that is subject to simple shear. The velocity field is presented in a set of markers moving together with the fluid.

In Figs. 2 and 3, we compare the result of computer simulation of sigmoidal inclusion trails in ellipsoidal porphyroblast with a rock sample found in nature. The classical explanation of these structures says that they are a manifestation of synkinematic growth during which a relative rotation of porphyroblast and the surrounding material containing foliations takes place. The foliations are then being caught by the crystallizing porphyroblast. One can use the geometry of inclusion trails in determining the kinematics of the deformation. This was the reason for many authors to study this subject.

Porphyroblasts are, as compared with the surrounding material, relatively rigid particles often of approximately spherical or ellipsoidal form. They thus offer a possibility to employ Jeffery's model of the motion of a rigid particle in viscous flow. However, such a work has not appeared in literature yet. Classical papers concerned with the modeling of the origin of inclusion trails in rotating porphyroblast were either purely experimental or exploited a geometrical approach. The first attempt to use the hydrodynamical approach is paper [9] of 1989 in which Masuda and Mochizuki were concerned with a computer simulation of the origin of inclusion trails in porphyroblasts based on the computation of the velocity field in the viscous fluid surrounding a rotating rigid spherical particle. They, however, did not employ the equations of motion of an ellipsoidal particle nor those of the velocity field around it derived by Jeffery and confined themselves to a simplified two dimensional

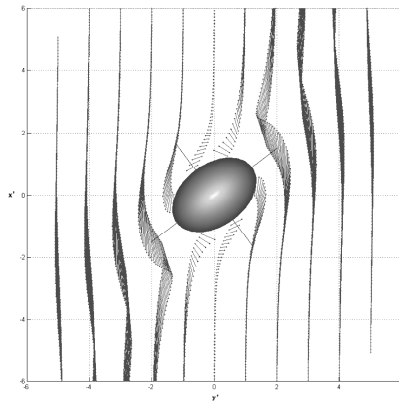


Fig. 1. Velocity field in the vicinity of an ellipsoidal particle that rotates in simple shear.

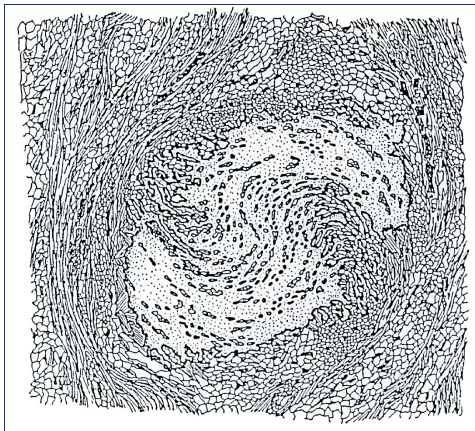
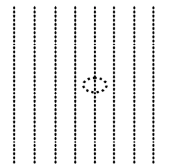


Fig. 2. Sigmoidal inclusion trails in ellipsoidal porphyroblast. Section of natural porphyroblast.

Inclusion Trails

Velocity Gradient Tensor
 .000 .000 .000
 .100 .000 .000
 000 000 000

Axial Ratio
 .75 : 1.00 : 1.20



Initial Position



Time Increment: 0.100
 Time Step: 740

Fig. 3. Sigmoidal inclusion trails in ellipsoidal porphyroblast. The result of computational treatment.

description of the rotation of a spheric particle in simple shear. They used their own formulae to describe the velocity field around the spherical particle.

The approach based on Jeffery's model that is the subject of this paper offers much more general possibilities: triaxial (i.e. asymmetric) particles and a general type of flow. We can thus expect that a more extensive comparison of results of the computer simulation with samples of rocks taken in nature will bring a new insight into the subject studied.

References

- [1] *A. Einstein*: Eine neue Bestimmung der Moleküldimensionen. *Ann. Physik* 19 (1906), 289–306, errata 34 (1911), 591–592.
- [2] *N. C. Gay*: The motion of rigid particles embedded in a viscous fluid during pure shear deformation of the fluid. *Tectonophysics* 5 (1968), 81–88.
- [3] *S. K. Ghosh, H. Ramberg*: Reorientation of inclusions by combination of pure shear and simple shear. *Tectonophysics* 34 (1976), 1–70.
- [4] *I. S. Gradshteyn, I. M. Ryzhik*: Table of Integrals, Series, and Products. 5th ed. Boston, Academic Press 1994.
- [5] *G. B. Jeffery*: The motion of ellipsoidal particles immersed in a viscous fluid. *Proc. Roy. Soc. London Ser. A* 102 (1922), 161–179.
- [6] *J. Ježek*: Software for modeling the motion of rigid triaxial particles in viscous flow. *Computers and Geosciences* 20 (1994), 409–424.
- [7] *J. Ježek, S. Saic, K. Segeth, K. Schulmann*: Three-dimensional hydrodynamical modelling of viscous flow around a rotating ellipsoidal inclusion. *Computers and Geosciences* 25 (1999), 547–558.
- [8] *J. Ježek, K. Schulmann, K. Segeth*: Fabric evolution of rigid inclusions during mixed coaxial and simple shear flows. *Tectonophysics* 257 (1996), 203–221.
- [9] *T. Masuda, S. Mochizuki*: Development of snowball structure: numerical simulation of inclusion trails during synkinematic porphyroblast growth in metamorphic rocks.. *Tectonophysics* 170 (1989), 141–150.
- [10] *W. H. Press et al.*: Numerical Recipes. The Art of Scientific Computing. Cambridge, Cambridge University Press 1986.
- [11] *L. J. Reed, E. Tryggvason*: Preferred orientations of rigid particles in a viscous matrix deformed by pure shear and simple shear. *Tectonophysics* 24 (1974), 85–98.
- [12] *S. Wolfram*: Mathematica. A System for Doing Mathematics by Computer. Reading, MA, Addison-Wesley 1993.

Authors' addresses: *Doc. RNDr. Josef Ježek, CSc.*, Faculty of Science, Charles University, Albertov 6, CZ-128 43 Praha 2, Czech Republic, e-mail: jezek@prfdec.natur.cuni.cz; *Doc. Ing. Stanislav Saic, CSc.*, Institute of Information Theory and Automation, Academy of Sciences, Pod Vodárenskou věží 4, CZ-182 08 Praha 8, Czech Republic, e-mail: ssaic@utia.cas.cz; *Doc. RNDr. Karel Segeth, CSc.*, Mathematical Institute, Academy of Sciences, Žitná 25, CZ-115 67 Praha 1, Czech Republic, e-mail: segeth@math.cas.cz.