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Control of a consumer-resource agent-based model using partial differential equation approximation

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Abstract

Agent-based models (ABMs) are increasing in popularity as tools to simulate and explore many biological systems. Successes in simulation lead to deeper investigations, from designing systems to optimizing performance. The typically stochastic, rule-based structure of ABMs, however, does not lend itself to analytic and numerical techniques of optimization the way traditional dynamical systems models do. The goal of this work is to illustrate a technique for approximating ABMs with a partial differential equation (PDE) system to design some management strategies on the ABM. We propose a surrogate modeling approach, using differential equations that admit direct means of determining optimal controls, with a particular focus on environmental heterogeneity in the ABM. We implement this program with both PDE and ordinary differential equation (ODE) approximations on the well-known rabbits and grass ABM, in which a pest population consumes a resource. The control problem addressed is the reduction of this pest population through an optimal control formulation. After fitting the ODE and PDE models to ABM simulation data in the absence of control, we compute optimal controls using the ODE and PDE models, which we them apply to the ABM. The results show promise for approximating ABMs with differential equations in this context.

KEYWORDS

agent-based model, optimal control, PDE approximation

1 | INTRODUCTION

Agent-based models (ABMs) allow biologists and social scientists to simulate and analyze populations as they interact with each other and their environment. Using rule-based computational logic, ABMs are easier to create than traditional aggregate models such as differential equations. Moreover, modelers can include many interesting and important features, especially heterogeneity of agent and environmental characteristics.[1] ABMs have shown great utility in a variety of application areas, including disease transmission,[2-6] risky alcohol use among college students,[7,8] wildlife ecology and management,[9-11] and cancer biology.[12,13] In these applications, problems of decision-making and performance optimization arise naturally, leading to questions of how best to use ABMs for control and optimization.

Optimal control and optimization techniques can frequently guide strategies for managing populations. Originally motivated by engineering problems, the mathematical and computational techniques of optimal control theory are effective in minimizing or maximizing an objective coupled with a differential equation, difference equation, or Markov transition matrix.[14-17] The mathematical techniques used to analyze optimal control problems typically fall into three basic categories. First, one may treat the optimal control problem as constrained optimization in an abstract function space,[18] applying iterative optimization methods. Second, characterization of the constrained optimization's Lagrange multipliers leads to two-point boundary value problems and Pontryagin's maximum principle.[15,16,19-20] Third, Bellman's optimality principle (whatever the current state and control, the remaining controls must be optimal for the state resulting from the current state and control) leads to the dynamic programming equation.[17] These three approaches allow optimization in applications in engineering,[15] economics,[21] and more recently, biological applications such as cancer treatments, wildlife management, and metabolic regulation.[14,22]

We acknowledge the widespread use of ABMs for a variety of biological and medical applications and often give insights about the biological mechanisms and the impact of various stochastic features. There is a need to design management strategies to guide the ABMs toward a desired goal. We are proposing that approximation by differential equations may be a useful approach for computing such management strategies. We note that there are variety of successful approaches to approximate interacting particle systems, stochastic microscopic population processes, and some ABMs.[23-27] Some ABMs have been also approximated using master equations and mean field approaches,[28,29] optimal controls may be found on a system that approximates an ABM. Implementing a version of an optimal control on the corresponding ABM may not be "optimal" but will often give reasonable choices for management actions, where "reasonable" might be judged by a chosen goal. Implementing the approximate system's optimal control on the corresponding ABM may not be optimal for the ABM, but it may provide a systematic means of improving the performance of the ABM with respect to the control objective.

ABMs, however, lack the mathematical structure that allows optimization of difference and differential equation models. The rule-based logic—exactly what makes ABMs widely accessible to scientists—limits their utility for systems-level studies like optimal design and control. The recent perspectives paper[30] offers a compelling call-to-arms for optimization and control tools for ABMs. Several approaches are described there, ranging from applying stochastic optimization techniques directly to the ABM to constructing a dynamical systems model that approximates the dynamics of the ABM (see also 31-33). Here we take the latter approach, developing a reaction–diffusion partial differential equation (PDE) approximation and using standard optimal control tools for PDEs. The use of PDEs as the approximating dynamical system involves computational challenges but offers the ability to treat heterogeneous spatial environments. We will illustrate such an approximation method on a specific ABM with varying levels of heterogeneity. We are not discussing valid issues about biological dynamics, stability, and extinction in our ABM model example,[34] rather the goal of this work is to illustrate techniques for constructing management strategies. We will point out how features of the ABM guide the choice of the structure of the PDE system. The ability to choose the structure of the approximating systems from understanding of ABM; the appropriate spatial heterogeneity in the approximating system is important to represent clearly. The goal of this work is to illustrate a technique for approximating ABMs with a PDE system to design some management strategies on the ABM. Optimal control of the PDE system will give control strategies for the corresponding ABM. We discuss our choices in approximation in a specific example to illustrate the technique.

The behavior of an ABM at the spatial boundaries will lead to specific types of boundary conditions in an approximation. If the spatial environment has "wrapping" torus-type conditions, then the approximation need to use such boundary conditions.

We will apply optimal control techniques to the rabbit-grass-weeds Netlogo ABM,[35-37] and connect with ideas of implementing management in ABMs. This ABM represents an ecosystem with rabbits, grass, and weeds, but we are using a simplified consumer (pest)-resource version without weeds. The rabbits move around randomly, and grass grows using a specified growth rate. Rabbits can eat the grass and gain enough energy to reproduce. If a rabbit does not have enough energy, it will die. We emphasize the approximation of this ABM by reaction–diffusion PDE for the rabbit population coupled with an ordinary differential equation (ODE) (in time with coefficients also depending on space) for the grass population. This system with spatial-temporal dependence extends the work by Federico et al.[38] which approximated this ABM by a system of two ODEs and used the optimal control for their ODE system as a random mortality rate in the ABM. Their approach worked well when the grass growth rates in the ABM were homogeneous across the environment, but did not work well even with a small amount of heterogeneity in the grass growth rate. We introduce "space" into our approximate system, using a PDE for the moving rabbit population and an ODE for the non-mobile grass population.

We investigate a variety of heterogeneous grass growth and use the approach of optimal control of PDEs to find controls for the ABM.

We note that there has been some success using PDE approximation and control in other ABM applications. A well-known ABM, Sugarscape, by Wilensky,[39] models agents that move spatially across an environment in search of sugar, a resource required for their survival. Sugar grows in a heterogeneous manner, making some areas more advantageous to agents than others. Agents differ in their vision and metabolism. Agents with greater vision can see farther across the landscape to move toward higher concentrations of sugar, while agents with high metabolism require more sugar in-take. An agent dies when its sugar is depleted. Christley et al.[40] approximated a Sugarscape model using a system of advection–diffusion PDEs to model directed motion and sugar levels of agents. The PDE system models the density of four types of agents: low or high vision, low or high metabolism. The control is the taxation of agents' sugar resources with the goal of maximizing agent population size and taxes collected. In the present article, we leverage some of the lessons learned in Reference 40 to explore the rabbits-and-grass model. Insights may be gained from the approximation of this specific ABM and the corresponding controls, which may lead to better schemes for managing other ABMs

In Section 2, we begin with discussing the importance of capturing key features in an ABM with its approximate system; having specific actions chosen for the management controls and the corresponding goal can guide the process. Then we describe the example ABM in more depth and discuss the construction of the approximation system. Section 3 gives the optimal control formulation and corresponding adjoint system and optimality conditions as one possible technique to find the corresponding optimal control. In this article, we use an adjoint system as a tool to find the optimal control for the approximate system. Then we present some numerical illustrations of our results, as the heterogeneity of the grass growth rate is varied in space. The resulting controls and approximation results are compared with results from the ODE system, as in Reference 38. We finish with some conclusions about the applicability of this approximation method.

2 | FROM AN ABM TO ITS APPROXIMATION

In most ABMs, certain agents can move. The rules behind the movement guide the selection of the spatial derivative terms. If the movement is random, the approximation may include diffusion. If some types of agents can choose to move in particular directions to some local knowledge of the location of resources, then including directed movement terms (advective) in the approximation is crucial. For example, in the PDE approximation of the Sugarscape ABM,[39] the agents have knowledge of the nearby locations containing needed energy, which give rise to advective terms (first derivative terms besides the time derivatives), representing directed movement; there is also random movement, which gives diffusive terms in the approximation. The features in the environment that may affect the movement of agents should be understood and included. Resources in the environment may have their own differential equation, possibly without spatial derivative terms due to lack of movement. If the resources are consumed by some agents resulting in changes in the environment, then terms in PDE system are needed to represent the corresponding effects. If the goal of such approximation is to devise management for an ABMs, the features to control in ABMs need to be translated into the approximate system, along with corresponding of the controls if applicable. In some ABMs, there may be type of "tax" on agents for consuming resources, like in Reference 39. Once the PDE system is built and calibrated with a least squares fit to the ABM, the corresponding objective functional would be chosen with an admissible control set. Then the optimal controls for the PDE system can be found numerically using some optimization method. Translating the optimal control from the PDE system into the ABM may be straightforward (or not), and then the resulting strategies can assessed in terms of its contribution to the ABM management goals.

To illustrate this process with our example, we briefly discuss the version of the rabbits/grass ABM used for this control problem. The habitat in the ABM is a grid of 45 by 45, and we use this as our spatial domain in our approximations. Rabbits and grass interact on a torus, which wraps around vertically and horizontally to avoid spatial edge effects. Grass grows randomly in each cell depending on a grass growth function. Each cell has a "grass growth rate" depending on its spatial coordinates. At each time step a random number between 0 and 1 is generated for each empty cell and if this number is less than its "grass growth rate," the cell turns into a grass cell. A cell remains grass until a rabbit enters the cell and eats the grass. Each rabbit moves randomly from its current cell to one of its eight neighboring cells each time step. Each rabbit has a unique energy state level, which is decreased by a constant amount upon each move, and increased a given amount each time it eats grass. If a rabbit's energy level is above a threshold, it reproduces. Reproduction creates a new individual with half of the energy level of its parent, while the parent's energy level is reduced by half. The offspring is located in the same cell as its parent. A rabbit dies when its energy level goes below another threshold level. See References 36 and 38 for more details, including some cases about extinction in the ABM. See the flowchart that depicts the possible changes in the state of an individual rabbit in Figure 1. After a rabbit eats grass in a grid box, the grass grows back randomly according to specified rates, which can vary spatially.

The work in Reference 38 constructed a system of 2 ODEs to represent the spatial average of the temporal dynamics of the grass and rabbit populations generated by the IBM. In this approximate system, N_1 represented the population size of grass, (number of grass cells) and N_2, the population size of rabbits, N_2, (number of rabbits). The time unit is days. Their general model to approximate this ABM is given by:

$$\frac{dN_1(t)}{dt} = a_1(a_2 - N_1(t)) - f(N_1(t))N_2(t),$$
$$\frac{dN_2(t)}{dt} = b_1 f(N_1(t))N_2(t) - b_2N_2(t) - u(t)N_2(t), \tag{1}$$
$$f(N_1(t)) = \frac{a_1a_3N_1(t)}{1 + a_3a_4N_1(t)}, \tag{2}$$

with initial conditions:

$$N_1(0) = N_{10}[\text{number of grass cells}], N_2(0) = N_{20}[\text{number of rabbits}].$$

In Reference 38, the forms of the growth for the grass N_1 and the consumer term $f(N_1)$ were chosen from considering a variety of functional forms and corresponding ODE system simulated data and completing a fitting to time series data from 100 ABM runs. Note that a_3, a_4, b_1, and b_2 were also selected with this fitting, while a_1 and a_2 came directly from the structure of the ABM. The ODE system approximates the average values of N_1 and N_2 in the ABM

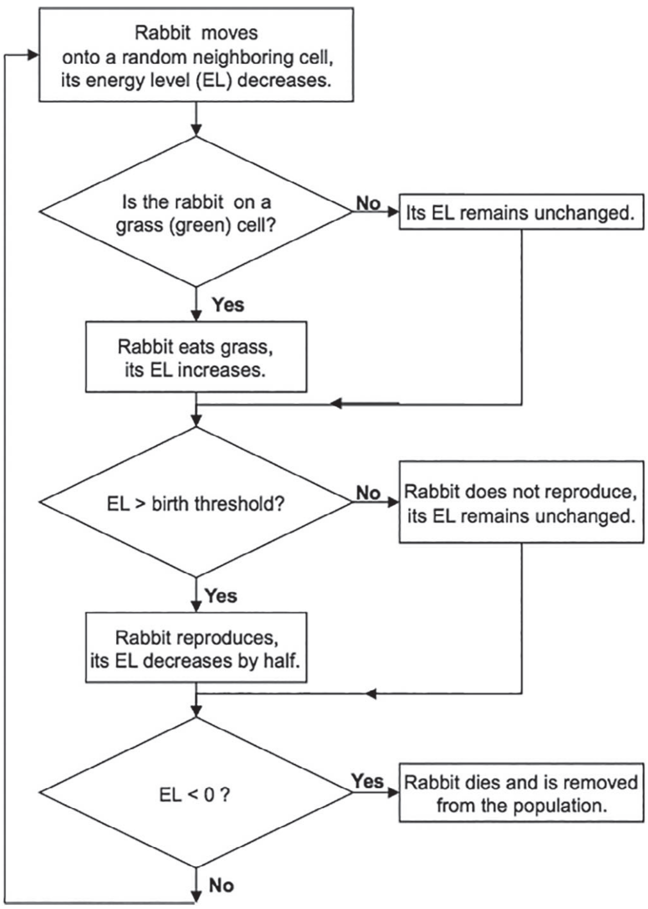

FIGURE 1 Flowchart of the rabbit actions in the ABM

well when the grass growth rate in the ABM is homogeneous in space and not so well with increasing heterogeneity. Note that the grass growth rate in the DE system is a constant (not varying in space). The control function $u(t)$ represents the harvest rate to reduce the "pest" rabbit population. In the ODE system, the objective functional to be minimized was

$$J(u) = \int_0^T (N_2(t) + c_1 u(t) N_2(t) + c_2 u^2(t)) dt,$$

which represents the minimizing the rabbit population while minimizing the cost of the harvest control actions. The corresponding optimal controls converted to control actions in the ABM, could easily be shown to be quite suboptimal when compared with some simple heterogeneous controls in the ABM, as illustrated in Reference 38.

The PDE system is formulated to represent average spatiotemporal dynamics of the grass and rabbit populations generated by the ABM. Now the state populations and the control will be functions of (x, y, t), space, and time. Starting with the movement of the rabbits randomly in space and they land on cells with specific grass levels by chance. This leads to a constant diffusion rate in the rabbit PDE, in both the x and y variables. In our ABM, the consumption of the grass by the rabbits increases their energy level, corresponding to a growth term in the rabbit PDE and a decay term in the grass equation. The grass population does not move, so we chose to use an equation without diffusion but with a time derivative; the grass growth rates can be functions of space to represent explicitly this heterogeneous feature. In the Federico approximation,[38] the grass growth rates had constant coefficients.

There are two major distinctions between the PDE and ODE approximation. First, the rabbit population diffuses across the environment in the PDE, allowing us to mimic the spatial distribution of rabbits that arises from the ABM's random walk: that is, rather than modeling the average total number of rabbits across the spatial grid, we model the average number of rabbits per unit area. Second, the grass may grow at different rates $g(x, y)$ in different spatial locations, allowing a heterogeneous landscape of resources for the rabbits to consume.

The state variables in the PDE model are $N_1(x, y, t)$, the population size of the grass at location (x, y) and time t, and $N_2(x, y, t)$, the population size of the rabbits at location (x, y) and time t. Let

$$Q = \{(x, y) \in R^2 | \; 0 < x < 45, 0 < y < 45\}$$

represent the square spatial domain in the ABM with size length L. The control $u(x, y, t)$ at location (x, y) and time $t$represents the harvest rate of the pest rabbits. The PDEs describing the two state variables are formulated as follows. For $(x, y) \in Q$ and $t > 0$, the PDE system for $(x, y, t) \in Q_T = Q \times (0, T)$ is

$$\frac{\partial N_1(x, y, t)}{\partial t} = g(x, y)(a_2 - N_1(x, y, t)) - f(N_1(x, y, t), x, y) N_2(x, y, t)), \tag{3}$$

$$\begin{aligned} \frac{\partial N_2(x, y, t)}{\partial t} - d\left(\frac{\partial^2 N_2(x, y, t)}{\partial x^2} + \frac{\partial^2 N_2(x, y, t)}{\partial y^2}\right) = {} & b_1 f(N_1(x, y, t), x, y) N_2(x, y, t) \\ & - (b_2 + u(x, y, t)) N_2(x, y, t), \end{aligned} \tag{4}$$

where

$$f(N_1(x, y, t), x, y) = \frac{g(x, y) a_3 N_1(x, y, t)}{1 + a_3 a_4 N_1(x, y, t)}. \tag{5}$$

We denote $f(N_1(x, y, t), x, y)$ as $f(N_1)$ for convenience, and we have

$$\frac{\partial f(N_1)}{\partial N_1} = \frac{g(x, y) a_3}{(1 + a_3 a_4 N_1(x, y, t))^2}.$$

State initial conditions are given by

$$N_i(x, y, 0) = N_{i,0}(x, y), \quad i = 1, 2,$$

with boundary conditions consistent with the torus boundary conditions of the ABM:

$$\begin{aligned}N_2(0,y,t) &= N_2(L,y,t),\\ N_2(x,0,t) &= N_2(x,L,t),\\ \frac{\partial N_2}{\partial x}(0,y,t) &= \frac{\partial N_2}{\partial x}(L,y,t),\\ \frac{\partial N_2}{\partial y}(x,0,t) &= \frac{\partial N_2}{\partial y}(x,L,t).\end{aligned}$$

The derivative boundary conditions are equivalent to flux-conservation:

$$\begin{aligned}\frac{\partial N_2}{\partial \eta}(0,y,t) &= -\frac{\partial N_2}{\partial \eta}(L,y,t),\\ \frac{\partial N_2}{\partial \eta}(x,0,t) &= -\frac{\partial N_2}{\partial \eta}(x,L,t),\end{aligned}$$

with η representing the outward normal vector direction. The system is a PDE extension of the ODE model in Reference 38, which will enable us to better handle the heterogeneity in the grass growth rate. The format of the interaction terms were chosen to be similar to those terms in that ODE model. The diffusion coefficient was chosen to be $d = 0.5$ to represent the movement in the ABM (see, e.g., Reference 17 for more on diffusions and random walks). The carrying capacity for the grass, N_1, is chosen to be $a_2 = 1$. The other parameters were estimated to obtain a reasonable fit to the average dynamics of the two populations as explained in more detail in Section 4 on numerical results. It is important to note that the PDE model can treat parameters like $a_1 = g(x, y)$ (grass growth rate) as spatially varying in order to capture spatial heterogeneity in the ABM.

3 | OPTIMAL CONTROL CHARACTERIZATION IN OUR PDE SYSTEM

Management of populations usually has goals with trade-offs between benefits and hazards of implementing control actions, and in many cases, the hazards or risks may be represented by costs. In managing an ABM, one would expect such trade-offs, or otherwise the desired control strategy would be obvious. In our example, a manager wants to balance the trade-off between the benefits of reducing a pest population (the rabbits) and the costs for the control actions (harvesting of the rabbits). Optimal control theory gives a tool to solve such a balancing optimization problem. In this illustration, there is a trade-off between harvesting rabbits and minimizing the cost of the control actions.

Choosing a goal to minimize a combination of the rabbit population and the cost of the implementing the control (like in Reference 38), the objective functional is:

$$J(u) = \int_{Q_T} (N_2(x,y,t) + c_1 u(x,y,t) N_2(x,y,t) + c_2 u(x,y,t)^2)\, dx\,dy\,dt. \tag{6}$$

Note that $c_1 u(x,y,t) N_2(x,y,t) + c_2 u^2(x,y,t)$ term represents the nonlinear cost of the control, includes a cost for the total number of rabbits harvested. For $M > 0$, the set of controls is given by

$$U = \{u \in L^2(Q \times (0,T)) |\ 0 \le u(x,y,t) \le M\}.$$

Note that the grass is not involved in the objective functional. For management of other ABMs, one must decide what actions can be implemented as controls and what is the corresponding goal.

The foundation of optimal control of PDEs was developed by Lions[16] and we will describe some of the basic steps needed to derive necessary conditions for an optimal control. This will lead to solving an optimality system, which will give a way to calculate the optimal control of the corresponding populations. For further developments and specific examples with analysis justification, see References 41 and 42 in solution spaces like $L^2(0, T; H^1(Q))$. We note that constructing an optimality system and solving that system numerically as done in this article is only one approach for finding optimal controls numerically for PDE. See References 43-50 for other numerical approaches, some with more direct optimization. Since this problem is bilinear in the control due to the uN_1 (product of the control and state), one can consider optimization approaches as in References 51 and 52. The introductory chapter of the book by Antil et al.[53] may be useful.

To derive the necessary conditions for the optimality system, we differentiate the map $u \mapsto J(u)$, in a directional derivative sense, which shows how the control affects the objective functional. The states contributes to the objective functional $J(u)$, so we also must differentiate the state with respect to the control, that is, differentiate the map $u \mapsto (N_1, N_2)(u)$.

The derivatives of this map satisfy sensitivity PDEs and are used to find the adjoint PDE system. We will choose the adjoint function such that the solution of the adjoint linear PDE system and the sensitivity system can be used to simplify that differentiation of J and then to obtain the explicit characterization of an optimal control. The population and adjoint PDEs and the optimal control characterization form the optimality system. More details are given in the appendix about deriving the sensitivity system and the optimal control characterization, and we present below the main points to obtain the optimality system, characterizing the optimal control.

The format of the terms and the boundary conditions from the adjoint system come from the boundary conditions for the sensitivity equations and the property of adjoint operators, that is, formally, in an appropriate L^2 space.

Using these limits to differentiate the control-to-states map for state system, with $u, l \in U$, and for $i = 1, 2$

$$\lim_{\epsilon \to 0} \frac{N_i(u + \epsilon l) - N_i(u)}{\epsilon} = \psi_i,$$

we can derive the system of sensitivity PDEs for the sensitivity functions ψ_1, ψ_2,

$$\frac{\partial \psi_1}{\partial t} + g(x, y)\psi_1 + \frac{\partial f(N_1)}{\partial N_1} N_2 \psi_1 + f(N_1)\psi_2 = 0, \tag{7}$$

$$\frac{\partial \psi_2}{\partial t} - d\frac{\partial^2 \psi_2}{\partial x^2} - d\frac{\partial^2 \psi_2}{\partial y^2} - b_1 \frac{\partial f(N_1)}{\partial N_1} N_2 \psi_1 - b_1 f(N_1)\psi_2 + b_2 \psi_2 = -u(x, y, t)\psi_2 - l(x, y, t)N_2, \tag{8}$$

with zero initial conditions and the same boundary conditions as the states:

$$\begin{aligned}
\psi_i(x, y, 0) &= 0, \quad i = 1, 2, \\
\psi_2(0, y, t) &= \psi_2(L, y, t), \\
\psi_2(x, 0, t) &= \psi_2(x, L, t), \\
\frac{\partial \psi_2}{\partial x}(0, y, t) &= \frac{\partial \psi_2}{\partial x}(L, y, t), \\
\frac{\partial \psi_2}{\partial y}(x, 0, t) &= \frac{\partial \psi_2}{\partial y}(x, L, t).
\end{aligned}$$

From the sensitivity system and the objective functional, we can obtain the adjoint system:

$$-\frac{\partial \lambda_1}{\partial t} + g(x, y)\lambda_1 + \frac{\partial f(N_1)}{\partial N_1} N_2 \lambda_1 - b_1 \frac{\partial f(N_1)}{\partial N_1} N_2 \lambda_2 = 0, \tag{9}$$

$$-\frac{\partial \lambda_2}{\partial t} - d\frac{\partial^2 \lambda_2}{\partial x^2} - d\frac{\partial^2 \lambda_2}{\partial y^2} + f(N_1)\lambda_1 - b_1 f(N_1)\lambda_2 + b_2 \lambda_2 + u(x, t)\lambda_2 = 1 + c_1 u. \tag{10}$$

Note that the nonhomogeneous terms of the adjoint system (on the right hand sides) come from differentiating the integrand of the objective functional with respect to the states:

$$\begin{aligned}
\frac{\partial (N_2 + c_1 u N_2 + c_2 u^2)}{\partial (N_1)} &= 0, \\
\frac{\partial (N_2 + c_1 u N_2 + c_2 u^2)}{\partial (N_2)} &= 1 + c_1 u.
\end{aligned}$$

The adjoint equation is backwards in time; note the format of the time derivative terms. Thus this system has final time and boundary conditions as follows:

$$
\begin{aligned}
\lambda_i(x,y,T) &= 0, \quad i = 1,2,\\
\lambda_2(0,y,t) &= \lambda_2(L,y,t),\\
\lambda_2(x,0,t) &= \lambda_2(x,L,t),\\
\frac{\partial \lambda_2}{\partial x}(0,y,t) &= \frac{\partial \lambda_2}{\partial x}(L,y,t),\\
\frac{\partial \lambda_2}{\partial y}(x,0,t) &= \frac{\partial \lambda_2}{\partial y}(x,L,t).
\end{aligned}
$$

From differentiating the objective functional with respect to the control at $u^\star$, we find the state and adjoint systems coupled with the optimal control characterization,

$$
u^\star(x,y,t) = \min\left\{M, \max\left\{0, \frac{N_2(x,y,t)(\lambda_2(x,y,t)-c_1)}{2c_2}\right\}\right\}. \tag{11}
$$

To understand this characterization, one can think of the λ_2 as the "shadow price" value of the N_2 population in achieving our goal, with $N_2(\lambda_2 - c_1)$ representing damage value of the rabbit population less the cost of implementing harvest (scaled by c_2). The state and adjoints systems with this characterization form the optimality system, which will be solved numerically in the next section for various cases of grass growth rates.

4 | NUMERICAL RESULTS

For computational purposes, we take a standard finite difference approximation to solve the PDEs in the optimality system and the forward-backward PDE system and $Q_{\Delta x} = \{(x_i, y_j) : x_i = i\Delta x, y_j = j\Delta x \ , i,j = 0,1, \dots, L/\Delta x\}$. The time interval $[0,T]$ is likewise discretized into $\{t_k : t_k = k\Delta t, k = 0,1, \dots, T/\Delta t\}$. The discretized forward system is given by

$$
\begin{aligned}
N_{1,i,j}^{k+1} &= N_{1,i,j}^{k} + \Delta t\left(g(i,j)(a_2 - N_{1,i,j}^{k}) - f(N_{1,i,j}^{k}, i,j)N_{2,i,j}^{k}\right),\\
N_{2,i,j}^{k+1} &= N_{2,i,j}^{k} + d\Delta t\frac{N_{2,i-1,j}^{k} + N_{2,i+1,j}^{k} + N_{2,i,j-1}^{k} + N_{2,i,j+1}^{k} - 4N_{2,i,j}^{k}}{\Delta x^2}\\
&\quad + b_1 f(N_{1,i,j}^{k}, i,j)N_{2,i,j}^{k} - b_2 N_{2,i,j}^{k} - u_{i,j}^{k} N_{2,i,j}^{k},
\end{aligned}
$$

with the adjoint or backward system approximation being

$$
\begin{aligned}
\lambda_{1,i,j}^{k-1} &= \lambda_{1,i,j}^{k} + \Delta t\left(-g(i,j)\lambda_{1,i,j}^{k} + b_1\frac{\partial f(N_{1,i,j}^{k})}{\partial N_1}N_{2,i,j}^{k}\lambda_{2,i,j}^{k} - \frac{\partial f(N_{1,i,j}^{k})}{\partial N_1}N_{2,i,j}^{k}\lambda_{1,i,j}^{k}\right),\\
\lambda_{2,i,j}^{k-1} &= \lambda_{2,i,j}^{k} + d\Delta t\frac{\lambda_{2,i-1,j}^{k} + \lambda_{2,i+1,j}^{k} + \lambda_{2,i,j-1}^{k} + \lambda_{2,i,j+1}^{k} - 4\lambda_{2,i,j}^{k}}{\Delta x^2}\\
&\quad + \Delta t\left(-f(N_{1,i,j}^{k})\lambda_{1,i,j}^{k} + b_1 f(N_{1,i,j}^{k})\lambda_{2,i,j}^{k} - b_2\lambda_{2,i,j}^{k} - u_{i,j}^{k}\lambda_{2,i,j}^{k} + 1 + c_1 u_{i,j}^{k}\right),
\end{aligned}
$$

with periodic boundary conditions. The discrete approximation for N_1 is

$$
N_{1,i,j}^{k} \approx \frac{1}{\Delta x^2}\int_{R_{i,j}} N_1(t_k, x, y)\, dxdy,
$$

with similar expressions for $N_2, \lambda_1, \lambda_2$, and with $R_{i,j} = \{(x,y) : |x - x_{i,j}| < \Delta x/2, |y - y_{i,j}| < \Delta x/2\}$. we implement the iterative forward-backward sweep algorithm.[19,54]

1. We solve the state N_1, N_2 system (3)–(4) forward in time,
2. With the current control and N_1, N_2 values, we solve the adjoint λ system (9)–(10) backward in time, and
3. With N_1, N_2 and λ_1, λ_2, we update the optimal control using the characterization (11).

The optimal control in the ODE system is implemented in the ABM by using $u^\star$ at times corresponding to the time steps in the ABM as a probability that any rabbit is harvested, and this result is that the fraction of the rabbits removed is approximately the harvest rate $u^\star$; thus at each time, the same harvest rate is applied to all rabbits across space. The optimal control in the PDE system is a function of space (x, y) and the resulting harvest control in the ABM for each rabbit depends on its location.

If the grass growth rate is constant, then as in Reference 38, the ODE approximation provides a reasonable control for the ABM. The spatial averages of the PDE approximation, integrating rabbit density and grass density over the domain, are indistinguishable from the ODE simulation results. But with heterogeneity in the grass growth rate, we have seen in Reference 38, that the controls applied in the ABM from the optimal controls of the approximation ODE system can be easily improved by including some spatial heterogeneity in the controls.

Using four cases of heterogeneity in the environment of our ABM model, we investigate the approximations by the ODE system and the PDE system and the corresponding optimal controls. The manner in which we experiment with heterogeneity is that we change the spatial distribution of the grass growth, maintaining a fixed geometric mean but allowing for non-uniformity across the environment. It is important to note here that the differential equation models contain parameters that do not directly translate from the parametric settings of the ABM. In order to determine the dynamical system parameters, we use standard least squares fitting of the solution of the ODE, with control set to zero, to the aggregate data of an ABM realization (also without control). The only parameters we carry from the ABM to the ODE are the known carrying capacity of 2025 cells of grass and the geometric mean growth rate of $0.02 = \left(\prod_{x,y} g(x, y)\right)^{(1/2025)}$. These parameters, as seen in Table 1, in some cases appropriately scaled to fit spatial-temporal averages, are then used in the PDE model to derive optimal controls for implementation in the ABM. The four cases increase in heterogeneity in the grass growth rate, and then we display the corresponding changes in the controls and objective functional values.

As the flowchart in Figure 1 indicates, the individual rabbits move according to random walks, and they consume grass, reproduce, and die as their energy levels change. The ABM dynamics will thus produce stochastic output for the abundance of rabbits over time. Thus, in our optimal control simulation experiments, we run the ABM for 100 realizations to estimate expected aggregate system dynamics and expected optimization objective functional values. We also provide ± 2 standard deviations of aggregate system dynamics to illustrate the variability arising from the ABMs. Since the optimal controls are computed from deterministic differential equation models, it is important to investigate how they operate in a stochastic environment.

4.1 | Case 1: Linearly varying grass growth rate

With grass growth rate of the form $g(x, y) = a + bx + cy$ in the ABM as seen in Figure 2, the spatial average of the harvest in the PDE system resembles the ODE control in Figure 3, but the PDE control is clearly different. To examine this feature more closely, in the 40 day time slice in Figure 4, the control from the PDE is becoming active with a small amount of

TABLE 1 Parameters for the NetLogo ABM

Parameter	Value
Movement cost	0.5
Grass energy	3
Energy for birth	8
Rabbit movement angle	$\pm 50°$
Initial rabbit population	200
Initial grass cells	500
Grid	45×45
Grass growth rate	Geometric mean of 0.02

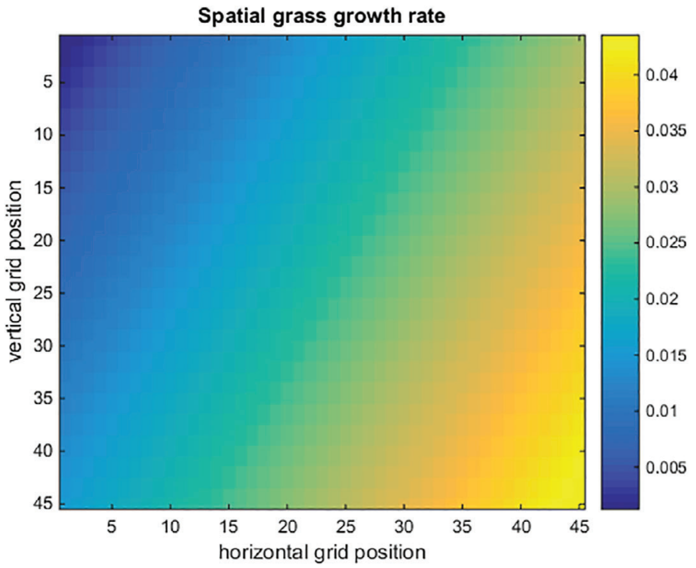

FIGURE 2 Case 1: Grass growth rate, linear varying

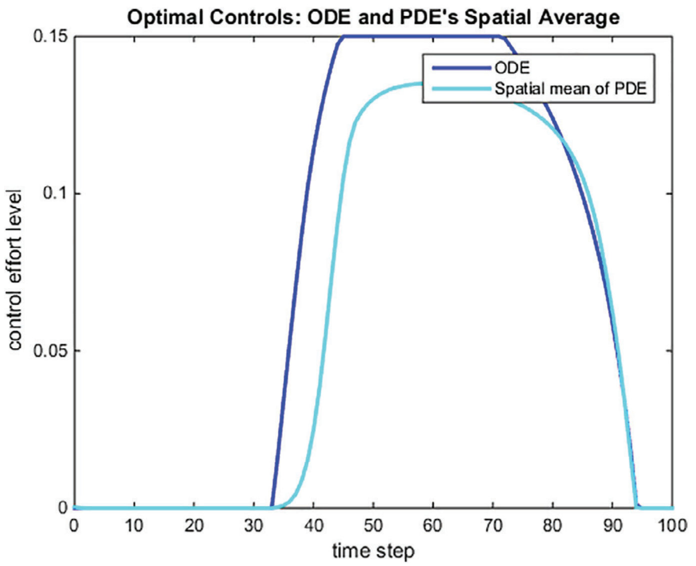

FIGURE 3 Case 1: For the linear grass growth rate, the spatial average of PDE control resembles ODE control but is no longer indistinguishable

heterogeneity. We compare the states averaged over time, from the ABM using the optimal controls from ODE system and from the PDE system; by running the ABM 100 times, those states are displayed with two standard deviations above and below the average ABM simulation results. The results in Figure 5 seem very close. To judge the difference, we record the average objective functional value J over 100 realizations. The PDE control is 13% better than the no control case, which is only slightly better than the corresponding 12% for the ODE control, as seen in Table 2. This particular heterogeneous growth rate varies smoothly with a gradual amount of change, with maximal difference of less than 0.045. Subsequent cases will consider larger and less smooth growth rate heterogeneities.

4.2 | Case 2: Sigmoid grass growth rate

With grass growth rate of the form $g(x, y) = a + \frac{b}{1+e^{cy}}$ in the ABM as seen in Figure 6, in the ABM, the approximations are not quite as good and we can see this reflected in the spatial averages of the controls from the ODE and PDE; those

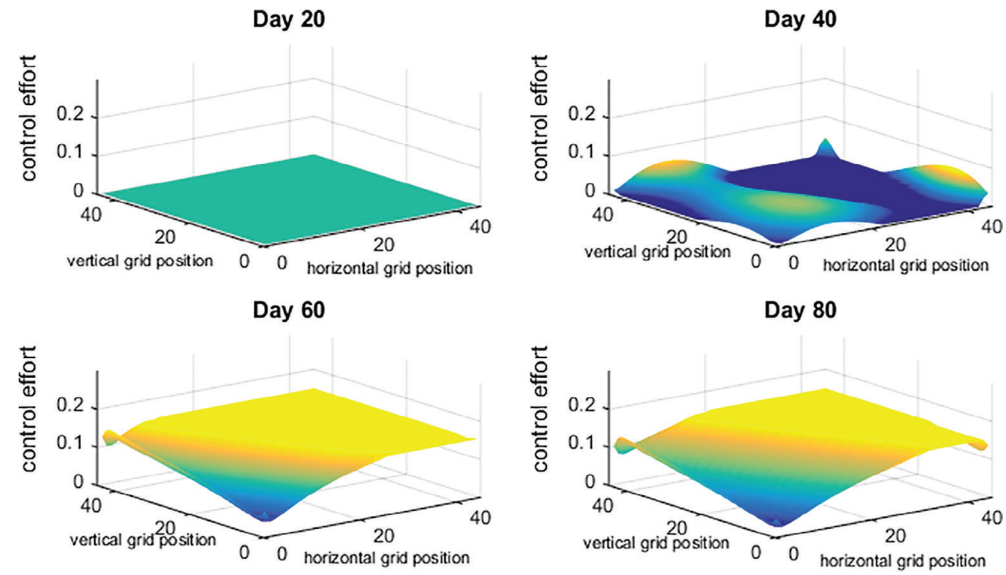

FIGURE 4 Case 1: For the linear grass growth rate, the control from the PDE starts to turn on at 40

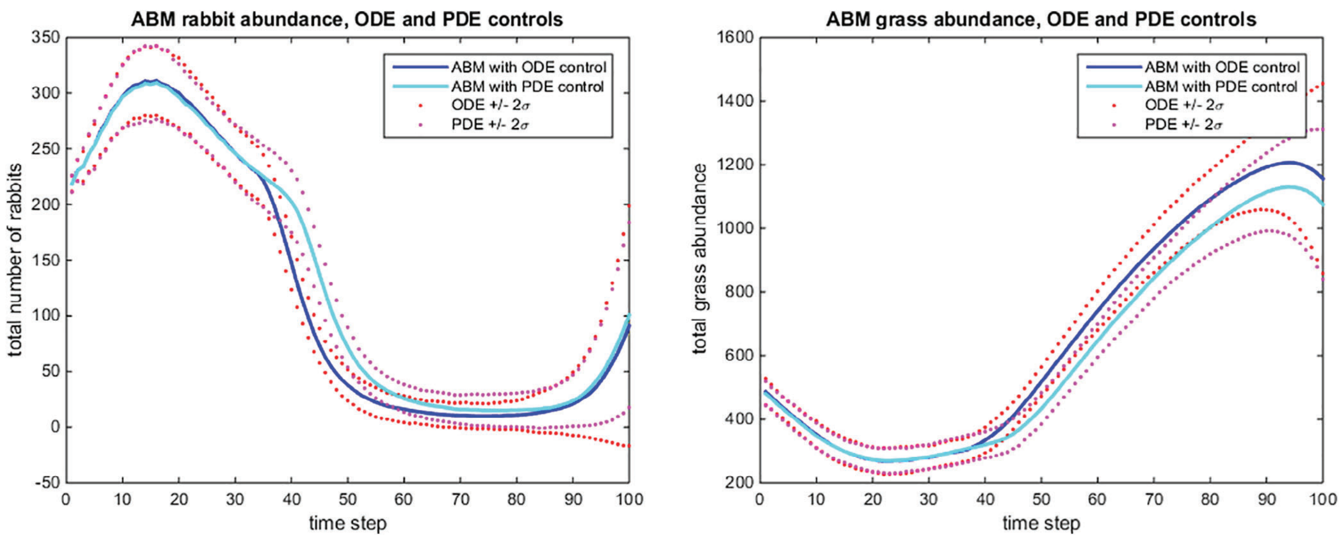

FIGURE 5 Case 1: For linear varying grass growth rate, rabbits and grass plots for ODE and PDE controls over 100 realizations

TABLE 2 Case 1: Comparison of objective functional values for linearly varying growth rate

Type of control	J_{avg}
No control	23,915
ODE control	20,947
PDE control	20,786

controls are quite different due to more heterogeneity in the space for the grass growth rate as seen in Figure 7. Looking more carefully at time slices of the control coming from the PDE in Figure 8, this control takes into account the spatial heterogeneity. Then comparing rabbits and grass populations over 100 realizations with ODE and PDE controls illustrates the difference, as seen in Figure 9. The optimal control for the ODEs make a quick transition from its lower bound to upper bound, while the optimal controls for the PDEs can manage the heterogeneity with a less drastic transition.

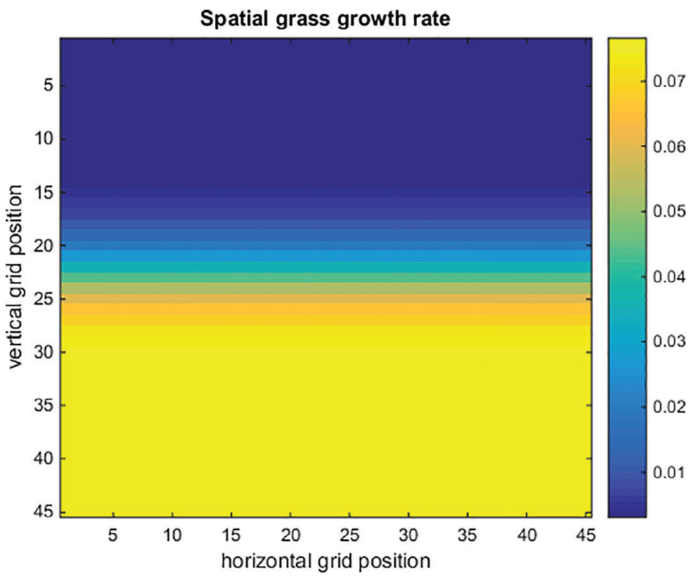

FIGURE 6 Case 2: Grass growth rate, sigmoid

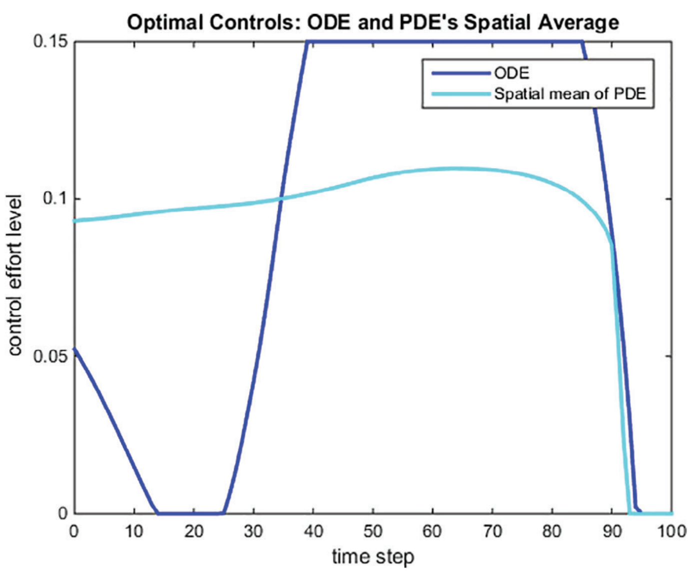

FIGURE 7 Case 2: For the sigmoid grass growth rate, the spatial average of PDE and ODE controls

Here the average J value for the PDE control are 30% better than for the no control case, as compared to 18% better for the ODE case. Table 3 details the outcomes of the objective.

4.3 | Case 3: Hot spot in growth rate

With grass growth rate of the form $g(x, y) = a + be^{((x-c)^4+(y-d)^4)}$ with geometric mean 0.02 in the ABM as seen in Figure 10, in the ABM, the approximation of the ABM by the PDE system is much better than that of ODE system as seen in Figure 11. As shown in Table 4, the average J value for ODE-based control was within 1% of the J value average of the uncontrolled ABM, while the PDE-based control brought a 22% reduction in J. The sharp discontinuity in the grass growth rate is accounted for in the PDE's spatial control, allowing differential pest management in the area where the pests are more likely to thrive.

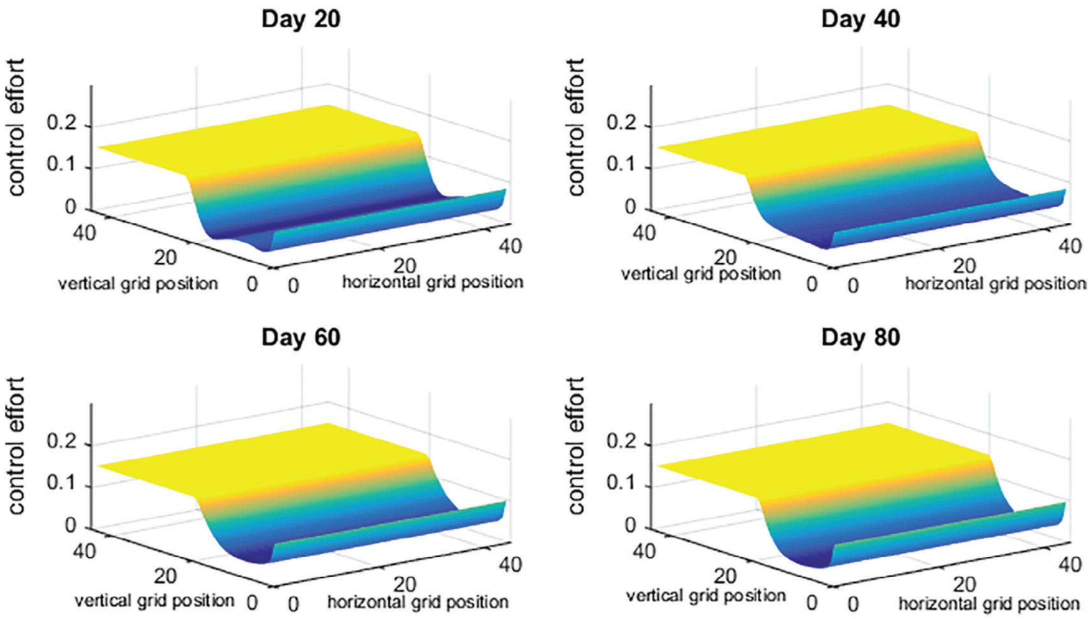

FIGURE 8 Case 2: For the sigmoid grass growth rate, PDE control shown over at 4 times

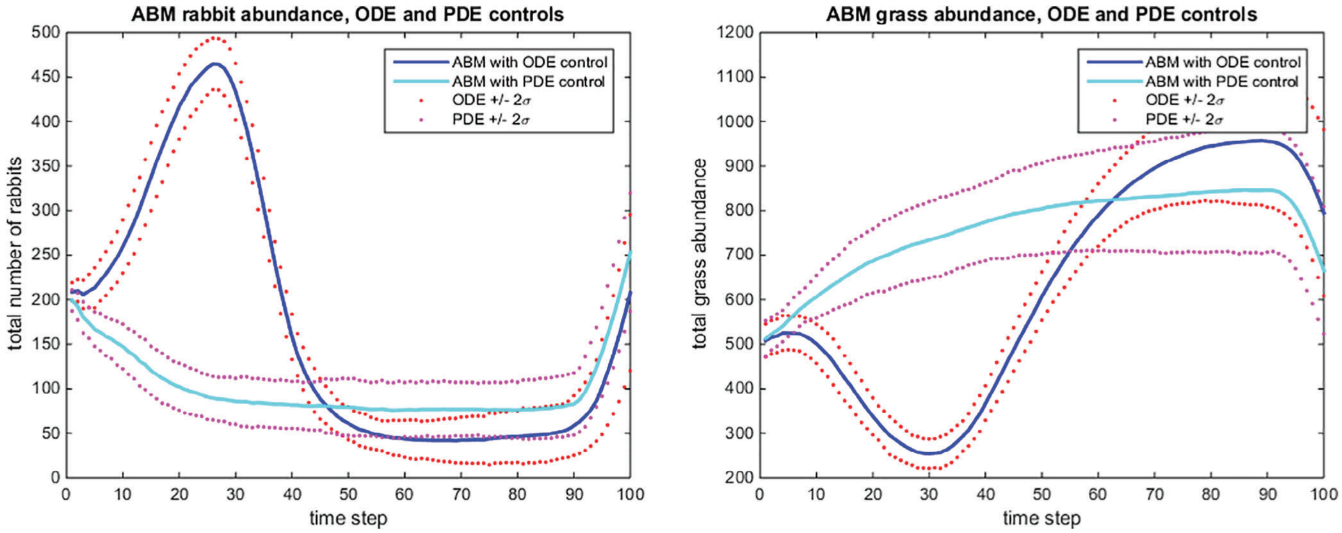

FIGURE 9 Case 2: With sigmoid grass growth rate, rabbits and grass plots with ODE and PDE controls over 100 realizations

TABLE 3 Case 2: Comparison of objective functional values for sigmoidal growth rate

Type of control	J_{avg}
No control	40,163
ODE control	32,840
PDE control	27,924

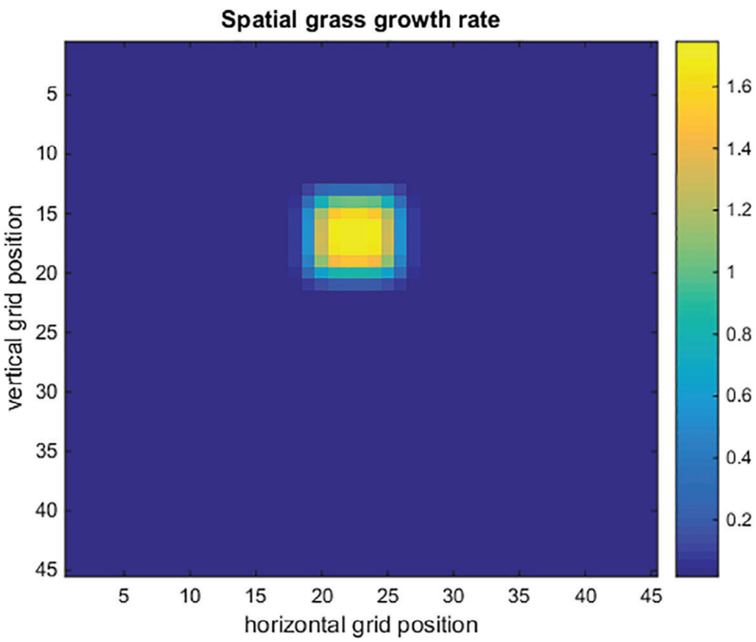

FIGURE 10 Case 3: Grass growth rate, one hot spot patch in the middle

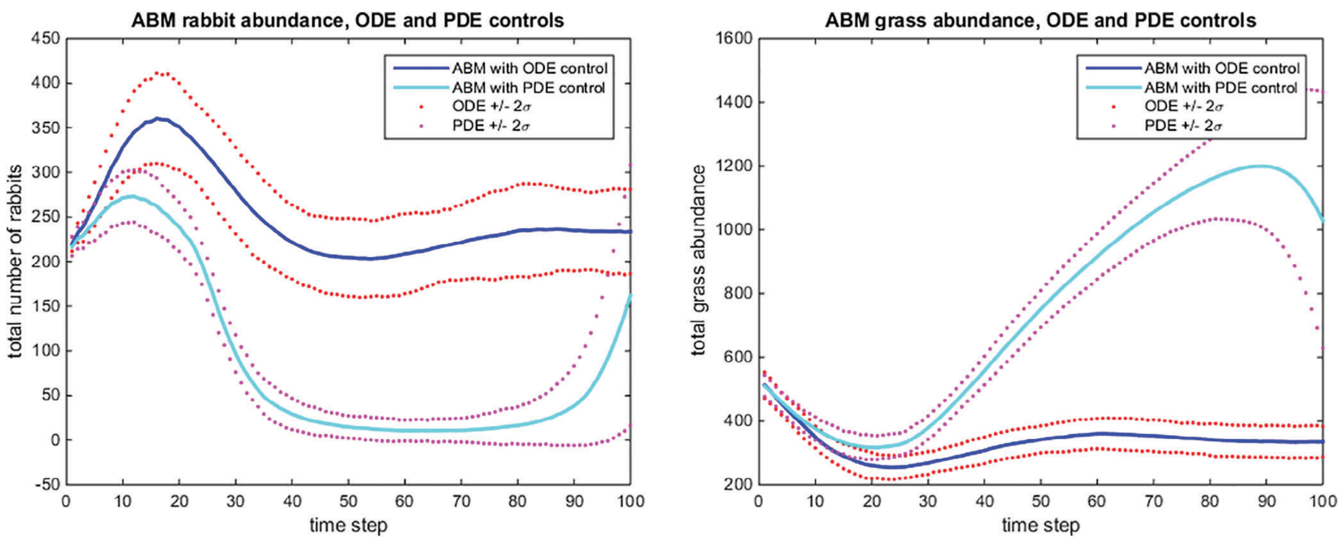

FIGURE 11 Case 3: With one hot spot, rabbits and grass plots with application of controls to ABM over 100 realizations

TABLE 4 Case 3: Comparison of objective functional values for growth rate with single hot spot

Type of control	J_{avg}
No control	25,268
ODE control	25,139
PDE control	19,571

4.4 | Case 4: Multiple hot spots in grass growth rate

With four hot spots in the grass growth rate, as shown in Figure 12, the ODE controls cannot capture any of this heterogeneity. The PDE controls do capture the effects of all four hot spots as in seen in Figures 13 and 14. In Figure 15, we see that the PDE-based control outperforms the ODE-based control in terms of aggregate rabbit and grass abundance. Similarly to Case 3, the averaged J values for the ODE-based control and the uncontrolled ABM are indistinguishable, while the PDE-based control results in a 28% reduction in average J from the uncontrolled ABM. Table 5 shows these J values. We emphasize here that in both Tables 4 and 5 the no control case and the ODE control case have about the same objective value. The PDE approach can tailor the control action to the heterogeneity of the environment and hence achieve improved performance.

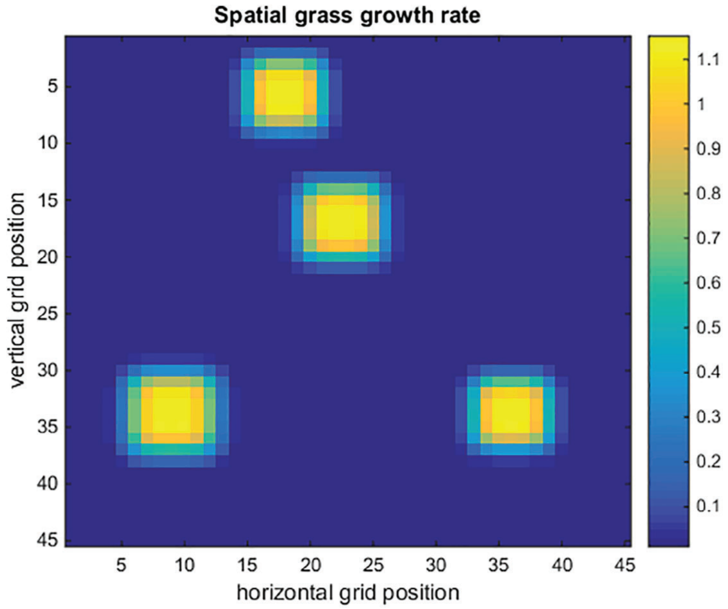

FIGURE 12 Case 4: Grass growth rate with multiple hot spots

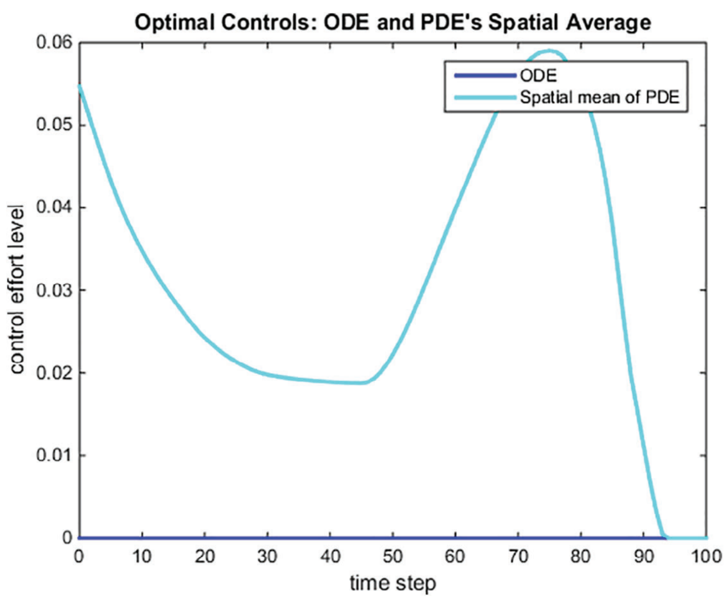

FIGURE 13 Case 4: With hot spots for grass growth rates, spatial average of PDE and ODE controls are shown

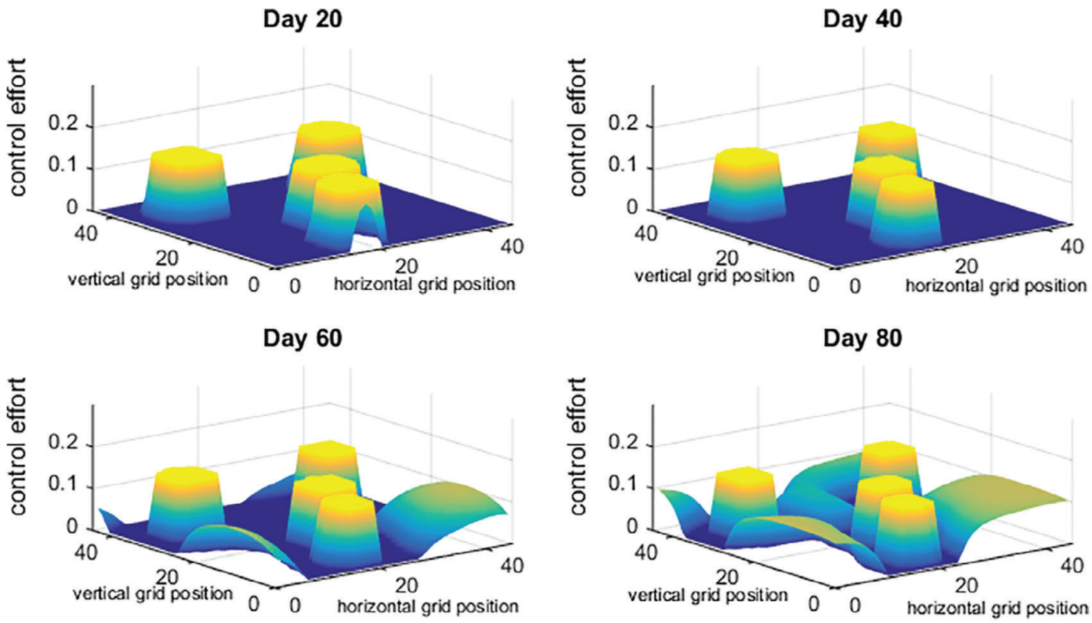

FIGURE 14 Case 4: With hot spots for grass growth rates, PDE control graphs are shown over at 4 times

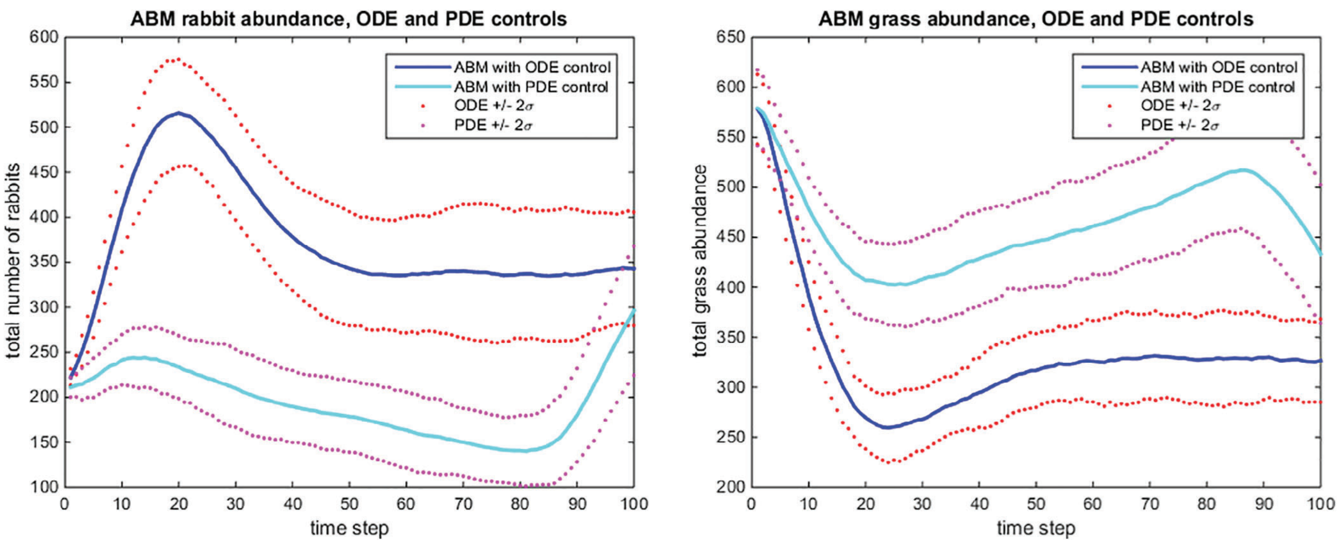

FIGURE 15 Case 4: With multiple hot spots for grass growth rates, rabbits and grass plots with application of controls to ABM over 100 realizations

TABLE 5 Case 4: Comparison of objective functional values for growth rate with multiple hot spots

Type of control	J_{avg}
No control	37,637
ODE control	37,375
PDE control	27,149

5 | CONCLUSIONS

Motivated by the need to choose management strategies for specific goals in ABMs, we show an approach to find appropriate controls using PDE approximations. We have not applied optimization directly to the ABM to determine these controls. However, the PDE controls do show consistent performance improvement over the ODE controls, which in turn reduce the cost of the pest population for the ABM. These controls may not be “optimal” in the ABM but should be more reasonable than most ad hoc controls. We have explained that the features of an ABM need to translate over to a PDE system for this approach. ABMs with a combination of random or directed movement may amenable to such approximations. The interactions between the environment and populations have to be understood in terms of functions of average levels.

As an illustration, we have approximated a simple ecological ABM that models diffusion and consumption by rabbits of a renewable grass resource,[36] with a reaction–diffusion PDE for the rabbit population coupled with a spatially distributed set of ODEs for the grass population. The heterogeneity of the grass growth presents some difficulties with the application of a simpler ODE model for control. We see that gradual changes of growth rates can be handled by the ODE with a modest increase in the objective functional average values (Figures 1–4) as seen in the similar objective functional average values for the no control, ODE control, and PDE control cases. But sharper changes in growth rate bring more significant penalties for the ODE controller and demonstrate the superiority of the PDE approach (Figures 5–13).

We note that the sharp boundaries between areas of low- and high-growth grass in Cases 2 and 3 could potentially be modeled by coupled systems of ODEs with appropriate continuity conditions across the boundaries of the resulting growth “subdomains.” Of course the difficulty with this approach is that each individual situation requires its own structure and code, while the PDE model merely needs to have as input the growth rate map.

We also note that our success in developing and implementing a PDE-based optimal control strategy for the rabbits-grass ABM should give some ideas for PDE approximation and corresponding controls for ABMs. As pointed out in Reference 30, challenges remain in optimization and control of ABMs. With the results of the current article, as well as the experience of Christley et al.[40] in controlling SugarScape using a PDE surrogate model, we expect that ABMs with relatively homogeneous agents that diffuse in space across a heterogeneous landscape would be most amenable to PDE approximation. In this article, the heterogeneity in the growth rate of the varying grass “environment” was considered. Additional features of the agents that vary in space and time may be included by adding additional underlying variables, like the “sugar” dependent variable in Reference 40.

But agents with complex features that would not fit easily into underlying continuous or simple discrete variables would cause problems for an approximation approach. Further work is needed in designing management strategies for ABMs, and some models may need approaches quite different from this approximation approach.

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DISCLAIMER

The views expressed in the present article are those of the authors and do not reflect the views or policies of the US Environmental Protection Agency (USEPA). Mention of trade names, products, or services does not convey and should not be interpreted as conveying official USEPA approval, endorsement, or recommendation.

DATA AVAILABILITY STATEMENT

Data sharing not applicable to this article as no datasets were generated or analyzed during the current study.

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APPENDIX

In this appendix, we sketch the idea of how to find the sensitivity equations and then show how to find the optimal control characterization.

The format of the terms and the boundary conditions from the adjoint system (9)–(10) come from the boundary conditions for the sensitivity system (7)–(8) and the property of adjoint operators, that is, formally, in an appropriate L^2 space. The sensitivity functions ψ_i (for $i = 1, 2$) represent directional derivatives of the states (rabbits, grass N_1, N_2) with respect to control u in the variation direction l. The sensitivity functions are found by limits of difference quotients, and their corresponding PDEs are formed formally by subtracting the PDEs (3)–(4) for the states with control $u + \epsilon l$ and the same PDEs but for the states with control u, and passing to the limit on difference quotients. *A priori* estimates for the quotients below justify the differentiation of the control-to-states map for state system,

$$\lim_{\epsilon \to 0} \frac{N_i(u + \epsilon l) - N_i(u)}{\epsilon} = \psi_i.$$

Then the sensitivity system can be derived to obtain PDEs (7)-(8) and corresponding initial and boundary conditions.

Using our adjoint and sensitivity systems, we can simplify the differentiation of J with respect to u at the optimal control to obtain the explicit characterization of an optimal control:

$$\begin{aligned} 0 &\le \lim_{\epsilon \to 0} \frac{J(u^\star + \epsilon l) - J(u^\star)}{\epsilon} \\ &= \int_{Q_T} [\psi_2 + c_1 u^\star \psi_2 + c_1 l N_2 + 2c_2 l u^\star] \end{aligned}$$

$$= \int_{Q_T} [< \psi_1, \psi_2 > \cdot < 0, 1 + c_1 u^\star > + c_1 l N_2 + 2 c_2 l u^\star]$$
$$= \int_{Q_T} [< \lambda_1, \lambda_2 > \cdot < 0, -l N_2 > + c_1 l N_2 + 2 c_2 l u^\star]$$
$$= \int_{Q_T} [-\lambda_2 l N_2 + c_1 l N_2 + 2 c_2 l u^\star]$$
$$= \int_{Q_T} [l(-\lambda_2 N_2 + c_1 N_2 + 2 c_2 u^\star)].$$

Through the properties of adjoint operators, one can convert from using the right hand side of the adjoint system to the right side of the sensitivity system. Note that l is an arbitrary variation of the control such that $u^\star + \epsilon l$ is in the control set U. We can conclude with a characterization (11) of an optimal control (using the last integral term above)

$$u^\star(x, y, t) = \min \left\{ M, \max \left\{ 0, \frac{N_2(x, y, t)(\lambda_2(x, y, t) - c_1)}{2c_2} \right\} \right\}.$$