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## Applied Mathematical Modelling

journal homepage: www.elsevier.com/locate/apm

## A computational modeling and simulation of spatial dynamics in biological systems

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#### ARTICLE INFO

Article history: Received 30 December 2014 Revised 8 October 2015 Accepted 10 November 2015 Available online 2 December 2015

Keywords: Meshless method Operator splitting Radial basis functions System of PDEs Epidemiological models

#### ABSTRACT

Most of the biological processes occurring in nature exhibit physical movements at macro and micro levels. These movements are convection–diffusion type and are studied due to the important role they play in the mathematical modeling and simulation of dynamical systems. Accurate simulation of complicated dynamical system models are quite challenging. The focus of the current work is to design an effective meshless procedure for the simulation of reaction–convection–diffusion type of epidemiological models. The simulation results of the proposed method show much realistic finite time blow-up, which occurs due to calamitous spatial movements of the susceptible class of the population. Numerical simulations obtained through the proposed method are carefully vetted and found consistent with the earlier results. In some cases, improvement in the earlier results is reported as well.

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#### 1. Introduction

The role of convection and diffusion modes of transport in natural and controlled occurrences is pivotal. Numerous real-world applications of convection–diffusion driven models can be found in biological and chemical sciences. These include, diffusion of different chemicals in living beings, electrical signaling of nerves, proper distribution of oxygen to the healing tissues, human population dispersal processes in space and time, etc. Ignoring the effects of spatial movements in the mathematical modeling of epidemiology could lead to erroneous simulation conclusions.

Kermack and McKendrick [1] have proposed a mathematical SIR model for the transmission of epidemic diseases of unstructured population. Later on, several forms of the model have been appeared in the literature (see [2–5] and the references therein). In [6], a modified SIR type of model was proposed on the bounded one-dimensional domain [0, *L*], L > 0. This model was complemented with diffusion phenomena having the diffusion coefficients  $k_1$  and  $k_2$  for S and I respectively.

The model [2] has incorporated a comparatively more realistic dynamics that the susceptible individuals were moving away from the focused area of the infected population whose movement was restricted due to the disease. This has led to overcrowding and finite time blow-up which was a prime factor responsible for the numerical difficulties for a number of well-known algorithms. The model [2] was in one space dimension, which has restricted its applicability to the real life applications. The case when  $k_1 = k_2$ , was discussed in [6].

Recently, in [7] the SIR type of model has been extended to two-dimensional geometry and numerically solved by using a hybrid approach based on the conventional FEM and Runge–Kutta Discontinuous Galerkin Methods. Many interesting aspects of

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http://dx.doi.org/10.1016/j.apm.2015.11.025





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the model have been simulated and thoroughly investigated. Various cases such as the avoidance of infection and the avoidance of overcrowding have been discussed in comprehensive manner for both one- and two-dimensional geometries.

In order to verify and improve the simulation results given in [7], we are proposing the so-called meshless collocation method for the simulation of the SIR model. This numerical procedure has been widely used in simulation of diverse applications in science and engineering. In general, meshless methods have the advantage of ease of implementation on nodes (uniform or scattered). Meshless methods have reduced the worries of complexity encountered in the implementation of conventional numerical methods, caused due to the curse of dimensionality. Some interesting applications of the RBFs based meshless algorithms can be found in [8–24] and the reference therein.

In this paper, our focus is on the numerical simulation of the SIR model [7] by a hybrid type of operator splitting meshless method. In the current work, we have concentrated our attention on the simulations results of increased finite blow-up time as well as a blow-up of smaller magnitude. For the purpose of comparison, some of the cases discussed in [7] are revisited and confirmed while some of the results discussed in [7] are modified in the light of new simulation results produced by meshless operator splitting method (MOSM). Some additional possibilities of the model are also considered. Ease of implementation of the MOSM has benefitted us a great deal in context of the SIR model. The dividends thus obtained are in the form of more accurate simulation results, delayed blow-up of smaller magnitude, simplicity of coding and less manual work.

The rest of the paper is organized as follows. In Section 2, a brief description of the model is given. In Section 3, time and space discretization procedures are elaborated. In Section 4, computation of numerical results and analysis are performed. In Section 5 some conclusions of the paper are given.

#### 2. Description of the model

An epidemic SIR model for a given total population (N) along with convection and diffusion dynamics as described in [7] comprises three classes (compartments), namely: the Susceptible(S), the Infected(I), and the Recovered(R) such that N = S+I+R.

In the two dimensional case a closed domain  $\Omega = [0, 1] \times [0, 1]$  is taken into consideration with the no flux condition on the boundaries of the domain. Diffusion–convection parameters for the susceptible and the infected classes are represented by  $d_1$  and  $d_2$  respectively. The infection is assumed to be transmitted from the infected population to the susceptible population at a rate  $\alpha > 0$  per head, and the infected population is assumed to recover at a rate  $\gamma > 0$  per head.

With these assumptions, the general form of the two dimensional model [7] is:

$$S_t = d_1 \nabla .(S \nabla N) + d_2 \nabla .(S \nabla I) - \alpha SI,$$
  

$$I_t = d_1 \nabla .(I \nabla N) + \alpha SI - \gamma I,$$
  

$$R_t = d_1 \nabla .(R \nabla N) + \gamma I,$$
(1)

where  $\nabla = (\frac{\partial}{\partial x})$  and  $\nabla = (\frac{\partial}{\partial x}, \frac{\partial}{\partial y})^T$  in one- and two-dimensional cases respectively. Expanded formulation of the above model can be written as:

$$\begin{split} S_{t} &= d_{1}S(S_{xx} + I_{xx} + R_{xx}) + d_{1}S_{x}(S_{x} + I_{x} + R_{x}) + d_{2}SI_{xx} \\ &+ d_{2}S_{x}I_{x} + d_{1}S(S_{yy} + I_{yy} + R_{yy}) + d_{1}S_{y}(S_{y} + I_{y} + R_{y}) \\ &+ d_{2}SI_{yy} + d_{2}S_{y}I_{y} - \alpha SI, \\ I_{t} &= d_{1}I(S_{xx} + I_{xx} + R_{xx}) + d_{1}I_{x}(S_{x} + I_{x} + R_{x}) \\ &+ d_{1}I(S_{yy} + I_{yy} + R_{yy}) + d_{1}I_{y}(S_{y} + I_{y} + R_{y}) + \alpha SI - \gamma I, \\ R_{t} &= d_{1}R(S_{xx} + I_{xx} + R_{xx}) + d_{1}R_{x}(S_{x} + I_{x} + R_{x}) \\ &\quad d_{1}R(S_{yy} + I_{yy} + R_{yy}) + d_{1}R_{y}(S_{y} + I_{y} + R_{y}) + \gamma I. \end{split}$$

$$(2)$$

The above system of nonlinear PDEs (1) or (2) is accompanied by the following non-negative initial conditions:

$$S(x, y, 0) = S_0,$$
  

$$I(x, y, 0) = I_0,$$
  

$$R(x, y, 0) = R_0.$$
(3)

and the no flux boundary conditions:

$$\left(d_1\frac{\partial N}{\partial n} + d_2\frac{\partial I}{\partial n}\right)(x, y, t) = d_1\frac{\partial N}{\partial n}(x, y, t) = 0,$$
(4)

where *n* is the outward unit normal vector on boundaries.

The positivity of the solution and its connection with the existence of the solution of the system of PDEs (1) and (4) has been proved in the following theorem.

**Theorem 1** [7]. If  $(S_0, I_0, R_0) > 0$ , any solution (S, I, R) of Eqs. (1) and (4) is positive as long as it exists.

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