rt
Anno 2009_Numero 111

rapporti tecnici INGV

Wolfram Mathematica® can provide an improper solution of an Ordinary Differential Equation: An intriguing example

111

Istituto Nazionale di Geofisica e Vulcanologia

Anno 2009_Numero 111

rapporti tecnici INGV

WOLFRAM MATHEMATICA® CAN PROVIDE AN IMPROPER SOLUTION OF AN ORDINARY DIFFERENTIAL EQUATION: AN INTRIGUING EXAMPLE

Andrea Bizzarri

INGV (Istituto Nazionale di Geofisica e Vulcanologia, Sezione di Bologna)

111

Table of contents

Introduction

Mathematica® is one of the most popular and powerful commercial softwares for scientific computation and solution of algebraic equations. With integrated symbolic computation, the user can work directly on precise models, by transforming, optimizing and solving them, only substituting approximate or specific numerical values where necessary (for instance for visualization purposes). It is developed and distributed by Wolfram Resarch (http://www.wolfram.com/company/background.html), a company founded in 1987 by Steven Wolfram, Ph.D. (http://www.stephenwolfram.com/about-sw/). Wolfram Research is now one of the world's most respected software companies, as well as a powerhouse of scientific innovation. After the first version of *Mathematica*® released on June 23, 1988, version 7 is now available. It now incorporates multi–core and platform–optimized numerical algorithms, making it suitable for the most computationally intensive problems. One of the key features of *Mathematica*® is that, in contrast to the typical fixed 16–digits limitation found in other computing systems, its numerics support platform–independent arbitrary precision across all functions.

The prominent objective of this report is to show, by considering a specific application described in the next section, that sometime the use of a third–party software as a black box can lead to solutions that are in contrast with the theoretical expectation coming from the mathematical analysis. In particular, we will consider a first–order Ordinary Differential Equation (ODE) with time–variable, real coefficients. We will show that the solution calculated by *Mathematica*® is not formally acceptable, since it is a function to complex values. We will show that only after a proper manipulation of the original analytical formulation of the given ODE, *Mathematica*® is able to find the proper form of the solution.

1. Scientific rationale

Belardinelli and Bizzarri (2009) compute the stress changes caused by an inflating source in a layered half–space in order to model the seismicity during the 1982–1984 unrest phenomenon, occurred at Campi Flegrei caldera (Southern Italy). The time dependent stress perturbations are used to evaluate the seismicity rate changes following the approach proposed by Dieterich (1994).

This model is formulated within the framework of the laboratory–derived rate– and state–dependent friction laws, that express the temporal evolution of the traction on a seismic fault as a function of several physical observables, such as fault the slip velocity (i.e., the slip rate) and a state variable (accounting for the previous slip episodes on the considered fault surface). The description of the model details — as well as the crucial importance of the formulation of a fault governing law — is beyond the intents of the present study; readers can refer to Bizzarri (2009) and references therein for an extensive discussion of these topics. Here we are mainly devoted to the intriguing technical details of the application of the Dieterich's model.

Dieterich (1994) proposes that the seismicity rate R can be described by a state variable γ, having dimensions of s/Pa, which evolves with time and stressing histories. More properly, the model expresses R as follows:

$$R = \frac{r}{\gamma\, \dot{\tau}_r} \tag{1}$$

where r is the steady state seismicity rate of the target region at the reference shear stressing rate $\dot{\tau}_r$. Physically, the rate R can be interpreted as a statistical measure of the expected earthquake rate for some magnitude interval in the considered area. To calculate R, assuming that r and $\dot{\tau}_r$ are known quantities, it is necessary to evaluate the state variable γ, which is given by the solution of the following equation:

$$\dot{\gamma} = \frac{1}{a\, \sigma_n^{eff}} \left[1 - \gamma\, \dot{\tau} + \gamma \left(\frac{\tau}{\sigma_n^{eff}} - \alpha_{LD} \right) \dot{\sigma}_n^{eff} \right] \tag{2}$$

In equation (2) a and α_{LD} are constitutive parameters, τ is the shear stress and σ_n^{eff} is the effective normal stress (see also Linker and Dieterich, 1992); over–dots indicate the time derivatives.

The specific objective of Belardinelli and Bizzarri (2009) is to calculate the seismicity rate R in several subsequent time intervals, each of whom is characterized by different (known) values of $\dot{\tau}$ and $\dot{\sigma}_n^{eff}$. This is accomplished by using a FORTRAN code iteratively, which in turn needs as input the values of state variable γ at the different time levels (in other words it requires the solution of equation (2)). Instead of trying to obtain numerically a solution of equation (2), it is computationally more convenient (both in terms of computational efficiency and accuracy) to look for an analytical solution of (2) and then to use this expression iteratively, through the subsequent time intervals.

While in some special cases, where τ and σ_n^{eff} are simple, given functions of time, relatively uncomplicated solutions of the previous equation (2) are obtained (see Dieterich, 1994 for some examples), the most general case — in which the temporal dependence on the time of τ and σ_n^{eff} is not explicitly given — can not be solved in closed–form. Therefore, in order to find an analytical solution of (2) in the general case, we express stressing histories as $\tau = \tau(t = 0) + \dot{\tau}\, t$ and $\sigma_n^{eff} = \sigma_n^{eff}(t = 0) + \dot{\sigma}_n^{eff} t$ and approximate equation (2) by considering its first–order Taylor expansion:

$$\dot{\tilde{\gamma}} = \frac{1}{c_0} \left(1 - c_1 \tilde{\gamma} - c_2 t + c_3 t \tilde{\gamma} \right) \tag{3}$$

in which the symbol ~ emphasizes the fact that the solution $\tilde{\gamma}$ of the equation (3) is an approximated solution of the original equation (2) and the coefficients $\{c_i\}$ are expressed in terms of the other relevant physical quantities of the problem:

$$
\begin{aligned}
c_0 &= a\,\sigma_n^{eff}(t=0) \\
c_1 &= \dot{\tau} - \left(\frac{\tau(t=0)}{\sigma_n^{eff}(t=0)} - \alpha_{LD} \right) \dot{\sigma}_n^{eff} \\
c_2 &= \frac{\dot{\sigma}_n^{eff}}{\sigma_n^{eff}(t=0)} \\
c_3 &= c_2 \left[2\dot{\tau} - \left(2\frac{\tau(t=0)}{\sigma_n^{eff}(t=0)} - \alpha_{LD} \right) \dot{\sigma}_n^{eff} \right]
\end{aligned}
\tag{4}
$$

We note that in equation (3), instead of having $\tau(t)$ and $\sigma_n^{eff}(t)$ as in equation (2), we have the known quantities $\tau(t = 0)$ and $\sigma_n^{eff}(t = 0)$. Equation (3) is associated to the initial condition

$$\tilde{\gamma}(t_{init}) = \gamma_{init} \tag{5}$$

where t_{init} is the instant of time at which an arbitrary temporal interval begins. Just for completeness, we mention here that at the beginning of the problem (i.e., when $t_{init} = 0$), the following initial condition is assumed: $\tilde{\gamma}(t = 0) = \gamma(t = 0) = \gamma_0 = 1/\dot{\tau}_r$. For brevity of notation, in the following we will indicate simply with γ_0 the initial condition of equation (3).

We emphasize that equations (2) and (3) are first–order ODEs, with real coefficients. As such, both of them admit a real–valued analytical solution. To date, this solution has not been presented in the literature and therefore this is one of the novelties of Belardinelli and Bizzarri (2009).

2. Analytical solution of the equation (3)

Typical values of the parameters of the problem for an arbitrary time interval are listed in Table 1.

Parameter	***Value***
γ_0	3.17×10^{-3} d/Pa
$\tau(t=0)$	$0.85 \times \sigma_n^{eff}(t=0) = 25.5$ MPa
$\sigma_n^{eff}(t=0)$	30 MPa
$\dot{\tau}$	3472.44 Pa/d
$\dot{\sigma}_n^{eff}$	– 476.74 Pa/d
a	0.004
α_{LD}	0.25

Table 1. Typical parameter values for the considered application (see Belardinelli and Bizzarri, 2009 for details about the physical constraints on these values).

With the following statements (see Wolfram *Mathematica*® 7 Documentation Center for details)

```
c0 = a * σ0;
c1 = τ̃ - ((τ0 / σ0) - αLD) * σ̃;
c2 = σ̃ / σ0;
c3 = c2 * (2 * τ̃ - (2 * (τ0 / σ0) - αLD) * σ̃);
Simplify[DSolve[{γ̃'[t] == (1 / c0) * (1 - c1 * γ̃[t] - c2 * t + c3 * t * γ̃[t]), γ̃[0] == γ0}, γ̃[t], t],
 t >= 0 && γ0 > 0 && σ̃ < 0 && τ̃ > 0 && τ0 > 0 && σ0 > 0 && a > 0 && αLD > 0]
```
(6)

it is possible to obtain with *Mathematica*® an analytical solution of the previous equation (3):

$$\tilde{\gamma}[t] = \Bigg(-e^{\frac{\left(-\overline{\tau}\sigma_0^2 + t\overline{\sigma}^2(\alpha_{LD}\sigma_0 - 2\tau_0) + \overline{\sigma}\sigma_0(2t\overline{\tau} - \alpha_{LD}\sigma_0 + \tau_0)\right)^2}{2a\overline{\sigma}\sigma_0^3(2\overline{\tau}\sigma_0 + \overline{\sigma}\alpha_{LD}\sigma_0 - 2\overline{\sigma}\tau_0)}} \sqrt{2\pi} \Bigg(\mathrm{Erf}\Big[\frac{\overline{\tau}\sigma_0 + \overline{\sigma}\alpha_{LD}\sigma_0 - \overline{\sigma}\tau_0}{\sqrt{2}\sqrt{a\overline{\sigma}}\sqrt{\sigma_0}\sqrt{2\overline{\tau}\sigma_0 + \overline{\sigma}\alpha_{LD}\sigma_0 - 2\overline{\sigma}\tau_0}}\Big] - \mathrm{Erf}\Big[\frac{\overline{\tau}\sigma_0^2 + \overline{\sigma}\sigma_0(-2t\overline{\tau} + \alpha_{LD}\sigma_0 - \tau_0) + \overline{\sigma}^2(-t\alpha_{LD}\sigma_0 + 2t\tau_0)}{\sqrt{2}\sqrt{a\overline{\sigma}}\,\sigma_0^{3/2}\sqrt{2\overline{\tau}\sigma_0 + \overline{\sigma}\alpha_{LD}\sigma_0 - 2\overline{\sigma}\tau_0}}\Big]\Bigg)\overline{\sigma}\sqrt{\sigma_0}\,\tau_0 - 2\left(-1 + e^{\frac{t\left(-2\overline{\tau}\sigma_0^2 + t\overline{\sigma}^2(\alpha_{LD}\sigma_0 - 2\tau_0) + 2\overline{\sigma}\sigma_0(t\overline{\tau} - \alpha_{LD}\sigma_0 + \tau_0)\right)}{2a\sigma_0^3}}\right)\sqrt{a\overline{\sigma}}\,\sigma_0\sqrt{2\overline{\tau}\sigma_0 + \overline{\sigma}\alpha_{LD}\sigma_0 - 2\overline{\sigma}\tau_0} + 2e^{\frac{t\left(-2\overline{\tau}\sigma_0^2 + t\overline{\sigma}^2(\alpha_{LD}\sigma_0 - 2\tau_0) + 2\overline{\sigma}\sigma_0(t\overline{\tau} - \alpha_{LD}\sigma_0 + \tau_0)\right)}{2a\sigma_0^3}}\overline{\sigma}^{3/2}\gamma_0(\alpha_{LD}\sigma_0 - 2\tau_0)\sqrt{a(2\overline{\tau}\sigma_0 + \overline{\sigma}\alpha_{LD}\sigma_0 - 2\overline{\sigma}\tau_0)} + \overline{\tau}\sigma_0\Bigg(e^{\frac{\left(-\overline{\tau}\sigma_0^2 + t\overline{\sigma}^2(\alpha_{LD}\sigma_0 - 2\tau_0) + \overline{\sigma}\sigma_0(2t\overline{\tau} - \alpha_{LD}\sigma_0 + \tau_0)\right)^2}{2a\overline{\sigma}\sigma_0^3(2\overline{\tau}\sigma_0 + \overline{\sigma}\alpha_{LD}\sigma_0 - 2\overline{\sigma}\tau_0)}} \sqrt{2\pi} \Bigg(\mathrm{Erf}\Big[\frac{\overline{\tau}\sigma_0 + \overline{\sigma}\alpha_{LD}\sigma_0 - \overline{\sigma}\tau_0}{\sqrt{2}\sqrt{a\overline{\sigma}}\sqrt{\sigma_0}\sqrt{2\overline{\tau}\sigma_0 + \overline{\sigma}\alpha_{LD}\sigma_0 - 2\overline{\sigma}\tau_0}}\Big] - \mathrm{Erf}\Big[\frac{\overline{\tau}\sigma_0^2 + \overline{\sigma}\sigma_0(-2t\overline{\tau} + \alpha_{LD}\sigma_0 - \tau_0) + \overline{\sigma}^2(-t\alpha_{LD}\sigma_0 + 2t\tau_0)}{\sqrt{2}\sqrt{a\overline{\sigma}}\,\sigma_0^{3/2}\sqrt{2\overline{\tau}\sigma_0 + \overline{\sigma}\alpha_{LD}\sigma_0 - 2\overline{\sigma}\tau_0}}\Big]\Bigg)\sqrt{\sigma_0} + 4e^{\frac{t\left(-2\overline{\tau}\sigma_0^2 + t\overline{\sigma}^2(\alpha_{LD}\sigma_0 - 2\tau_0) + 2\overline{\sigma}\sigma_0(t\overline{\tau} - \alpha_{LD}\sigma_0 + \tau_0)\right)}{2a\sigma_0^3}}\sqrt{a\overline{\sigma}}\,\gamma_0\sqrt{2\overline{\tau}\sigma_0 + \overline{\sigma}\alpha_{LD}\sigma_0 - 2\overline{\sigma}\tau_0}\Bigg)\Bigg) \Big/ \left(2\sqrt{a\overline{\sigma}}\,(2\overline{\tau}\sigma_0 + \overline{\sigma}(\alpha_{LD}\sigma_0 - 2\tau_0))^{3/2}\right) \tag{7}$$

In equation (7) Erf(.) is the error function, defined as

$$\mathrm{erf}(z) = \frac{2}{\sqrt{\pi}}\int_0^z e^{-t^2}\,dt \tag{8}$$

and, in the interest of simplicity, we have omitted the indices in $\dot{\sigma}_n^{eff}$ (briefly referred as $\dot{\sigma}$) and we have indicated $\tau(t=0)$ and $\sigma_n^{eff}(t=0)$ as τ_0 and σ_0, respectively.

At a first glance, the previous solution (7) might appear correct. However, by considering the values of the model parameters (listed in Table 1), we can easily discover that (7) is an imaginary–valued function. In fact, the terms containing square roots of $\dot{\sigma}_n^{eff}$, which is a negative quantity, give imaginary values. This clearly contradicts the theoretical expectation coming from the mathematical analysis that the solution of the equation (3) has to be a real–valued function.

Finally, we want to emphasize that in the `DSolve` statement above we have already introduced the constrain on the sign of $\dot{\sigma}_n^{eff}$ (see the directive $\dot{\sigma} < 0$).

3. The proper solution of the problem

Independently on the noticeable complication of the very long expression previously found for $\tilde{\gamma}$, it is evident that equation (7) is not practically usable neither in a FOTRAN implementation, nor for general purposes, since it is not a real–valued function, as required by the realness of coefficients in the ODE to be solved (equation (2) or (3)).

Let us we now solve equation (3) by leaving unspecified the coefficients $\{c_i\}$. We then find:

$$\tilde{\gamma}[t] = \frac{1}{2\sqrt{c_0}\,c_3^{3/2}}\left(-e^{\frac{(c_1-t c_3)^2}{2 c_0 c_3}}\sqrt{2\pi}\left(\mathrm{Erf}\left[\frac{c_1}{\sqrt{2}\sqrt{c_0}\sqrt{c_3}}\right]+\mathrm{Erf}\left[\frac{-c_1+t c_3}{\sqrt{2}\sqrt{c_0}\sqrt{c_3}}\right]\right)c_1 c_2 + e^{\frac{(c_1-t c_3)^2}{2 c_0 c_3}}\sqrt{2\pi}\left(\mathrm{Erf}\left[\frac{c_1}{\sqrt{2}\sqrt{c_0}\sqrt{c_3}}\right]+\mathrm{Erf}\left[\frac{-c_1+t c_3}{\sqrt{2}\sqrt{c_0}\sqrt{c_3}}\right]\right)c_3 + 2\sqrt{c_0}\sqrt{c_3}\left(c_2+e^{\frac{t(-2c_1+t c_3)}{2c_0}}(-c_2+c_3\gamma_0)\right)\right) \quad (9)$$

Now, by considering the values tabulated in Table 1, we realize that c_0 and c_1 are positive, while c_2 and c_3 are negative (see Table 2).

Coefficient in (3)	*Value*
c_0	0.12 MPa
c_1	3758.49 Pa/s
c_2	$-1.58914 \times 10^{-5}\ \mathrm{d}^{-1}$
c_3	$-0.121349\ \mathrm{Pa/d}^2$

Table 2. Values of the four coefficients $\{c_i\}$ of equation (3) for the typical values of model parameters listed in Table 1.

Therefore, from equation (9) we learn that imaginary values originate from the coefficient c_3. This causes the multiplicative factor $1/\left(2\sqrt{c_0}\ c_3^{3/2}\right)$ to be pure imaginary and the arguments of the error functions to have real and imaginary parts (these parts are of the comparable order of magnitude). Moreover, one of the arguments of the error function evolves with time.

Let us now rewrite equation (3) in the following form:

$$\dot{\tilde{\gamma}} = \frac{1}{c_0}\left(1 - c_1\,\tilde{\gamma} - c_2 t - \left| c_3 \right| t\,\tilde{\gamma}\right) \tag{10}$$

that differs from equation (3) because we have now $-\ |c_3|$ instead of $+\ c_3$. This equation is numerically equivalent to equation (3), even it is different from a formal, mathematical point of view.

Now, if we solve equation (10) with *Mathematica*®, using again the `DSolve` directive, we obtain the following expression:

$$\tilde{\gamma}[t] = \frac{1}{2\,\mathrm{Abs}[c_3]^{3/2}\sqrt{c_0}} \left(e^{-\frac{(t\,\mathrm{Abs}[c_3]+c_1)^2}{2\,\mathrm{Abs}[c_3]\,c_0}} \left(\sqrt{2\pi}\,\mathrm{Abs}[c_3] \left(-\mathrm{Erfi}\left[\frac{c_1}{\sqrt{2}\sqrt{\mathrm{Abs}[c_3]}\sqrt{c_0}}\right] + \mathrm{Erfi}\left[\frac{t\,\mathrm{Abs}[c_3]+c_1}{\sqrt{2}\sqrt{\mathrm{Abs}[c_3]}\sqrt{c_0}}\right]\right) + 2\left(e^{\frac{c_1^2}{2\,\mathrm{Abs}[c_3]\,c_0}} - e^{\frac{(t\,\mathrm{Abs}[c_3]+c_1)^2}{2\,\mathrm{Abs}[c_3]\,c_0}} \right)\sqrt{\mathrm{Abs}[c_3]}\sqrt{c_0}\,c_2 + \sqrt{2\pi}\left(-\mathrm{Erfi}\left[\frac{c_1}{\sqrt{2}\sqrt{\mathrm{Abs}[c_3]}\sqrt{c_0}}\right] + \mathrm{Erfi}\left[\frac{t\,\mathrm{Abs}[c_3]+c_1}{\sqrt{2}\sqrt{\mathrm{Abs}[c_3]}\sqrt{c_0}}\right]\right) c_1\,c_2 + 2\,e^{\frac{c_1^2}{2\,\mathrm{Abs}[c_3]\,c_0}}\,\mathrm{Abs}[c_3]^{3/2}\sqrt{c_0}\,\gamma_0 \right)\right) \tag{11}$$

In the previous equation Erfi(.) is the imaginary error function, defined as:

$$\mathrm{Erfi}(z) = \mathrm{Erf}(iz)/i \tag{12}$$

being i the square root of unity ($i^2 = -1$). Interestingly, we note that for real values of the argument z the imaginary error function gives a real number (i.e., $z \in \Re \Rightarrow \mathrm{Erfi}(z) \in \Re$). Moreover, now all the terms appearing in equation (11) are such that it is a real–valued function for all times t.

For completeness, in Figure 1 we plot the time evolution of $\tilde{\gamma}$ over a one month–long time interval.

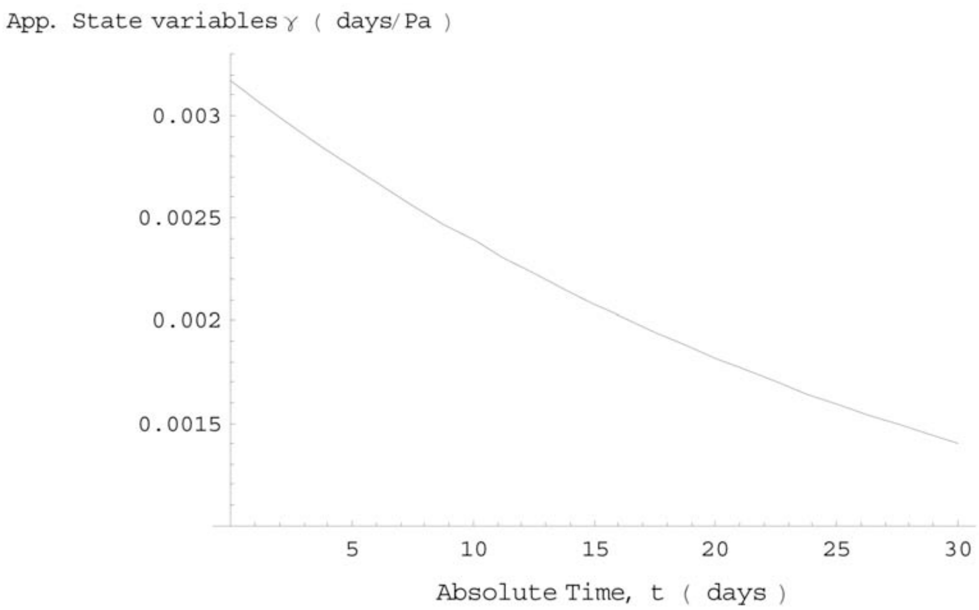

Figure 1. Plot of the time evolution of the analytical solution of the ODE, $\tilde{\gamma}$, expressed as in equation (11).

It is interesting to note that the implementation in FORTRAN of the equation (11) is straightforward; the imaginary error function Erfi(.) can be easily calculated by exploiting the special function (`COMPLEX *16`) `ZERFE`, embedded within the Visual Numerics *IMSL*® numerical library package (http://www.vni.com/products/imsl/). After a simple algebra (see also Visual Numerics *IMSL*® Documentation for the formal definition of `ZERFE`) we find that the following relation holds:

$$\mathrm{Erfi}(z) = \frac{e^{z^2}\,\mathtt{ZERFE}(z) - 1}{i} \tag{13}$$

In our specific case, the complex input argument z of the function `ZERFE` has null imaginary part (specifically, the arguments of imaginary error functions appearing in the previous equation (12) are $\frac{c_1}{\sqrt{2}\,\sqrt{\mathrm{Abs}[c_3]}\,\sqrt{c_0}}$ and $\frac{t\,\mathrm{Abs}[c_3] + c_1}{\sqrt{2}\,\sqrt{\mathrm{Abs}[c_3]}\,\sqrt{c_0}}$).

4. Summary and concluding remarks

We have considered a first–order Ordinary Differential Equation (ODE; equation (3)) with real, time variable coefficients (equation (4)) and initial condition as in equation (5). Such an equation admits a real–valued solution.

We have used Wolfram *Mathematica*® in order to obtain analytically the solution of that ODE. Due to the specific scientific problem, focused on the effects on seismicity rate of stress perturbations arising from an inflating source in a layered medium (see section 1), we need to found such an analytical solution and implement it in a FORTRAN code.

In this report we have shown that, even imposing the specific constrains on the sign of the model parameters, *Mathematica*® gives an analytical expression with imaginary values (see equation (7)). This result, also obtained with older version of *Mathematica*®, contradicts the theoretical expectation from the mathematical analysis and can not be implemented in a FORTRAN code.

We have also shown that only after a proper manipulation of the ODE to be solved we obtain a numerically equivalent ODE (equation (10)), which can be solved by *Mathematica*®. The solution that we obtain in this case (equation (11)) has now real values, as expected. Finally, we have indicated that the encoding in FORTRAN of such a solution is straightforward.

This intriguing example, originated by a specific, well–motivated scientific problem, highlights the fact that, as for other third–party commercial software packages, a black box is not a panacea.

Acknowledgements

I wish to acknowledge Maurizio Bonafede and Maria Elina Belardinelli for insightful discussions. I' m grateful to Daniele Melini and to an anonymous referee for their useful comments.

References

Belardinelli, M. E., Bizzarri, A. (2009). A model for seismicity rates observed during the 1982–1984 unrest at Campi Flegrei caldera (Italy). paper in preparation

Bizzarri, A. (2009), What does control earthquake ruptures and dynamic faulting? A review of different competing mechanisms. Pure Appl. Geophys., 166, Nos. 5−7, 2009, 741−776, doi: 10.1007/s00024−009−0494−1

Dieterich, J. H. (1984). A constitutive law for rate of earthquake production and its application to earthquake clustering. J. Geophys. Res., 99, No. B2, 2601−2618

Linker, M. F., Dieterich, J. H. (1992). Effects of variable normal stress on rock friction: observations and constitutive equations. J. Geophys. Res., 97, No. B4, 4923−4940

Visual Numerics *IMSL*® Documentation. The technical documentation available online at http://www.vni.com/products/imsl/documentation/index.php

Wolfram *Mathematica*® 7 Documentation Center. The complete product guide and manuals available online at http://reference.wolfram.com/mathematica/guide/Mathematica.html

Coordinamento editoriale e impaginazione
Centro Editoriale Nazionale | INGV

Progetto grafico e redazionale
Laboratorio Grafica e Immagini | INGV Roma

Via di Vigna Murata, 605
00143 Roma
Tel. +39 06518601 Fax +39 065041181

http://www.ingv.it

Istituto Nazionale di Geofisica e Vulcanologia