An agent-based computational framework for simulation of competing hostile planet-wide populations

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Abstract

The increase in readily available computational power raises the possibility that robust agent-based modeling can play a productive role in the analysis of population dynamics. Accordingly, the objective of this work is to develop a robust agent-based computational framework to investigate the emergent structure of initially intermeshed hostile, competing, populations on a global scale. Specifically, we develop a model based on discrete entities (agents), each with their own interaction rules with their immediate neighbors, innate skill sets, reproductive rates, mobility and lifespans to represent a population. The global population is then allowed to evolve according to these local rules over many generations. *The biological systems-level applications are numerous, stemming from human conflict on the macroscale to microbes on the microscale.* Numerical examples are provided to illustrate the model construction and the results of such an approach.
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1. Introduction

The objective of this work is to develop a computationally-amenable agent-based model to investigate the behavior of competing populations by directly working at the individual level of interaction. The ubiquitous availability computational power raises the possibility that robust agent-based modeling can play a significant role in the analysis of population dynamics. The essential feature of the model is that discrete entities (agents) are used to represent a population, each with their own interaction rules with their immediate neighbors, skill sets, reproductive rates, mobility and lifespans. The global population is then allowed to evolve according to these local rules. *There are a large number of applications.* However, before proceeding with the construction of such an approach, it is useful to review basic concepts in the study of population dynamics, which dates back over two centuries to the work of Thomas Malthus. In 1798, he postulated that a population, denoted p, at a future time $(t + \Delta t)$, is related to the current population (at time t) by

$$p(t + \Delta t) = \lambda p(t), \tag{1.1}$$
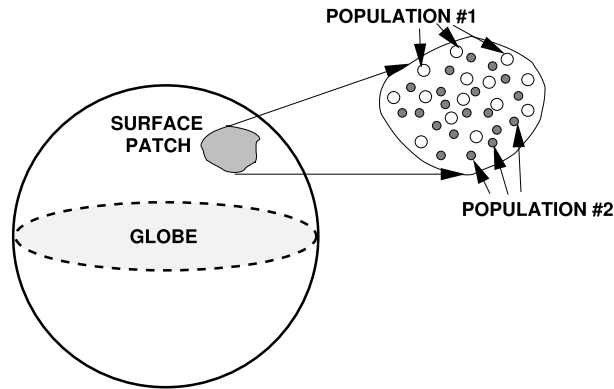
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Fig. 1. A model problem of a "planet" with two intermeshed different populations, which suddenly become hostile.

where $\lambda = 1 + b - d$, where $bp(t)$ is the number of births at time t and where $dp(t)$ is the number of deaths at time t. One may write

$$p(t + \Delta t) - p(t) = (\lambda - 1)p(t), \tag{1.2}$$

leading to, in the limit as $\Delta t \to 0$,

$$p(t) = p(0)e^{(\lambda-1)t} = p(0)e^{(b-d)t}, \tag{1.3}$$

provided that λ is constant.

Virtually all subsequent, more complex phenomenological continuum models build upon the Malthusian approach. For extensive reviews, see Murray [1]. Extensions of such models to describe competing populations, such as the Lotka–Volterra predator–prey relations, were developed in the 1920's. For example, consider an overly simplified, yet illustrative, phenomenological model for two interacting populations (p_1 and p_2, Fig. 1), given by

$$\dot{p}_1 = rp_2 - \tau p_1, \tag{1.4}$$

where r represents p_1's growth dependency on p_2, τ represents p_1's growth dependency on p_1 and

$$\dot{p}_2 = ap_1 - \gamma p_2, \tag{1.5}$$

where a represents p_2's growth dependency on p_1, γ represents p_2's growth dependency on p_2. For both populations to grow, we must have

$$\dot{p}_1 = rp_2 - \tau p_1 > 0 \tag{1.6}$$

and

$$\dot{p}_2 = ap_1 - \gamma p_2 > 0. \tag{1.7}$$

Thus there are four parameters, and clearly many possible combinations which can lead to growth, coexistence, extinction, etc.

With some difficulty, one can further extend these phenomenological approaches to simple spatial domains. These approaches require extensive, complex, discretization techniques and are of limited value for studies on population dynamics with underlying complex interaction between populations.[1] Such models have limited predictive capability and are computational expensive due to the extremely fine discretization needed to achieve tolerable numerical accuracy. Independent of the numerical difficulties, such modeling approaches attempt to develop continuum type field equations, by passing to the limit as $\Delta t \to 0$, $\Delta x \to 0$ make somewhat unrealistic assumptions in order to obtain tractable partial differential equations. At best, historically, most approaches apply asymptotic analysis to the resulting

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[1] As an example, the appendix provides more on such spatio-temporal "PDE-based" approaches, in particular for biological applications on the cellular/microbial level.
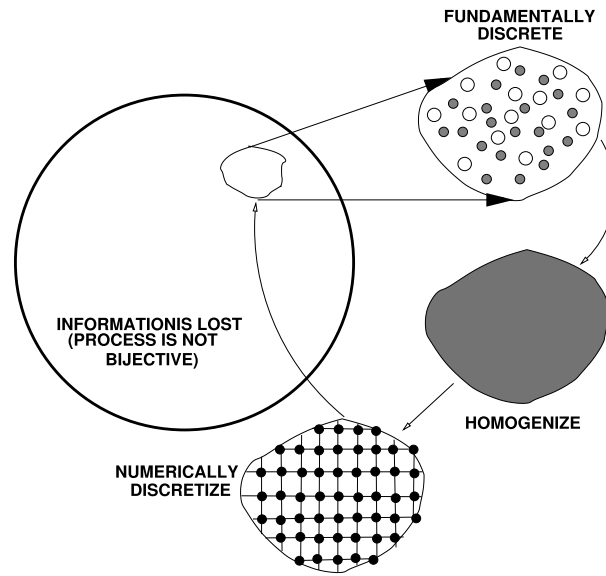
Fig. 2. The usual process of developing a continuum model from an inherently discrete system, which is then re-discretized.
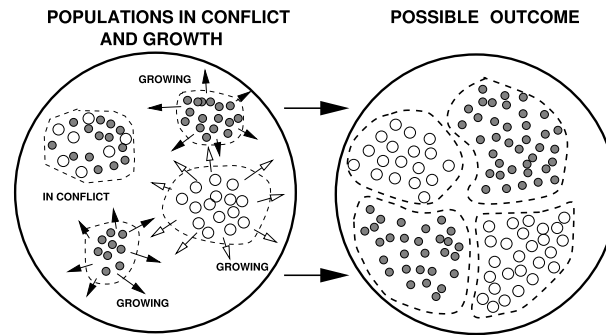

Fig. 3. Growing populations producing boundaries.

equations in order to extract some qualitative estimates of the model behavior. *Furthermore, one must question the process of first homogenizing a discrete population's characteristics to develop continuum models, resulting in partial differential equations and then discretizing them back again into nodal values. This process is not bijective, in other words, one does not recover the original discrete system (Fig. 2).* Also, because of the simplifying assumptions on interaction, births, age structuring, etc., that are typically made, in order to obtain tractable field equations, the resulting discrete equations are not as physically meaningful as the true discrete population interaction which is based on complex rule-driven processes that are not amenable to smooth (tractable) continuum representations. *Finally, in dealing with small populations, or populations which become quite small and heterogeneously dispersed during the time-history of interaction, the assumptions behind regularization techniques leading to continuum models, may be difficult to justify. This motivates the approach which we will present.*

2. Objectives of this work

As mentioned in the outset, the objective of this work is to develop a robust agent-based computational procedure to investigate the behavior of initially intermeshed hostile species populations by directly working at the rule-driven level of interaction. The global populations are then allowed to engage and to evolve according to the local rules. Generally, one should expect that (Fig. 3), if the two hostile groups were initially uniformly dispersed over some area, were of equal number and had similar characteristics: (1) both groups would suffer massive fatalities, leaving only well separated, "enclaves" of homogeneous species, where one group had locally dominated over the other, (2) the

enclaves would then grow, unrestrictedly, until they would eventually encounter one another again, resulting in "border conflicts" and (3) the growing, hostile, groups would develop well defined boundaries. Some of the key parameters are:

- The reproductive rates of the respective populations,
- The nominal life-spans of the respective populations,
- The "combat skills" of the respective populations and
- The mobility of the populations.

This approach allows one to study the spatio-temporal evolution of interacting populations, age-structuring and other demographic information. Furthermore, when coupled to a robust inverse algorithm one can determine optimal strategies for a desired demographic outcome, such as "parity points", i.e. multiple parameter sets which yield stable population coexistence.

Remarks. Although it is obvious to draw an analogy to human conflict at the macroscale, a problem of perhaps more concern is the microscale world. For example, during the last decade there has been a renewed interest in the study of epidemics, typified by the recent outbreaks of the Ebola and Zika viruses. Furthermore, interest has now grown in the area of astro-biology, specifically concerned with so-called "forward-contamination", defined as Earth-based microbes infesting celestial bodies, carried by Earth-based spacecraft. Safeguards against contamination are driven by the COSPAR regulations (Committee on Space Research) and the various outer space treaties signed over the last 50 years. Forward-contamination has become a timely issue since the recent discovery of water on Mars, as well as on the moons of Saturn and Jupiter. For example, it has been reported over the last few years that on Mars, water in liquid state could form seasonally on the surface where snow has been deposited on soils with saline content (Martinez and Renno [2]). This is critical, since terrestrial bacteria can grow in brines. Furthermore, because the lack of a magnetic field and minimal atmospheric shielding (the Martian overhead airmass is 16 g/cm^2 instead of the terrestrial 1000 g/cm^2), there are intense radiation sources reaching Mars (100 times that of Earth), however, there still exist a wide range of microbes which can survive. Additionally, while it would be difficult to maintain life directly on the surface of Mars, life in the subsurface could be possible. Space agencies such as NASA have long reported that *spores of Bacillus subjected to years of the vacuum of space and cosmic and extraterrestrial solar radiation, as well as temperature fluctuations, can survive if they are somewhat shielded by the exterior of a spacecraft and then deposited into the immediate subsurface upon landing.* Of course, reverse (backward) contamination is perhaps of more concern, namely if astronauts become contaminated it is possible they could bring these potential pathogens back to Earth. Thus, while there exist test protocols to guard against such contamination, for example plans developed by the NASA Planetary Protection Office, concerns remain. We refer the reader to Beaty [3], Fischer et al. [4], Martinez and Renno [2], Summons et al. [5], Michalski [6] and Debus [7] for details.

3. Direct agent-based interaction models

We now construct a model problem based on discrete rule-driven interaction between agents of two populations. One can consider an agent as an individual or a small group of individuals (a "meta-person").

3.1. Rules of engagement

Consider the following construction, for the "rules of engagement" for two hostile populations, which are either in close proximity to one another or intermeshed (Fig. 4):

- If two agents of the opposing populations, denoted (1) and (2), come within a certain conflict distance,

$$\|\boldsymbol{r}_i^{(1)} - \boldsymbol{r}_j^{(2)}\| \le d_{ij}^{(1-2)}, \tag{3.1}$$

  then two are said to engage in a "local" conflict.
- The agents alert all "support agents" of their respective populations, within a certain "support distance",

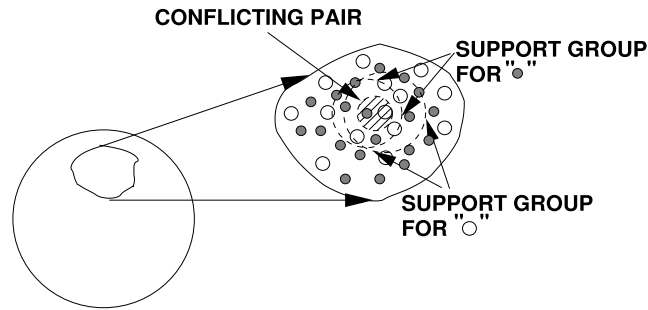$$\|\boldsymbol{r}_i^{(1)} - \boldsymbol{r}_j^{(1)}\| \le s_{ij}^{(1-1)}, \tag{3.2}$$

Fig. 4. The interaction between two groups.

and

$$\|\boldsymbol{r}_i^{(2)} - \boldsymbol{r}_j^{(2)}\| \leq s_{ij}^{(2-2)}, \tag{3.3}$$

in order to aid in the local conflict.

- The "combat skills" of the two populations may be different. Consider a certain number of the agents (subgroup) of population (1), p_1, which are engaged in a local conflict and (2), p_2, which are engaged in the same local conflict. The percentage of each group in the local conflict are

$$\phi_1 = \frac{p_1}{p_1 + p_2} \quad \text{and} \quad \phi_2 = \frac{p_2}{p_1 + p_2}. \tag{3.4}$$

Consider the following rules for victory:
1. If $w^{(1)}\phi^{(1)} = w^{(2)}\phi^{(2)}$ then all agents of both populations, that are involved in the local conflict, perish.
2. If $w^{(1)}\phi^{(1)} > w^{(2)}\phi^{(2)}$ then all agents of population (2) perish and $min(p_1, (w^{(1)}\phi^{(1)} - w^{(2)}\phi^{(2)})(p_1 + p_2))$ of population (1) survive.
3. If $w^{(1)}\phi^{(1)} < w^{(2)}\phi^{(2)}$ then all agents of population (1) perish and $min(p_2, (w^{(2)}\phi^{(2)} - w^{(1)}\phi^{(1)})(p_1 + p_2))$ of population (2) survive.

- An agent of either population cannot participate in two local conflicts simultaneously.
- Once an agent of either population perishes, it cannot participate in any further conflicts.
- If an agent of a population survives beyond a certain number of conflict periods then it produces offspring, and then perishes. The offspring are placed randomly within an "offspring" radius, centered at the spatial location of the parent. The number of children possible that an individual can have, at maturity, is given by (it is a gender-neutral rule)

$$\textit{offspring} = \text{integer}(\phi \times M) \tag{3.5}$$

where $0 \leq \phi \leq 1$ is a random number and where M is the maximum. The function "integer" extracts the nearest integer from $(\phi \times M)$. After giving birth to the offspring once, the agent cannot have offspring again.

The development of a continuum approximation and corresponding rediscretization, would be extremely tedious, if not impossible. The relative ease at which one can generate two populations, and step them through several conflict periods is rather obvious. *This is straightforward to implement.*

3.2. Algorithm

The algorithm is as follows:

- STEP 1: Select:
- (a) The initial number of agents in the populations.
- (b) The conflict distance.
- (c) The support distances for populations.
- (d) The local conflict manpower weight for the populations.
- (e) The age to maturity for an agent for reproduction.
- (f) The lifespan of an agent in each population.

- (g) The total simulation time, T.
- (h) The conflict cycle time $= \delta t^*$. (The number of conflict rounds is $\frac{T}{\delta t^*}$.)
- (i) The maximum number of children for an agent in each population.
- STEP 2: Generate the initial population locations on the globe.
- STEP 3: For each population, loop over each agent, and check if there is an agent from the other population in the conflict radius. If so, according to the "rules of engagement" in the previous section, compute the interaction of the pair with their respective support agents who are within their respective support radii.
- STEP 4: Compute the survivors and deaths of the existing agents for the conflict period.
- STEP 5: Compute the births of new agents and their locations according to the placement formula in the previous section for the conflict period.
- STEP 6: Update the ages of the entire population and compute any natural deaths.
- STEP 7: Repeat STEPS 2–6 for the next conflict period until the overall simulation time is complete.

4. A model problem

4.1. Parameter selection

As an example, consider two populations, each starting with 2000 agents (Fig. 5). We consider two main cases:

- Case 1 (Fig. 5): the populations are uniformly mixed across the globe, then become mutually hostile and mobile and
- Case 2 (Fig. 6): the populations are uniformly mixed in an isolated zone then become mutually hostile and mobile.

Consider the following parameters:

- The initial number of agents in population 1: $p_1(t = 0) = 2000$.
- The initial number of agents in population 1: $p_2(t = 0) = 2000$.
- Globe radius, $R = 1$.
- The conflict distance: $d_{ij}^{(1-2)} = 0.05R$.
- The support distance for population 1: $s_{ij}^{(1-1)} = 0.025R$.
- The support distance for population 2: $s_{ij}^{(2-2)} = 0.025R$.
- The local conflict manpower weight for population 1: $w^{(1)} = 0.5$.
- The local conflict manpower weight for population 2: $w^{(2)} = 0.5$.
- The number of conflict periods until viable offspring are produced for an agent in population $1 = 3$.
- The number of conflict periods until viable offspring are produced for an agent in population $2 = 3$.
- The number of conflict periods for the lifespan of an agent in population $1 = 15$.
- The number of conflict periods for the lifespan of an agent in population $2 = 15$.
- The maximum number of children for an agent in population $1 = 6$.
- The maximum number of children for an agent in population $2 = 6$.
- The age to maturity of an agent for reproduction in population $1 = 3$.
- The age to maturity of an agent for reproduction in population $2 = 3$.
- Total simulation time: $T = 70$.
- Conflict cycle time $= \delta t^* = 0.1$.
- The random location of each offspring is computed by $r^{parent} + (v^{rand} + v^{mean}) \times \delta t^*$, which is then projected back onto the sphere. In this case, we have chosen each component of v^{rand} to be between $-0.1 \leq v^{rand} \leq 0.1$ and $\|v^{mean}\| = 0$.
- For the second example (Fig. 8) of two populations initially isolated and intermeshed in a "patch", both populations are placed at random on the globe, but with the following restrictions at $t = 0$:

$$-0.5R = r_{2xi}^- \leq r_{2xi}^- \leq r_{2xi}^+ = 0.5R \tag{4.1}$$

and

$$-0.5R = r_{3xi}^- \leq r_{3xi}^- \leq r_{3xi}^+ = 0.5R, \tag{4.2}$$

where r_{1x} is allowed to be arbitrary, with the only restriction being that the agent resides on the globe surface.
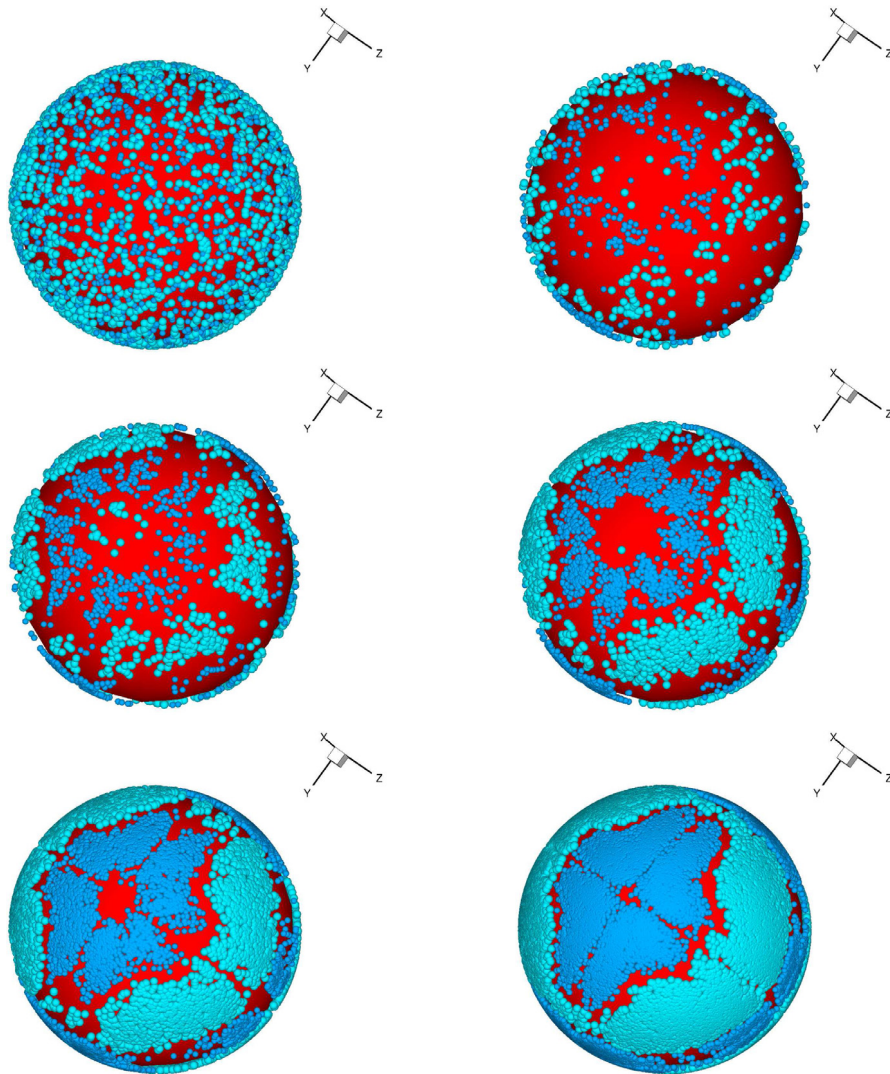
Fig. 5. Case 1-globally-intermeshed: Starting from left to right and top to bottom, the progressive growth of two *initially* intermeshed populations. Shown are after 1, 10, 20, 30, 40, 50 conflict periods. The system progresses from (1) intermeshed to (2) small enclaves to (3) larger homogeneous populations with stable border conflicts.

4.2. Observations

- Fig. 5 illustrates the overall growth of the populations for Case 1. It indicates that when the populations are strongly intermeshed, initially almost all perish. Fig. 6 illustrates the similar behavior for Case 2, with a more pronounced initial die-off due to closer proximity for conflict.

- Afterwards, the populations grow, however, with distinct boundaries evolving between them.

- There are two main types of boundaries: (1) Boundaries between growing hostile populations where neither population has a clear advantage and (2) Boundaries between growing hostile populations where eventually one is squeezed between two populations, and two like populations meet and eventually merge together.

- Typically, for such systems with a finite number of agents, there will be slight variations in the behavior for different random starting configurations. This is discussed further later. However, if one wished to extract some overall statistical behavior, a number of different starting realizations must be tested and then the overall results averaged.

- In Figs. 7 and 8, the average age and the population size are depicted. Classical models usually incorporate so-called "Leslie Matrices" (Leslie [8]), which stagger the growth rate process over the population based upon age.
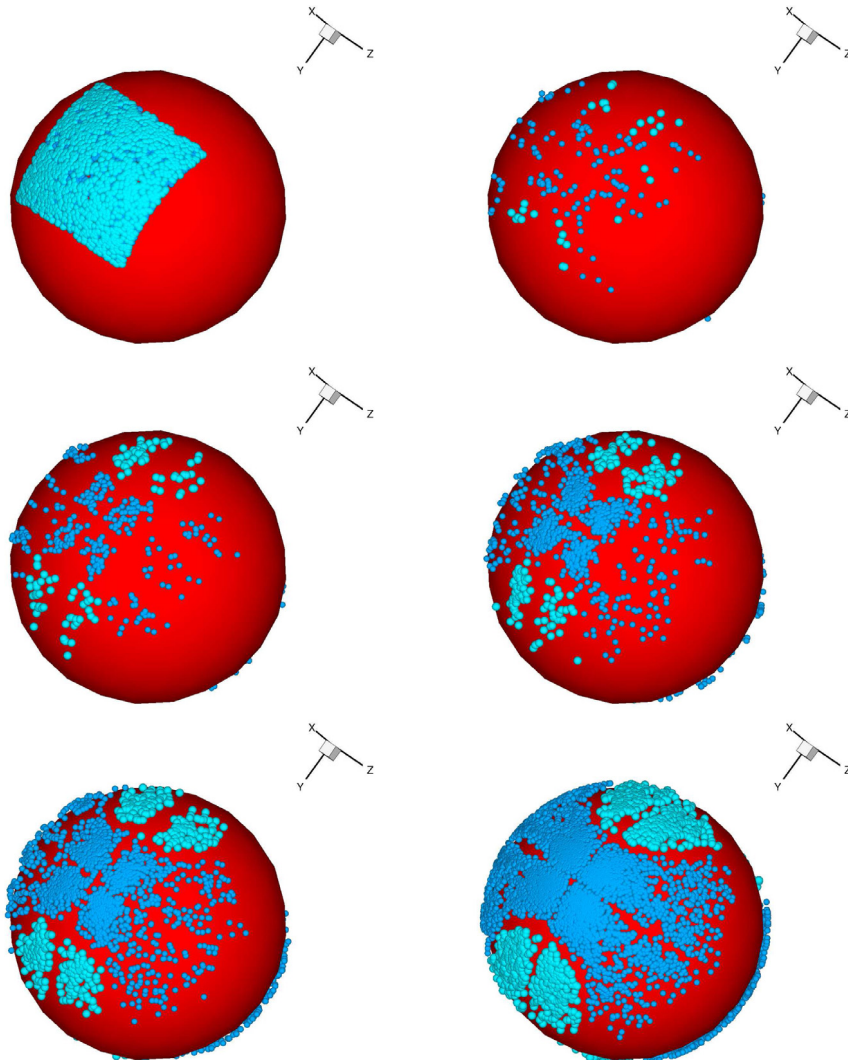
Fig. 6. Case 2-initially-isolated and intermeshed: Starting from left to right and top to bottom, the progressive growth of two *initially* intermeshed populations. Shown are after 1, 10, 20, 30, 40, 50 conflict periods. The system progresses from (1) intermeshed to (2) small enclaves to (3) larger homogeneous populations with stable border conflicts.

This is complex to incorporate in classical models. *However, in the discrete agent-based method pursued in the paper, age-structuring is produced automatically.* The total population growth is oscillatory behavior due to the interaction between populations. This effect can also be qualitatively predicted by classical analytical methods. For the coupled model system (Eqs. (1.4) and (1.5)), by differentiating and substituting we obtain:

$$\frac{d^2 p_1}{dt^2} + (\gamma + \tau)\frac{dp_1}{dt} + (\tau\gamma - ra)p_1 = 0 \tag{4.3}$$

and

$$\frac{d^2 p_2}{dt^2} + (\gamma + \tau)\frac{dp_2}{dt} + (\tau\gamma - ra)p_2 = 0. \tag{4.4}$$

Thus, if the initial conditions are the same, the solutions are identical for this simple model. Let us put the equation in classical form:

$$\ddot{p}_1 + 2\zeta\omega_n\dot{p}_1 + \omega_n^2 p_1 = f(t), \tag{4.5}$$
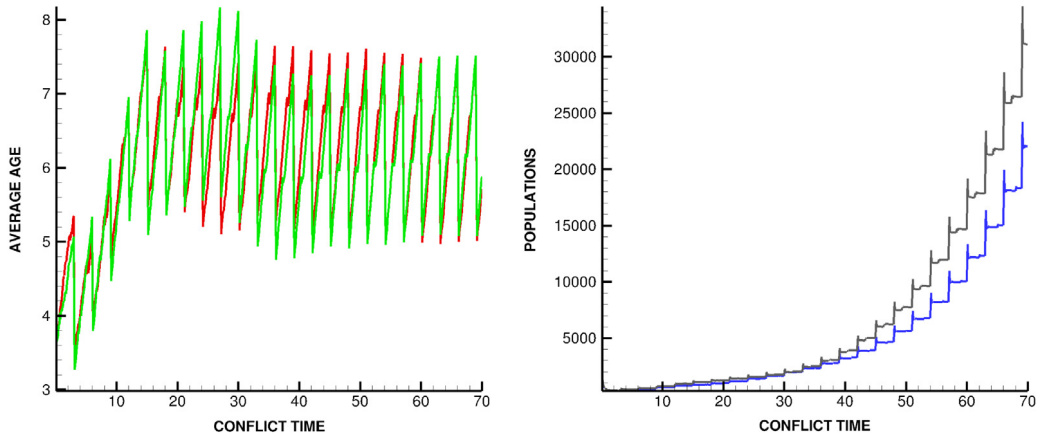
Fig. 7. Case 1-globally-intermeshed. Left: The average age of each population. Right: The total population growth. Notice the oscillatory behavior due to the interaction between populations, as qualitatively predicted by the analytical models.
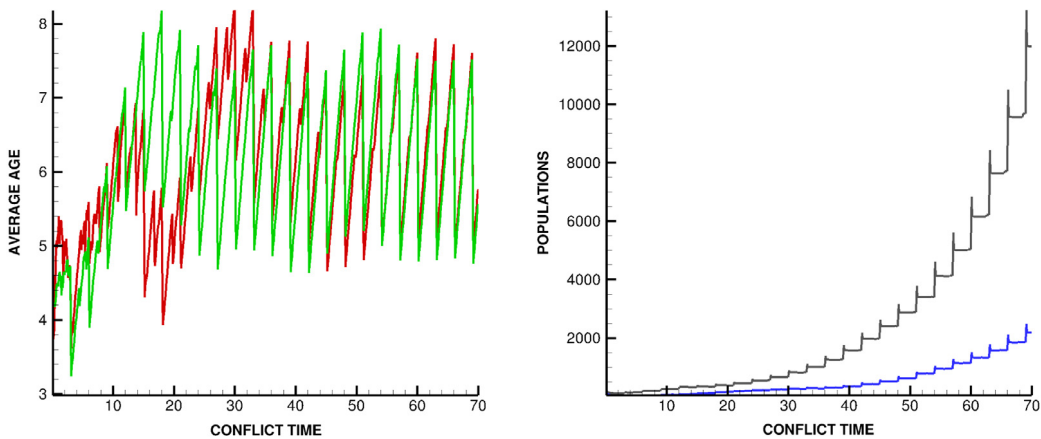

Fig. 8. Case 2-initially-isolated and intermeshed. Left: The average age of each population. Right: The total population growth. Notice the oscillatory behavior due to the interaction between populations, as qualitatively predicted by the analytical models.

where, assuming $\tau\gamma - ra \geq 0$ and $\tau + \gamma \geq 0$

$$\omega_n = \sqrt{\tau\gamma - ra} \tag{4.6}$$

and

$$\zeta = \frac{1}{2}\frac{(\gamma + \tau)}{\sqrt{\tau\gamma - ra}}. \tag{4.7}$$

This is the form of a forced damped oscillator. Depending on the value of ζ, the solution will have one of three distinct types of behavior: (1) $\zeta > 1$, overdamped, leading to no oscillation, where the value of p_1 approaches equilibrium for large values of time, (2) $\zeta = 1$, critically damped, leading to no oscillation, where the value of p_1 approaches equilibrium for large values of time, however faster than the overdamped solution and (3) $\zeta < 1$, underdamped, leading to damped oscillation, where the value of p_1 approaches equilibrium for large values of time, in an oscillatory fashion. In the case considered here, the populations would continue to grow, albeit in an oscillatory manner, unless they were resource limited.

Remark. We note that, if desired, incorporation of "forbidden regions" i.e. "uninhabitable zones" within the domain is relatively easily to enforce by checking at each time step whether an individual has entered such an area. If so, then the individual is moved back outside, and a new position is recalculated with a different trajectory.

5. Conclusions and extensions

The utility of the presented computational approach is that one can trivially modify the "rules of engagement", population sizes, reproduction rates, etc., *and provide quantitative spatial and temporal information.* Clearly, *such a computational technique is easy to implement, and it is no extra effort to increase the number of population character parameters.* For example, one could include a so-called epidemic effect, which is a relevant issue of concern for backward contamination. In classical models, the most basic type of epidemic is a so-called "S-I-R" model, which identifies three classes of individuals (Murray [1]):

- (1): S = "Susceptible", that can contract diseases,
- (2): I = "Infected", that can transmit the disease and who are infected and
- (3): R = "Removed" (dead), where the typical assumptions include: (a) the gain in the infected class is at a rate proportional to the number of infected and susceptible, that is $k_1 S I$, $k_1 > 0$ (b) the rate of removal of the infected is proportional to the number of infected, $k_2 I$, $k_2 > 0$ and (c) the incubation period is short enough to be negligible.
- (4) In addition, if it is assumed that the various classes are uniformly mixed:
- (I) $\frac{dS}{dt} = -k_1 S I$,
- (II) $\frac{dI}{dt} = k_1 S I - k_2 I$ and
- (III) $\frac{dR}{dt} = k_2 I$.
- Adding all of the populations together,

$$\frac{dS}{dt} + \frac{dI}{dt} + \frac{dR}{dt} = 0, \tag{5.1}$$

where $S + I + R = p$ (p being the total population), $S(0) = S_o > 0$, $I(0) = I_o > 0$ and $R(0) = 0$, $k_1 > 0$ is the infection rate and $k_2 > 0$ is the death rate.

A crucial question is, given k_1, k_2, S_o and I_o, whether the infection will spread or not, and if it does, how it develops with time, and crucially when it starts to decline. Clearly, from $\frac{dI}{dt} = k_1 S I - k_2 I$, we have

$$\left.\frac{dI}{dt}\right|_{t=0} = I_o(r S_o - k_2), \tag{5.2}$$

where $\frac{dI}{dt}|_{t=0} > 0$ if $S_o > k_1/k_2$ and $\frac{dI}{dt}|_{t=0} < 0$ if $S_o < k_1/k_2$. If $S_o < k_1/k_2$, then $\frac{dS}{dt} = -k_1 S I$ implies $\frac{dS}{dt} < 0$ and $\frac{dI}{dt}|_{t=0} = I_o(r S_o - k_2) < 0$ for all $t \geq 0$, in which case $I_0 > I(t) \to 0$ as $t \to \infty$, and so the infection dies out; that is no epidemic can occur. On the other hand, if $S_o > k_1/k_2$, then $I(t)$ initially increases, and we have an "epidemic". The term "epidemic" means that $I(t) > I_o$ for some time $t > 0$. Thus, in summary, we have a "threshold" phenomenon:

- (a) If $S_0 > S^* = k_1/k_2$ an epidemic will occur,
- (b) If $S_0 < S^* = k_1/k_2$ no epidemic will occur.

The parameter k_1/k_2 is sometimes called the relative removal rate, while its reciprocal is called the infectious contact rate. Using agent based methods, more complex features, such as spread of disease/epidemics and emergent age-structuring of populations, can easily be incorporated. For example, if a susceptible individual is near an infected one, then they become infected. The lifespan of an infected person, after contraction of the disease, is T_i. In the appendix, an algorithm for systematic parameter determination, based on genetic algorithms, is provided.

Another extension to the overall modeling is to provide more detail on the movement of the agents. In the model described in the body of the paper, the offspring were placed around the spatial location of the parent. However, we could have allowed for them (as well as the parents) to move according to more physical rules. For example, swarm-like movement to avoid predators is often advantageous for biological groups. This behavior is often decentralized, which reduces the group vulnerability, and makes the decision making is relatively simple and rapid for each individual. The overall behavior is however quite sophisticated. Modeling of this sort dates back, at least, to Breder (1952) [9]. The usual approach to modeling such systems is to use a combination of short-range and long-range interaction forces (Gazi and Passino [10], Bender and Fenton [11], Kennedy and Eberhart [12] and Zohdi [13,14]). Early approaches that rely on decentralized organization can be found in Beni [15], Brooks [16], Dudek et al. [17], Cao et al. [18] and Liu and Passino [19]. However, there are alternative rule-driven swarms where the interaction is

not governed by forces, but by proximal instructions such as: (a) if a fellow swarm agent gets close to me, attempt to retreat as far as possible, (b) follow the leader, (c) stay in clusters, etc. For example, ant colonies (Bonabeau et al., [20]) exhibit foraging-type behavior, in addition to the trail-laying-trail-following mechanism for finding food sources, where they deposit a chemical substance, called *pheromone*, which decays over time. The fellow swarm agents detect paths with a high pheromone concentration (where the food source is highly concentrated) and follow them (Kennedy and Eberhart [12] and Bonabeau et al. [20], Dorigo et al., [21], Bonabeau et al. [20], Bonabeau et al. [22] and Fiorelli et al. [23]). For certain swarms, the "visual field" of the individual agents may play a significant role, while in others, this is a non-issue, for example if the agents are robots or UAVs where the communication is electronic. Still, in some systems, agents interact with a specific set of swarm agents, *regardless* of whether they are far away (Feder [24]). For example, based on a number of careful observations, Starlings (Sturnus vulgaris), Ballerini et al. [25] conclude, that such birds communicate with a certain number of birds surrounding it, *regardless of the distance away*, attributing this to a perceptual limit in of the number of objects that they can track (the sixth or seventh nearest neighbor). These issues are currently under investigation by the author.

Acknowledgments

Appendix A. Rule parameter identification

As with all mathematical models, the identification of parameters is important. Typically, for the class of problems considered in this work, the corresponding formulations depend in a nonconvex and nondifferentiable manner on the system parameters. Classical gradient-based deterministic optimization techniques are not robust, due to difficulties with objective function nonconvexity and nondifferentiability. Classical gradient-based algorithms are likely to converge only toward a local minimum of the objective functional if an accurate initial guess to the global minimum is not provided. Also, usually it is extremely difficult to construct an initial guess that lies within the (global) convergence radius of a gradient-based method. These difficulties can be circumvented by the use of a certain class of nonderivative search methods, usually termed "genetic" algorithms (GA), before applying gradient-based schemes. Genetic algorithms are search methods based on the principles of natural selection, employing concepts of species evolution, such as reproduction, mutation and crossover. Implementation typically involves a randomly generated population of fixed-length elemental strings, "genetic information", each of which represents a specific choice of system parameters. The population of individuals undergo "mating sequences" and other biologically-inspired events in order to find promising regions of the search space. There are a variety of such methods, which employ concepts of species evolution, such as reproduction, mutation and crossover. Such methods primarily stem from the work of John Holland (Holland [26]). For reviews of such methods, see, for example, Goldberg [27], Davis [28], Onwubiko [29], Kennedy and Eberhart [12] and Goldberg and Deb [30].

Adopting the approaches found in Zohdi [13], a genetic algorithm has been developed to treat nonconvex inverse problems involving various aspects of multiobject mechanics. The central idea is that the system parameters form a genetic string and a survival of the fittest algorithm is applied to a population of such strings. The overall process is (a) A population (S agents in total) of different *parameter sets* are generated at random within the parameter space, each represented by a ("genetic") string of the system (N) parameters, (b) The performance of each parameter set is tested, (c) The parameter sets are ranked from top to bottom according to their performance, (d) The best parameter sets (parents) are mated pairwise producing two offspring (children), i.e. each best pair exchanges information by taking random convex combinations of the parameter set components of the parents' genetic strings and (e) The worst performing genetic strings are eliminated, new replacement parameter sets (genetic strings) are introduced into the remaining population of best performing genetic strings and the process (a–e) is then repeated. The term "fitness" of a genetic string is used to indicate the value of the objective function. The most fit genetic string is the one with the smallest objective function. The retention of the top fit genetic strings from a previous optimization generation (parents) is critical, since if the objective functions are highly nonconvex (the present case), there exists a clear possibility that the inferior offspring will replace superior parents. When the top parents are retained, the minimization of the cost function is guaranteed to be monotone (guaranteed improvement) with increasing optimization generations.

There is no guarantee of successive improvement if the top parents are not retained, even though nonretention of parents allows more new genetic strings to be evaluated in the next optimization generation. Numerical studies conducted by the author imply that, for sufficiently large populations, the benefits of parent retention outweigh this advantage and any disadvantages of "inbreeding", i.e. a stagnant population. For more details on this "inheritance property" see Davis [28] or Kennedy and Eberhart [12]. In the upcoming algorithm, inbreeding is mitigated since, with each new optimization generation, new parameter sets, selected at random within the parameter space, are added to the population. Previous numerical studies of the author (Zohdi [13]) have indicated that not retaining the parents is suboptimal due to the possibility that inferior offspring will replace superior parents. Additionally, parent retention is computationally less expensive, since these parameter sets do not have to be re-evaluated in the next optimization generation. For example, such algorithms can be used to search for parameter sets yield populations having similar stable sizes after many conflicts. Mathematically speaking, this couple be expressed by writing $\min_{\boldsymbol{\Lambda}} \Pi(\boldsymbol{\Lambda})$, where

$$\Pi(\boldsymbol{\Lambda}) = \frac{|p_1 - p_2|}{|p_1 + p_2|}, \tag{A.1}$$

where $\boldsymbol{\Lambda} \stackrel{\text{def}}{=} \{d_{ij}^{(1-2)}, s_{ij}^{(1-1)}, s_{ij}^{(2-2)}, w^{(1)}, w^{(2)}, etc.\}$ and where p_1 and p_2 are populations after a set number of conflict periods for a given $\boldsymbol{\Lambda}$. The goal would be to find the sets of $\boldsymbol{\Lambda}$ that minimize Π, other than the trivial parity parameter set, namely that both of the populations have identical characteristics. In particular, one could determine what factors (parameters) can counterbalance one another for population coexistence. An implementation of such optimization ideas follows (Zohdi [13]):

- **STEP 1:** Randomly generate a population of S starting genetic strings, $\boldsymbol{\Lambda}^i$, $(i = 1, \ldots, S)$:

  $\boldsymbol{\Lambda}^i \stackrel{\text{def}}{=} \{ \Lambda_1^i, \Lambda_2^i, \Lambda_3^i, \Lambda_4^i, \ldots, \ldots \Lambda_N^i \}$
- **STEP 2:** Compute fitness of each string $\Pi(\boldsymbol{\Lambda}^i)$, $(i = 1, \ldots, S)$
- **STEP 3:** Rank genetic strings: $\boldsymbol{\Lambda}^i$, $(i = 1, \ldots, S)$
- **STEP 4:** Mate nearest pairs and produce two offspring, $(i = 1, \ldots, S)$

  $\boldsymbol{\lambda}^i \stackrel{\text{def}}{=} \Phi^{(I)} \boldsymbol{\Lambda}^i + (1 - \Phi^{(I)}) \boldsymbol{\Lambda}^{i+1}, \boldsymbol{\lambda}^{i+1} \stackrel{\text{def}}{=} \Phi^{(II)} \boldsymbol{\Lambda}^i + (1 - \Phi^{(II)}) \boldsymbol{\Lambda}^{i+1}$
- **NOTE:** $\Phi^{(I)}$ and $\Phi^{(II)}$ are random numbers, such that $0 \leq \Phi^{(I)}, \Phi^{(II)} \leq 1$, which are different for each component of each genetic string
- **STEP 5:** Kill off bottom $M < S$ strings and keep top $K < N$ parents and top K offspring (K offspring + K parents + $M = S$)
- **STEP 6:** Repeat STEPS 1–6 with top gene pool (K offspring and K parents), plus M new, randomly generated, strings
- **OPTION:** Rescale and restart search around best performing parameter set every few optimization generations
- **OPTION:** We remark that gradient-based methods are sometimes useful for post-processing solutions found with a genetic algorithm, if the objective function is sufficiently smooth in that region of the parameter space. In other words, if one has located convex portion of the parameter space with a global genetic search, one can employ gradient-based procedures locally to minimize the objective function further. In such procedures, in order to obtain a new directional step for $\boldsymbol{\Lambda}$, one must solve the following system, $[\mathbb{H}]\{\Delta\boldsymbol{\Lambda}\} = -\{\boldsymbol{g}\}$, where $[\mathbb{H}]$ is the Hessian matrix ($N \times N$), where $\{\Delta\boldsymbol{\Lambda}\}$ is the parameter increment ($N \times 1$), and $\{\boldsymbol{g}\}$ is the gradient ($N \times 1$). We shall not employ this second (post-genetic) stage in this work. Reviews of these methods can be found in the texts of Luenberger [31] and Gill, Murray and Wright [32].

To compute the fitness of a parameter set one must go through the procedure above, requiring a full-scale simulation. It is important to scale the system variables, for example, to be positive numbers and of comparable magnitude, in order to avoid dealing with large variations in the parameter vector components. Typically, for populations with a finite number of agents, there will be slight variations in the performance for different random starting configurations. In order to stabilize the objective function's value with respect to the randomness of the starting configuration, for a given parameter selection ($\boldsymbol{\Lambda}$), a regularization procedure is applied within the genetic algorithm, whereby the performances of a series of different random starting configurations are averaged until the (ensemble) average converges, i.e. until the following condition is met: $\left| \frac{1}{Z+1} \sum_{i=1}^{Z+1} \Pi^{(i)}(\boldsymbol{\Lambda}^I) - \frac{1}{Z} \sum_{i=1}^{Z} \Pi^{(i)}(\boldsymbol{\Lambda}^I) \right| \leq TOL \left| \frac{1}{Z+1} \sum_{i=1}^{Z+1} \Pi^{(i)}(\boldsymbol{\Lambda}^I) \right|$, where index i indicates a different starting random configuration ($i = 1, 2, \ldots, Z$) that has been generated and Z indicates

the total number of configurations tested. In order to implement this in the genetic algorithm, in STEP 2, one simply replaces *compute* with *ensemble compute*, which requires a further inner loop to test the performance of multiple starting configurations. Similar ideas have been applied to other types of randomly dispersed multibody systems in Zohdi [13].

Appendix B. Continuum formulations of spatio-temporally coupled models

In order to illustrate a classical continuum spatio-temporal formulation of competing populations, in this case microbial cells and chemical regulators, following Zohdi [33], a spatio-temporal system constructed, comprised of two conservation laws:

- **Microbial cell proliferation** ($p_1 = c$): which is comprised of (a) rate of change of microbial cells, (b) cellular migration, (c) cellular proliferation controlled by a cell mitosis regulating chemical and (d) cell apoptosis.
- **Environmental chemical regulator** ($p_2 = s$): which is comprised of (a) rate of change of the microbial cell mitosis chemical regulator, (b) regulator diffusion, (c) regulator production by cells and (d) regulator decay.

To simplify things, we consider *infinitesimal deformations* of the medium $\dot{()} = \frac{\partial ()}{\partial t}|$. In other words, the domain does not change its shape or geometry with changes in concentration. The microbial cell concentration in an arbitrary volume of material denoted ω, consists of

$$\underbrace{\frac{d}{dt} \int_\omega c\, d\omega = \frac{\partial}{\partial t} \int_\omega c\, d\omega}_{storage} = \underbrace{-\int_{\partial\omega} \boldsymbol{m}(c) \cdot \boldsymbol{n}\, da}_{migration} + \underbrace{\int_\omega r(s)\, d\omega}_{production} - \underbrace{\int_\omega \tau(c)\, d\omega}_{apoptosis}, \tag{B.1}$$

where c is a concentration (storage) term, $-\boldsymbol{m} \cdot \boldsymbol{n}$ is an inward normal migration flux term, $r(s)$ is a proliferation term, and $\tau(c)$ is a cell apoptosis term and

$$\underbrace{\frac{d}{dt} \int_\omega s\, d\omega = \frac{\partial}{\partial t} \int_\omega s\, d\omega}_{storage} = \underbrace{-\int_{\partial\omega} \boldsymbol{f}(s) \cdot \boldsymbol{n}\, da}_{diffusion} + \underbrace{\int_\omega p(c)\, d\omega}_{production} - \underbrace{\int_\omega \gamma(s)\, d\omega}_{decay}, \tag{B.2}$$

where s is the cell mitosis regulator concentration, $-\boldsymbol{f} \cdot \boldsymbol{n}$ is an inward normal migration flux term, $p(c)$ is a production term and $\gamma(s)$ is a regulator loss term. After using the divergence theorem on the flux terms, since the volume ω is arbitrary, one obtains a diffusion–reaction model in strong form (assuming a Fickian-type law, $\boldsymbol{m} = -\mathbb{D} \cdot \nabla c$ and $\boldsymbol{f} = -\mathbb{K} \cdot \nabla s$)

$$\frac{\partial c}{\partial t} = \nabla \cdot \mathbb{D} \cdot \nabla c + r(s) - \tau(c) \tag{B.3}$$

and simultaneously the balance of a mitosis regulating chemical (s)

$$\frac{\partial s}{\partial t} = \nabla \cdot \mathbb{K} \cdot \nabla s + p(c) - \gamma(s). \tag{B.4}$$

There is a vast amount of literature on the construction of the functions $r(s)$, $\tau(c)$, $p(c)$ and $\gamma(s)$ for specific types of problems, such as wound healing. See Murray [1] for an extensive review, with early experimental studies dating back at least to Lindquist [34] Van den Brenk [35], Crosson et al. [36], Zieske et al. [37], Franz et al. [38] and Sherratt and Murray [39]. Such a coupled model can represent a variety of biological systems, such as growth in biological scaffolding, proliferation of damaged cellular tissue, etc. However, for the reasons outlined in the body of the text, such models computationally expensive and of limited physical usefulness for true, complex, population dynamics studies. However, the modeling of outlined here has a close similarity to multicomponent diffusion–reaction industrial processes, where it is quite useful and enjoys wide usage in engineering. We refer the reader to Zohdi [33,40–43] for more details.

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