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Numerical Verification for the Asian Rust Dispersion in Paraná

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Abstract. This work aims to study the discretization error of a numerical model describing the atmospheric transport of the Asian Rust spores in Paraná. The model was obtained from the discretization of a two-dimensional Partial Differential Equation with diffusive, convective, and reactive terms by the finite difference method. To study the behavior of the discretization error, *a priori* and *a posteriori* analyzes were performed. From the verification process, it was found that the apparent order converged to the asymptotic order. Thus, the process of estimating numerical errors through the Richardson Estimate presented promising results.

Keywords: Asian rust, Discretization error, Richardson estimator.

1 Introduction

Several physical phenomena that occur in nature can be modeled by Partial Differential Equations (PDE). Depending on the initial and boundary conditions it is not possible to obtain analytical solutions. An alternative is to take a numerical approach, which consists of approximating the derivatives with a discretization method. However, this approach generates an accumulation of errors that can be caused in various ways, such as truncation, iteration, or rounding errors [1]. Among these sources, the truncation error arises when a continuous mathematical concept is replaced by a discrete concept. It constitutes the most significant portion that influences the quality of numerical solutions. Although this error cannot be eliminated, it must be studied and at least minimized.

When the numerical error is influenced only by the truncation error, it is called a discretization error. The ways of estimating the discretization error can be divided into two types: *a priori* and *a posteriori* estimates. The *a priori* estimates are used to predict the behavior of the discretization error before obtaining any numerical solution. On the other hand, *posterior* estimates are used to effectively estimate the magnitude of the discretization error using numerical solutions. In general, numerical verification procedures are used to identify the extent to which a mathematical model is adequately solved using a numerical method [1]. Several methods can be used *posterior* to estimate the discretization error. In this work, Richardson estimator [2] will be used to study the discretization error of a numerical model that describes the two-dimensional atmospheric transport of Asian Rust spores in the state of Paraná.

This work is structured as follows: Section 2 presents details on the Asian Rust, necessary to understand the physical characteristics of the problem. Section 3 presents the model mathematician that describes the transport of spores of Rust Asian. Section 4 presents the numerical model obtained by discretizing a mathematical model using the finite difference method. In Section 5, the theory of numerical error is presented, necessary to estimate the discretization error of the numerical model. Section 6 presents the results obtained in this work. Finally, in Section 7 some considerations are presented.

2 Asian Rust

Asian Rust is the main disease that affects soybean plantations in the state of Paraná. Its etiological agent is a biotrophic fungus called *Phakopsora pachyrhizi* which depends on living hosts to survive and multiply. The fungus that causes this disease can survive outside hosts through micro-organisms, called spores. These spores are structures, like seeds, that serve to spread the fungus to other plants and places through the winds [3]. Spores can remain viable during atmospheric transport for long periods, resulting in contamination of large soybean-producing areas. Literature, some works study the influence of atmospheric currents on the transport of Asian Rust spores, such as [4–9].

In the state of Paraná, most of the contamination of soybean crops that occurred in the field was during the off-season period, due to the existence of secondary hosts for the fungus. As a way of reducing the number of cases of the disease in the off-season and delaying the occurrence of the disease during the harvest, a period of 60 to 90 days without live plants in the field, called the soybean-free period, was implemented in Paraná. However, new cases of the disease were being identified in the state after the period of the sanitary vacuum and after the occurrence of cold fronts. The wind regime that occurs in Paraná is directly influenced by the terrestrial rotation in the east-west direction. On the other hand, during the occurrence of cold fronts, atmospheric currents move in the opposite direction. Until 2018/2019, the period of sanitary void was not practiced in countries neighboring the state of Paraná, such as Paraguay, where soybean cultivation was constant throughout the year. In the work presented by [9], it was found that cold fronts may be responsible for the atmospheric transport of Asian Rust spores to the state of Paraná in the 2018/2019 harvest. This phenomenon was modeled and studied through an EDP.

3 Mathematical Model

The equation that describes the two-dimensional atmospheric transport of Asian Rust spores, through cold fronts, presented in [9], is given by an EDP with diffusive, convective, and reactive terms.

$$\underbrace{\frac{\partial C}{\partial t}}_{\text{temporal term}} = \underbrace{D\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2}\right)}_{\text{diffusion term}} - \underbrace{\left(\frac{\partial (Cv_x)}{\partial x} + \frac{\partial (Cv_y)}{\partial y}\right)}_{\text{convective term}} - \underbrace{\lambda C}_{\text{reactive term}} . \quad (1)$$

In (1), the function representing the concentration of spores is represented by $C(x, y, t)$, which depends on two spatial variables x and y, and a temporal variable t. The parameter D represents the molecular diffusion coefficient of spores during atmospheric transport. The velocity field representing cold fronts is given by the terms $v(x, y, t) = v_x(x, y, t)\hat{i} + v_y(x, y, t)\hat{j}$ and, finally, λ represents the spore mortality rate during atmospheric transport.

4 Numerical Model

The discretization of the model (1) is performed by the finite difference method over a two-dimensional domain $[0, 1000] \times [0, 700]$ that includes the physical geometry of the state of Paraná and its surroundings. The first-order derivative of the temporal term is approximated by the regressive finite difference formula. The second-order derivatives of the diffusive term are approximated by the central finite difference formula. In the first-order derivatives of the convective term, the scheme is applied *First Order Upwind* (FOU).

In order to simplify the notation, the points of the computational mesh are labeled by cardinal points, so that $P = (i, j)$, $E = (i + 1, j)$, $W = (i - 1, j)$, $N = (i, j + 1)$, $S = (i, j - 1)$, $EE = (i + 2, j)$, $WW = (i - 2, j)$, $NN = (i, j + 2)$ and $SS = (i, j - 2)$. The spacings between mesh points in the spatial domains x and y, and in the temporal domain t, are denoted by h_x, h_y and h_t, respectively. In this way, the model's discretized equation (1) is given by

$$C\Big|_P^{k+1} = d\left[r_x\left(C\Big|_E^{k+1} + C\Big|_W^{k+1}\right) + r_y\left(C\Big|_N^{k+1} + C\Big|_S^{k+1}\right) - \frac{\overline{\delta}_E}{2h_x}C\Big|_{EE}^{k+1} + \right.$$
$$\left. + \frac{\delta_W}{2h_x}C\Big|_{WW}^{k+1} - \frac{\overline{\delta}_N}{2h_y}C\Big|_{NN}^{k+1} + \frac{\delta_S}{2h_y}C\Big|_{SS}^{k+1} + \frac{1}{h_t}C\Big|_P^k\right]. \quad (2)$$

In the equation (2), the terms,

$$r_x = \frac{D}{(h_x)^2} \qquad r_y = \frac{D}{(h_y)^2} \qquad \delta_E = v_x|_E \left(\frac{1+S_E}{2}\right) \qquad \overline{\delta}_E = v_x|_E \left(\frac{1-S_E}{2}\right)$$

$$\delta_W = v_x|_W \left(\frac{1+S_W}{2}\right) \qquad \overline{\delta}_W = v_x|_W \left(\frac{1-S_W}{2}\right) \qquad \delta_N = v_y|_N \left(\frac{1+S_N}{2}\right) \tag{3}$$

$$\overline{\delta}_N = v_y|_N \left(\frac{1-S_N}{2}\right) \qquad \delta_S = v_y|_S \left(\frac{1+S_S}{2}\right) \qquad \overline{\delta}_S = v_y|_S \left(\frac{1-S_S}{2}\right)$$

$$d = \left[\frac{1}{h_t} + 2r_x + 2r_y + \frac{\delta_E}{2h_x} - \frac{\overline{\delta}_W}{2h_x} + \frac{\delta_N}{2h_y} - \frac{\overline{\delta}_S}{2h_y} + \lambda\right]^{-1},$$

appear in order to simplify the notation

The equation (2) requires the calculation of the spore concentration at the mesh points $E = (i+1, j, k+1)$, $W = (i-1, j, k+1)$, $N = (i, j+1, k+1)$, $S = (i, j-1, k+1)$, $EE = (i+2, j, k+1)$, $WW = (i-2, j, k+1)$, $NN = (i, j+2, k+1)$, $SS = (i, j-2, k+1)$ and $P = (i, j, k)$, resulting in an implicit scheme, so that k and $k+1$ represent the previous and current time level, respectively, which leads to the resolution of a system of linear equations at each time level to generate the numerical solution.

5 Numerical Error

The truncation error E of a numerical approximation (ϕ) can be represented, generically, by [1]

$$E(\phi) = C_1 h^{p_L} + C_2 h^{p_2} + C_3 h^{p_3} + ... \tag{4}$$

where C_1, C_2, C_3, ... are coefficients that are independent of h. The terms, p_L, p_2, p_3, ... are the true orders of $E(\phi)$; ϕ is the variable of interest; h is the size of the mesh elements. In this work, the numerical approximation (ϕ) is represented by the variable C which represents the concentration of spores.

In the equation (4) the smallest exponent of h is defined as asymptotic order p_L. This term is a positive integer that satisfies the condition $p_L \geq 1$. When the size of h approaches zero in the equation (4), the first term (p_L) is the main component.

The numerical error (E) of a variable of interest is defined as the difference between the analytical solution (Φ) and its numerical solution (ϕ), i.e.

$$E(\phi) = \Phi - \phi. \tag{5}$$

As the model (1) has no known analytical solution [9], it is not possible to calculate the numerical error using the equation (5). Thus, it is necessary to estimate the numerical error. This estimate is also called the uncertainty (U) of the numerical solution, calculated by the difference between the estimated analytical solution (ϕ_∞) and its numerical solution (ϕ), that is

$$U(\phi) = \phi_\infty - \phi. \tag{6}$$

The value of (ϕ_∞) in (6) can be calculated using Richardson Extrapolation based on asymptotic order,

$$\phi_\infty(p_L) = \phi_1 + \frac{(\phi_1 - \phi_2)}{(q^{p_L} - 1)}, \tag{7}$$

or based on apparent order,

$$\phi_\infty(p_U) = \phi_1 + \frac{(\phi_1 - \phi_2)}{(q^{p_U} - 1)}, \tag{8}$$

so that

$$p_U = \frac{\log\left(\frac{\phi_2 - \phi_3}{\phi_1 - \phi_2}\right)}{\log(q)}. \tag{9}$$

6 Results

The results presented in [9] were considered the influence of nine cold fronts for the atmospheric transport of Asian Rust spores to the state of Paraná, between October 2018 and February 2019, which corresponds to the harvest period in the state. Numerical results were obtained by iteratively solving the equation (2) by the Gauss-Seidel method, considering as stopping criterion, the relative error between two consecutive iterations with a tolerance of $\varepsilon = 10^{-6}$. In this work, the discretization error of the equation 2 will be analyzed, considering only the influence of a cold front with a duration time of $t_f = 3$ hours, according to the simulations carried out in [9].

6.1 Estimation of the *a priori* discretization error

In the model (1), the discretization error $E(h_x, h_y, h_t)$ is given by

$$E(h_x, h_y, h_t) = \frac{h_t}{2!}\frac{\partial^2 C}{\partial x^2}\bigg|_P^{k+1} - \frac{(h_t)^2}{3!}\frac{\partial^3 C}{\partial t^3}\bigg|_P^{k+1} - \frac{(h_x)^2}{3}\frac{\partial^3 Cv_x}{\partial x^3}\bigg|_P^{k+1} - \frac{(h_y)^2}{3}\frac{\partial^3 Cv_y}{\partial y^3}\bigg|_P^{k+1} + \\ +\mathcal{O}(h_t^3) - \mathcal{O}(h_x^3) - \mathcal{O}(h_y^3). \tag{10}$$

Comparing the equations (10)-(4), it can be seen that the asymptotic order of the discretization error of the model (1) is $p_L = 1$.

With the equation (9) it is possible to verify the behavior of the apparent order (p_U) with the reduction of the spacing between the mesh points: h_x, h_y and h_t. The results obtained are shown in Table 1. The terms M_x, M_y and M_t that appear represent the number of partitions performed in the spatial and temporal domains, respectively.

Table 1. Behavior of (p_U) with constant refining ratio $q = 2$ between meshes. Asymptotic order, $p_L = 1$.

M_x	h_x	M_y	h_y	M_t	h_t	p_U
20	50	20	35	40	0,075	–
40	25	40	17.5	80	0.0375	–
80	12.5	80	8.75	160	0.01875	1.210479
160	6.25	160	4.375	320	0.009375	1.198745
320	3.125	320	2.1875	640	0.0046875	1.087947

The apparent order (p_U) calculations presented in Table 1 were performed considering the magnitude of the results obtained by the equation (2) in five spatial grids $(20, 40, 50, 80, 160$ and $320)$, in the standard L_1. From the behavior of the apparent order presented, it can be observed that $p_U \to p_L$, when h_x, h_y and $h_t \to 0$.

6.2 Estimation of *a posteriori* discretization error

To estimate the magnitude of the discretization error *a posteriori* the uncertainty (U) of the numerical solution (equation 5) was calculated. For this, the estimated analytical solution (ϕ_∞) was obtained, according to the equations (6)-(7). Table 2 shows the behavior of the estimated analytical solution calculated using the Richardson Extrapolation based on asymptotic and apparent orders.

Table 2. Estimated Analytical Solution (ϕ_∞) - Richardson extrapolation based on asymptotic and apparent orders.

M_x	h_x	M_y	h_y	M_t	h_t	$\phi_\infty(p_L)$	$\phi_\infty(p_U)$
20	50	20	35	40	0,075	–	–
40	25	40	17.5	80	0.0375	–	–
80	12.5	80	8.75	160	0.01875	0.17595661	0.17734123
160	6.25	160	4.375	320	0.009375	0.17891442	0.17818012
320	3.125	320	2.1875	640	0.0046875	0.17907412	0.17917156

To analyze the behavior of the uncertainty (U) of the results, the Figure 1 was obtained, so that, $U_{(pL1)}$, $U_{(pL2)}$, $U_{(pL3)}$, $U_{(pU1)}$, $U_{(pU2)}$ and $U_{(pU3)}$, represent the respective mesh sequences $(40, 80)$, $(80, 160)$ and $(160, 320)$, used to calculate the uncertainty (U) based on asymptotic and apparent orders.

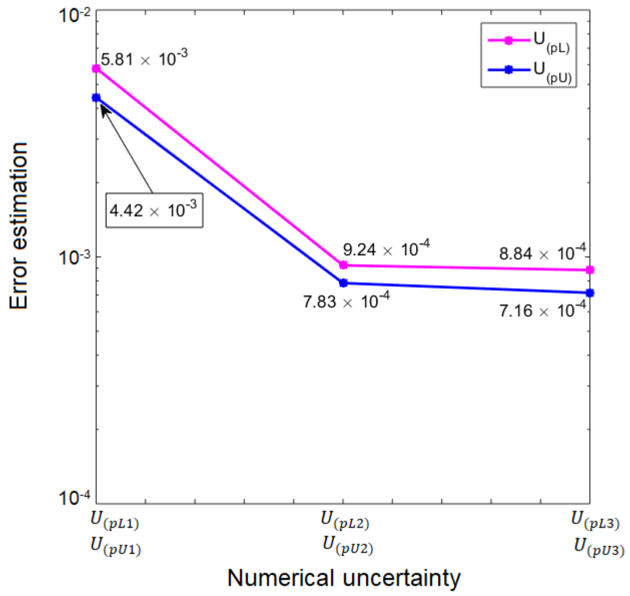

Figure 1. Numerical uncertainty (U) *versus* h

From the results presented by Figure 1, it can be seen that as the mesh refinement is performed, the uncertainty of the numerical solution decreases, reaching an order of 10^{-4} for the meshes (80 and 160) and (160 and 320).

7 Conclusions

The present work aimed to study the behavior of the discretization error of a numerical model that describes the atmospheric transport of spores from the Asian Rust to the state of Paraná due to the influence of cold fronts.

From the results obtained in this work, it was verified that the discretization error is minimized as the mesh refinement is performed. This behavior was expected, since the more points are used to obtain the numerical solution, the closer the numerical model is to the continuous model. In this work, only the behavior of a source of numerical error was studied. As a proposal for future work, a study can be carried out on other sources of errors that influence the quality of numerical solutions, such as iteration and rounding errors.

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