# Some interesting title

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**Abstract**

This paper explores the notion that dynamically changing the representation of submodels within an ensemble of models may provide a means of optimising the overall utility of a model. DESCRIPTION. TOY MODEL. RESULTS.

## 1 Introduction

Many models are constructed as an ensemble of submodels. Often these submodels are integrated almost seamlessly and the aggregate system presents itself, like an organism, as an indivisible entity. At the other end of the spectrum models may be comprised of quite distinct submodels which retain their independence and stand, in some sense, as models in their own right.

There are quite a number of well established ways of integrating submodels, many of which achieve efficiency, either in run-time or accuracy, by running different components of the model at different, possibly varying temporal or spatial scales. There may still be scope for improvement, however.

The scope of ecosystem models is steadily increasing (NWS, ATLANTIS, EcoSIM/EcoPath/EwE, ATLAS) [REFS]. Our models are including more functional groups within the ecosystem and the interactions between components are becoming more detailed. As our climate changes and the environment we live in and use drifts further from its familiar state, there is a corresponding need to manage our interactions with the ecosystems around us more carefully, and this often implies a greater reliance on detailed modelling of the system. This explosion of demand for detail is costly in terms of computational load – modelling whole populations of some endangered species at an individual level may be very good at capturing the population's vulnerability to exceptional events, but it takes a long time. Worse still, much of the simulation time may be spent with the model in a largely unchallenging part of its state-space.

As a simple illustration we might consider the motion of a mass capable of acceleration, say a rocket or a car. The rules of Newtonian motion make a good model as long as our mass doesn't move too quickly, and while relativistic motion is accurate at low speeds, it is more expensive to calculate. A simulation of a spacecraft (or car) that approaches the speed of light would spend a lot of time calculating relativistic motion when a simpler model would be adequate. It is easy to imagine that we might use Newton's equations when the velocities are low (most of the state space), but shift to relativistic motion when we stray from the areas where Newton is comfortably accurate.

So the notion is that we might change the *representation* of a submodel based on its location in its state-space, or indeed the state of the model as a whole. In some sense we do this in our simulation models anyway. In the most simple case, time-steps or spatial resolutions are changed, but beyond that clauses may be by-passed if the local state of the simulation meets certain criteria, and additional calculations might be performed to reduce the error when the state is changing rapidly.

The experience garnered in the several large scale MSE-style ecosystem modelling projects has shown that a more systematic approach is needed. The burden of maintaining all of a complex model's state when it is in a region where a simple state may perform better is unnecessary, and the potential for significant improvements in run-time and the reduction of error seem achievable. There are a number of aspects of the notion that need to be teased out and examined closely: how the state of a sub-model changes through transitions (mutations) in representation, how we decide *when* to change representation and how expensive that might be, and how to manage the error associated with the potential loss of state information are all important issues which need investigation. More fundamentally there needs to be, *prima facie*, a demonstration that the notion might be worth pursuing; this is the intent of this paper.

This approach to the problem has been developed in the light of experience with several large scale human-ecosystem interaction models. In these studies work [PMEZ, NWS, and now Ningaloo], a number of submodels are run concurrently, many of which represent individuals or small aggregations of individuals. One of the significant components in each of these projects is simulating the interaction between simulated organisms and contaminant plumes. This particular facet of the models has very expensive in terms of run-time – in the NWS model it increased the time taken by roughly an order of magnitude. In these PMEZ and NWS, a considerable amount of time was unprofitably spent by the submodels in areas of the state space of the model where no interaction with contaminant plumes was possible. Alas, heuristics can only go so far and so our search for alternative ways of reducing the computational load without undue loss.

### 1.1 Scope

The aim of this paper is not to develop a complete body of work supporting the use of models which mutate according to where they might be in their state-space, rather it is to establish that the idea is reasonable. This is a specific example which has been carefully constructed to maximise its chance of supporting the hypothesis, and though we might make general observations that lie outside this unassuming target, the pursuit of their implications lie outside our immediate intent.

We will consider a model of organisms moving along a simple migratory path which intersects a region with varying levels of contamination. The model isn't really intended to be an accurate representation of any real system; since its role is to help explore some of the issues associated with changing representations and to test the hypothesis that we might gain efficiency in simulation time, representational accuracy, or both, its proximity to any real situation must be viewed as happy coincidence.

Our toy uses rather obvious basic representations of individuals and populations as the "natural variants" and the mutating model simply oscillates between them. The population model makes the assumption that the contaminant contact with the population is distributed through the population according to the density function which describes the population and that this is adequate to characterise the uptake based on the likelihood of an individual being at any given location within the population's radius, while the individual-based simulation makes the assumption that the individual trajectories have an important impact on the contaminant loads of the individuals . Unlike the example of Newtonian and Relativistic motion, the state-spaces of the basic models we consider differ, though in only a small way. Individuals follow trajectories whose mean is (more or less) the migratory circle. Most of this position information is not pertinent for the population model – it's natural representation is to simply position itself at the appropriate point on the migratory path for any given time. The transition from individuals to population and population to individuals involves the loss and reconstruction of this fine-scale position data. In this context, we assume that the location of any given individual would be thoroughly randomised over the interval of time usually spent in a population representation, and so we can reconstruct a plausible location based on the distribution of individuals within the population's domain.

## 2 Experimentation

The comparison of the three modelling schemes is based on the run-times for each representation, the correspondence between the total contaminant loads across the biomass through time, a comparison of variability in contaminant load through time amongst the representations, and the sensitivity to variability in the nature of the plume.

Our strategy is to first establish the equivalence of the mutating model and the individual-based representation in terms of their results. This component of the study also provides us with data for comparing the relative efficiency of the representations in terms of run-time. We generate forty trials each simulating forty individuals for both the individual-based and mutating models. The population models are deterministic and one run is sufficient.

Second, we incorporate the data from the mutating model in a matching set to double the sample size, and run a corresponding set of trials using an asymmetric plume. These runs are compared with each other and with corresponding symmetric and asymmetric runs of the population-based representation. Ideally, the results with an asymmetric plume would be consistent across the model representations, though the results will show this is not the case.

## 2.1 Basic model structure

There are a number of attributes of the system which are common to all of its representations. Each of the submodel representations can be viewed as analogous to a process running in a multitasking operating system. There is a central queue which passes control to each agent in its queue in turn and, when given control, each agent runs for a time step. The machinery which supports this structure is the same for each representation, and the system is quite capable of running an arbitrary number of populations, and individuals at the same time.

An alternative view is of the model as a whole as a sequence of mappings, $s$: $\boldsymbol{S} \rightarrow \boldsymbol{S}$, each of which maps an element of of the state space, say $\boldsymbol{s}_t \in \boldsymbol{S}$, to some other element, $\boldsymbol{s}_{t+\delta t}$, in $\boldsymbol{S}$. In all three representations the number of entities modelled remains the same, but in the mutating model the number of mappings applied at each time may change. This is a substantial formal difference and we will address it in the discussion at the end of the paper.

For the moment will will only consider the two "pure" models: the population-based representation and the individual-based representation. In these cases, each submodel would correspond to some subset of the ordinates in a state vector and the mapping $\check{s}_i$ or $\tilde{s}_j$ would manipulate only the ordinates corresponding to the population $i$ or the individual $j$. Thus, each of these mappings is pertinent only to a particular part of the state vector $\boldsymbol{s}_t$, and the update step corresponds to the mapping of the whole state from one step to the next. So we might write

$$\boldsymbol{s}_{t+\delta t} = \check{s}_1 \circ \tilde{s}_2 \circ \tilde{s}_3 \circ \check{s}_4 \ldots s_n(\boldsymbol{s}_t) \equiv \boldsymbol{s}_{t+\delta t} = \left( \bigodot_{s_i \in \mathcal{A}} s_i \right)(\boldsymbol{s}_t),$$

where each $s_i$ on the right hand side is either $\check{s}_i$ (for a population's update) or $\tilde{s}_i$ (for an individual's update). This update is performed for each time step until the defined end of the simulation. It is important to note that in these cases, the function composition is commutative: the individuals and the populations do not interact with each other, so the order of application isn't important.

These views of the system are compatible. Indeed, this duality lies at the heart of the mapping between the representations in this toy model.

The issue of whether an individual-based approach or a population-based approach is the best representation for modelling real situations really lies outside the scope of this paper, but for our purposes we will assume that (for whatever reason) the dynamics of the system which we wish to capture are best elicited by an individual-based representation. In the models which had a formative influence on this exploration, individual-based models were used to model the contact and uptake of contaminant. The primary reason for this is that in both of the earlier studies the initial exploration suggested that the structure of the plumes would be quite fine with a rapid decay from their peak values and that a Lagrangian approach might be more sensitive to the dynamics of the system.

## 2.2 Distributions and compatibility

The toy model has two basic representations of a group of organisms which proceed around a circular migratory path on an annual basis. Within one region which intersects this path there is a plume of some contaminant with an intensity which varies sinusoidally at a frequency which is relatively prime to the annual migration cycle. The contaminant load of the modelled entities is subject to constant decay, but when the group (or members of the group) are inside the boundary of the plume, their contaminant load increases. The processes of uptake and depuration are represented by an equation which relates the contaminant load at the end of the time step to their load at the beinging of the time step and the level of contact they experience over their path.

The first representation of the group is as a set of individual agents whose movement is a directed random walk around the migratory circle. At each time step the trajectory of each individual incorporates a directional component toward the "target location" on the migratory path which corresponds to the notional ideal centre of the group at that time. Each agent (instance of the submodel) maintains its own contaminant load, and its location and trajectory is independent of the others.

Our second approach is to represent the individuals as an aggregate entity. This is a mean-field representation of the population: we can, in some way, smear the individuals symmetrically around the disk to give us a representative entity which possesses a centroid and a radial distribution around that centroid which is consistent with the distribution of the individuals in the first representation. The density of the simulated individuals around their target location arising from their movement model closely follows the probability density function of a normal distribution. This is an ideal situation – in practice there may be a number of environmental influences which make a such a simple population distribution unrealistic. The actual distribution of individuals is slightly skewed by their motions along the migratory circle, but we optimistically decide that the error introduced with the approximation is worth the resulting simplicity, particularly in light of the population's relatively slow motion around the migratory circle. From this representation of the individuals' density, we define the population's density, $\rho(p)$, to be the value of the standard 2D normal distribution with a mean of zero in each ordinate and a variance which is experimentally determined to match that of the individuals. More explicitly

$$\rho(|p|) = S_L \frac{1}{2\pi\sigma^2} \exp\left( -\frac{p_x^2 + p_y^2}{2\sigma^2} \right),$$

where $p = (p_x, p_y)$ is the position in the population disk relative to its centre, $S_L$ is a scaling parameter (equal to 1.015) which ensures that the population density, $\rho$, integrated over the finite disk with a radius, $\tau$, is one, and $\sigma^2$ is the variance for the distribution. If the distribution of individuals around the point $m(t)$ arising from the movement model and the distribution of the population around $m(t)$, which is identified with its centroid, were not consistent, then the contaminant exposure of the two models would be incompatible and the sort of mutation error discussed above becomes significant. The effective radius, $\tau$, of the population is statically "tuned" to reflect the observed distribution of the individual-based model. The variance in the distance of the individuals from $m(t)$ was calculated and used as the variance for the population density. We took the value $\tau = 9408.75$ which was three standard deviations from the centre of the observed distribution.

The general aim is to construct mappings between representations which preserve as much information as possible without undue burden. Clearly the significant information which the individual-based representation possesses and the population representation does not is the variation in contaminants amongst the individuals within the group. The role of the individual locations of these individuals is not really a significant factor for a large portion of the state-space since the interval between conversions from individuals to aggregates is large enough to ensure a thorough randomisation of relative position (though if the contaminant load exerted some influence on behaviour, such as the speed of the individual, this may not be so). We will discuss the construction of our third form of the system, the mutating model, in greater detail later.

# 3 Formulating the basic models

The basic representations play a dual role in the experiment. Not only do they provide comparison data in their own right, but each forms an unmodified component of the mutating model. This is accomplished by providing each of the basic models with enough extra machinery to report its state to a "supervisor" which manages the swap from one representation to another.

The population-based and individual-based models have been kept as similar as practicable in order to minimise the sources of divergence. Both models simulate migration around the same path and use the same contaminant uptake equations. Differences arise in the calculation of the contact with the contaminant, since the interactions of an individual moving through the plume is, in some sense, an integration across a path, while the population's expected interactions are more analogous to the integration over the domain of the population.

## 3.1 The migratory circle and the plume

The migratory path is a circle which can be defined by the equation

$$\boldsymbol{m}(t) = R \cdot (\cos(2\pi t/Y), \sin(2\pi t/Y)),$$

where $\boldsymbol{m}(t)$, denotes the "location at time $t$" on the migratory path, $R$ is the radius of the migratory path and $Y$ is the period. This circle is used for all the variant models of the system.

The plume is modelled as an elliptical cloud. Its centroid is positioned on the migratory circle. The plume is modelled as an intensity at a location with an attenuation function. The intensity at a point, $\boldsymbol{r}$, within the plume at time $t$ is given by

$$I(t, \boldsymbol{r}) = \frac{1}{2}(1 + \cos(2\pi t/p))(|\boldsymbol{r} - \boldsymbol{m}(t)|^2 + (1 - \frac{< r, \boldsymbol{m}(t) >}{< r, \boldsymbol{m}(t) > + 1})^{0.01})^{-1},$$

where $p$ is the period of the plume and $r$ is a distance from the source, and $< \boldsymbol{a}, \boldsymbol{b} > = |\boldsymbol{a} - \boldsymbol{b}|$. The intensity is made asymmetric by instead taking $< \boldsymbol{a}, \boldsymbol{b} > = (\boldsymbol{a} - \boldsymbol{b}) \cdot (\sqrt{2}, \frac{1}{\sqrt{2}})^{\frac{1}{2}}$. In the model's code, this intensity function is represented in cartesian coordinates rather than polar coordinates. The effective radius of the symmetric plume in the model is approximately 3684m, while the radius of the migratory circle, $R$, is 100000m and the period, $Y$, is 12 years.

## 3.2 Contaminant load and contact

The strategy for modelling the contact, uptake and depuration of our contaminant is the same for both representations. Initially a "total contact" is calculated for the time step. As might be expected, the total contact for a population is calculated in a different way to the total contact of an individual. In either case, this resulting contact is fed through the uptake-depuration o.d.e.

$$dC/dt = uM - \lambda C$$

which is solved numerically for the value of $C$ given a contact mass, $M$, and an initial contaminant value or vector of values for $C$. Later, when we explore the time series resulting from the trials of the three representations, we will take $C_{rkj}(t)$ to represent the time series associated with individual $j$ in trial $k$ of representation $r$, $C_{rk}(t)$ to be the mean over all the individuals in the indicated representation and trial, and $C_r(t)$ denotes the time step generated by taking the mean of $C_{rk}(t)$ across the values of $k$ for the indicated representation.

For individuals, the mass of contaminant which is available for uptake is taken to be the result of integrating the intensity of the plume over the path of the individual, $\boldsymbol{P}_t$ to $\boldsymbol{P}_{t+\delta}$,

$$M = \int_{\boldsymbol{P}_t}^{\boldsymbol{P}_{t+\delta}} I(\boldsymbol{p})\ |\boldsymbol{p}|\, d\,\boldsymbol{p}$$

where we assume that the motion between $(t,\ \ell_t)$ and $(t + \delta_c,\ l_{t+\delta})$ is linear. Populations are somewhat more complex. Here, we calculate the definite integral

$$M = \int_{\boldsymbol{P}_t}^{\boldsymbol{P}_{t+\delta}} 2 \int_{\boldsymbol{\Omega}} I(\boldsymbol{p} + \boldsymbol{\omega})\ \rho(\boldsymbol{p} + \boldsymbol{\omega})\ d\,\boldsymbol{\omega}\, d\,\boldsymbol{p}$$

where $\mathbf{\Omega}$ is an area over which we assess the effective area of the population and $\omega + \boldsymbol{p}$ denotes the area $\mathbf{\Omega}$ translated so that its centroid corresponds to $\boldsymbol{p}$. A fourth-order Runge-Kutta algorithm was used to solve the contact equation and a simple adaptive quadrature algorithm was used for calculating $M$.

### 3.2.1 The homogeneous population model

The significant state variables for the population model consist of the time, a location, an effective radius and a contaminant load level. A population is effectively a radial density function, $\rho$, for which $\int_{\mathbf{\Omega}} \rho(\boldsymbol{\omega})\, d\,\boldsymbol{\omega} = 1$; the disk we integrate over, $\mathbf{\Omega}$, moves uniformly with its centre on migratory circle, $\boldsymbol{m}(t)$, in accord with the annual migration. The vector of contaminant loads (possibly empty or only a single quantity) is updated at each time step in the same way as the individuals according to the contact during that interval, and the uptake and depuration rates. The populations are also given a nominal number of members, though this datum is not useful unless we are considering a mutating model.

### 3.2.2 The homogeneous individual-based model

Individuals are basically represented by a location, a subjective time, a velocity vector and a contaminant load. There are obviously other parameters which influence their contaminant load: rates of uptake and depuration, and the parameters which condition their drunkard's walk around the migratory circle. In our case, these attributes really only contribute to the rate of progress around the migratory circle (the frequency and duration of contact) and the distribution of the spatial coverage of the group of individuals around $\boldsymbol{m}(t)$, and hence the effective radius of the population. So, the details of the mechanics of the movement of the individuals are also relevant only in so far as they help inform the construction of the population model.

## 4 The mutating model

The mutating model tests our hypothesis: that that it may be more efficient in terms of time or representational accuracy to change the representation of components of the model, depending on the nature of the region of the state-space a submodel. The specific example we are dealing with, individuals interacting with a highly local plume, is very simple – almost simplistic – but it possesses many of the properties which the general problem of an *ad hoc* animal/plume interaction might be expected to exhibit, namely the test for coincidence, generating a random walk for each individual, and evaluating the uptake and decay of the contaminant load. Over a long period of infrequent contact, we would expect quite a lot of time to be spent generating random walks and evaluating the contact and uptake in places where there is no likelihood of contact at all. Our strategy is to adopt, over particular regions in the state space, appropriate representations which preserve enough fidelity in the basic properties of the system to reconstitute any missing data required for another representation without incurring undue error or operational overhead. This is, fundamentally, about managing the often competing demands of representational accuracy, mathematical tractibility, and run-time.

In order to test the hypothesis, each of the possible representations the mutating model may assume is identical to one or the other basic, "homogeneous" representations. In the case of the mutating model's population-based representation, the contaminant value (a 1-tuple) is replaced by a vector consisting of the contaminant loads of the individuals with non-zero contaminant levels, the levels of the remaining members of the aggregate represented by the population are assumed to be zero. The values in each ordinate of the $n$-tuple are decayed independently as time progresses.

Individuals are mapped into a population by adding their contaminant level to the contaminant vector of an appropriate population after their movement and contaminant decay have been calculated. When a population-based model is mapped back to an individual-based representation, the non-zero contaminant levels are first mapped onto new individuals whose random locations are chosen to be consistent with the distribution for the population around its centroid. This mapping preserves the contaminant load present in the system and the likelihood of an encounter between a contaminated individual and new contaminants. In this way the distinct contamination levels within the system are maintained with a minimum of cost.

Some overhead is incurred in managing the swap from one representation to another. The actual conversion is done by a routine which is integrated with the scheduler which manages the transition from one time-step to the next. Each of the models is able to indicate to the scheduler that a change in representation may be reasonable when it determines that it has left its domain of efficiency.

## 4.1 Heuristics: When do we swap

The contraints we impose on this toy model are quite stringent so the heuristics we can use to decide when to change representation may thus assume a great deal more than might be the case in a general situation: we know where the contaminants are at all times, the movement of the populations and the individuals are controlled, and the behaviour of the simulated organisms does not change through the run. In the general case, the heuristics might be much more complex and require a great deal more data. Deciding when to change the representation is central to the optimisation of the system: changing at the wrong time might sacrifice accuracy, efficiency or both.

In our case, the principal issue is whether or not an agent (population-based or individual-based) may encounter contaminants: in our case it is simple, there is a single source and the mean movement toward or away from that source is quite predictable. As a population enters the region of contaminants we can immediately determine that it will encounter contaminants quite consistently for some non-trivial period, and a mapping is called for.

The which determines if an individual is mapped into a population is similarly straightforward: an individual is mapped into a population if it is far enough outside the region of contaminants that there is no chance that it might encounter them in the next few time-steps, and it is close enough to a population. If there is no suitable population, a new one is created in order to accomodate it. This spatial constraint is stringent enough, when combined with the speed of migration, that the system hasn't needed to create more than one population in any of the annual cycles in the trials. This fortunate state of affairs is largely due to strong contstraints on the movement associated with the annual trek around the migratory circle.

The transition rules in this model, from population to individual or from individual to population, can be based solely on the distance to the contaminant source, the time-step and the speed at which the simulated group of organisms moves around its annual path. Our heuristic could be generalised to systems where there were multiple, dynamically instanciated sources, when the sources of contamination could be determined at the beginning of a time-step. This particular model attempts to present a greatly simplified version of the general case – if the hypothesis were to fail in this case it would be reasonable to assume that it would fail in most cases.

## 4.2 Sensitivity to plume distribution

The issue of whether the configuration of the plume has an different effect on the results of a simulation depending on the representation of the organisms is important. It is easy to imagine calibrating a population-based representation with data from fine-scale individual simulations in order to make the most of the economies a population-based model affords, but this may not be a good idea if there is poor correspondence between the two models over their domain.

Additional trials of the standard (symmetric) plume model were run to extend the data available, and a corresponding series of trials with an asymmetric plume were run for comparison. Our analysis in these trials is based on a total of eighty trials of forty individuals with each trial covering twelve years. The asymmetric plume covers the same area as the symmetric plume and the integral over the area of the plumes are the same, up to the numerical error in the quadrature.

# 5 Results

The analysis in this section is based on three sets of runs. The first set is comprised of forty trials of each of the model representations (purely individual, mutating and population based). Each trial tracked either forty individuals or a population which nominally represented forty individuals. The contaminant plume was symmetric and its centroid was on the migratory circle. This set of runs was conducted to establish the relative cost in cpu-time of the three approaches and to experimentally verify (at least to some degree) the equiuvalence which ought to exist between the purely individual-based model and the mutating model. The second trial consisted of another set of forty replicates of the mutating model, mirroring the mutating trials in the first set. The third set consisted of eighty trials of the mutating model, and one of the population mode. The principal difference between the second and third set is that the second, when combined with the first gives us eighty replicates using a symmetric plume, while the third set replaces the plume with an asymmetric plume which is tangential to the migratory circle. Our initial analysis will only consider the trials in the first set of runs, and a comparison of the reponses to the asymmetric plume will be treated separately.

Both population-based and individual-based representations may use a heuristic which suppresses contact evaluation when they are sufficiently far from the contaminant source. No other significant optimisations of the code have been made, and as far as possible the same routines are used in both representations. The motivation for this approach is to provide a common baseline which we can use to measure the utility of the adaptive representation.

To ensure that run-time comparisons are meaningful all of the simulations in the first set of trials were run on the same computer. Each of the configurations simulated forty organisms for twelve years.

## 5.1 Contaminant load correspondence between representations

The set of trajectories arising from the various representations aren't directly comparable. Our individual-based representation produces a time series of contaminant levels for each individual, while the population-based model produces a "mean load" across the whole group of entities it is representing. The mutating model sits between the two, sometimes producing individual time series and sometimes mean time series for varying parts of the population. In order to compare the dynamics of the system we generate mean time series for each of the $k$ trials in the individual-based and mutating sets, $C_{ik}(t)$ and $C_{mk}(t)$, paying special attention to generating the correct mean in the mutating model from time steps which have a mixture of individual trajectories and mean trajectories. Each of these mean time series corresponds to the mean contaminant load of the population, $C_p(t)$, produced by the population-based model; averaging them – constructing $C_r(t) = \frac{1}{k}\Sigma_{j=1}^{k} C_{rj}(t)$, where $r$ is one of $i$ or $m$ – is equivalent to running many stochastic trials and averaging to fit the population model.

Using $C_{ik}(t)$, $C_{mk}(t)$ and $C_p(t)$ we find the maximum value attained for each representation, $\hat{C}_r$. We are also interested in the mean value across time of each representation, $\bar{C}_r = \frac{1}{T}\Sigma_{t\in T} C_r(t)$ These quantities are listed in Table 1.

| Time series | $\hat{C}_r$ | $\bar{C}_r$ |
|---|---|---|
| $C_i$ | 0.1787 | 0.0390 |
| $C_m$ | 0.1821 | 0.0392 |
| $C_p$ | 0.1387 | 0.0350 |

**Table 1.** Maxima and Means

## 5.2 Contaminant load variability

Several measures of variability in the time series were calculated using the aggregated time series $C_{ik}(t)$ and $C_{mk}(t)$ and their respective means across the $k$ trials, namely $C_i(t)$ and $C_m(t)$. We'll take

$$\hat{\sigma}_{ab} = \max_{t\in[1,T]} \left[ \frac{1}{k} \sum_{j=1}^{k} \left(C_{ak}(t) - C_b(t)\right)^2 \right]^{1/2}$$

and

$$\sigma_{a\,b} = \left[ \frac{1}{T} \sum_{t=1}^{T} \left[ \frac{1}{k} \sum_{j=1}^{k} \left( C_{a\,k}(t) - C_b(t) \right)^2 \right] \right]^{1/2},$$

where $T$ is the total number of timesteps taken. Clearly we can write $\sigma_{rr}$ as $\sigma_r$ without introducing ambiguity, and similarly for $\hat{\sigma}_r$. The values for these measure of of variability are presented in Table 2.

| StdDev | $C_i$ | $C_m$ | $C_p$ |
|---|---|---|---|
| $\hat{\sigma}_i$ | 0.0083 | 0.0084 | 0.0534 |
| $\sigma_i$ | 0.0024 | 0.0024 | 0.0096 |
| $\hat{\sigma}_m$ | 0.0090 | 0.0090 | 0.0538 |
| $\sigma_m$ | 0.0024 | 0.0024 | 0.0096 |

**Table 2.** Deviations amongst the model runs with respect to a given mean

## 5.3 Sensitivity to asymmetry in the plume

We will use the same notation as Section 5.2 for the data derived from the symmetric plumes, while we will add a prime symbol to the data derived from the asymmetric plumes. Thus, the mean value time series for the mutating model would be denoted $C'_m$ and the mean value of that time series is $\bar{C}'$.

The data for the symmetric plume is presented in Table 3 and the data for the asymmetric plume is presented in Table 4.

| Time series | $\hat{C}_r$ | $\bar{C}_r$ | StdDev | $C_m$ | $C_p$ |
|---|---|---|---|---|---|
| $C_m$ | 0.1738 | 0.0392 | $\hat{\sigma}_m$ | 0.0088 | 0.0535 |
| $C_p$ | 0.1387 | 0.0350 | $\sigma_m$ | 0.0024 | 0.0098 |

**Table 3.** Symmetric plume results

| Time series | $\widehat{C'}_r$ | $\overline{C'}_r$ | StdDev | $C'_m$ | $C'_p$ |
|---|---|---|---|---|---|
| $C'_m$ | 0.1856 | 0.0394 | $\hat{\sigma}'_m$ | 0.0087 | 0.0616 |
| $C'_p$ | 0.1763 | 0.0445 | $\sigma'_m$ | 0.0025 | 0.0092 |

**Table 4.** Asymmetric plume results

## 5.4 Run-time

Each run collected data regarding the amount of time spend in different parts of the model. As a basis of comparison, the overall amount of time spent running on the cpu (linux/unix "cpu seconds") for the whole run is the most important figure, though the time spent in other parts provipdes illumination into just where the effort is concentrated. Predictably, most of the effort is in calculating contact and updating contaminant loads.

The optimisation of supressing the contact calculations when a population is outside the area of potential contact seemed to make very little difference to the run-time of population model (of the order of 3%), and seems unlikely to make a great deal of difference to the mutating model. In the case of the purely individual-based model, this sort of optimisation is likely to play a much bigger role in that a three second penalty would be multiplied by the number of entities simulated.

The population-based model ran for 98.7. This model is deterministic and the amount of cpu time used is very stable, so only a single run is considered for comparison. The purely individual-based models took just over a mean time of 4205 cpu seconds with a standard deviation of barely more than 16 seconds and the mean of the mutating model's run time was 1157 cpu seconds with a standard deviation of slightly over 11 seconds.

# 6 What the toy model tells us

The initial sets of runs have two aims, namely to establish the relative speeds of the three approaches and to support the assertion that the mutating model possesses the same essential dynamics as the purely individual-based representation. The essential equivalence of the individual-based and mutating representations is well supported and there is a significant benefit in run-time with the mutating model when compared to the individual-based model. The population model, while fastest by several orders of magnitude, showed responses to the contaminant plume which were significantly different to those of the other two models.

## 6.1 Means, maxima and variation

In terms of the formulation of the mutating model, it is difficult to see how there could be a significant difference between it and the purely individual-base model, at least in terms of the contaminant loads in the group of individuals. The means, maxima and the various calculations of deviation between the individual-based and mutating models were very close and this supports the belief that they can be treated as essentially identical in terms of modelling the contaminant load in the group of simulated organisms. Both of these representations, however, differed noticably from the population-based model; the population's mean value, $\bar{C}_p$, was about 10% lower than that of the either $\bar{C}_i$ or $\bar{C}_m$, and the root mean square error of either the individual-based model and the mutating model from the population's mean value was about four times greater than from either of the individual-based or mutating means.

The discrepancy between the population-based uptake and individual-based uptake is enough to suggest that the formulation of the population distribution was not quite consistent with the spatial dynamics of the individuals, that the tuning of the population model with respect to the individuals was inadequate or, most likely, that both of these errors contribute to the difference. This is the sort of situation alluded to in section 4.2: the fundamental models exhibit different dynamics over the domain of the simulation, and this is one of the niches which a mutating approach might be most advantageous. It is difficult to accurately describe a wild population's distribution across the whole of its domain – changes in the behaviour of individuals (arising from predation, drought or other stressors) may engender quite different population distributions, so even in the case of a purely population-based representation an argument can be made for changing the underlying representation based on the local state.

## 6.2 Run-time

The population-based model is clearly much faster than either of the other two representations, and for situations where we can reasonably make mean-field assumptions and our distribution model fits well with the observed data it is likely that the economies afforded by the speed of execution and the well established mathematical understanding of such models will outweigh benefits of individual-based representations. In situations where mean-field assumptions are not tenable it is similarly clear that there are benefits to using mutating models. Purely individual-based models entail significant overhead, which in our context contributes nothing to the outcome. In a richer environment with diverse responses to the local state, an individual-based model's 'non-productive' overhead may be competitive with the overheads associated with the management and transition of mutating models.

## 6.3 Symmetry and asymmetry

The data in the second set of trials had means, maxima and deviations for the mutating model which were largely between the symmetric and asymmetric contaminant fields. This matches our expectations since the total areas covered, the total contaminant load over the area are the same for the two representations are the same, and the speed of the agents through the plume is relatively slow. In contrast, the symmetric and asymmetric trials of the population-based model had markedly different maxima and mean values through time.

The data suggest that the individual-based representation is reasonably robust with respect to the plume shape (at least in the context of this experiment). The population model did not behave as expected and it may be that the model of the distribution of individuals which formed the basis of the population model may have systematic problems with the population wide sampling of the plume – the increase in mean and maximum levels when the plume was asymmetric and oriented tangentially along the track of the population suggests that the centre of the population is oversampled. The implications of this are that we must choose our population distribution carefully, and a simple gaussian distribution about a centroid may not behave well with respect to the plume dynamics.

Set against this, the numeric modelling of populations is well established. It is quite likely that the individual-based model would fail to meet expectations with regard to the dynamics of recruitment and mortality, had those aspects of the life history of a population been included in the model. In such a situation, the mutating model would have performed best overall – largely maintaining the fidelity of each of the representations across the state-space.

# 7 Discussion

In this section, we move from the specific to the general: having established that there is a *prima facie* case for mutating models, we discuss some of the issues which have arisen. Loosely speaking, we will group our discussion in terms of *formal notation*, *optimisation*, *transition heuristics*, and *model transitions*.

The formal notation is presented as a means of aiding the discussion, and to begin to establish some sort of mathematical basis for the strategy. In itself it contributes nothing but clarity, and, with luck, a little illumination.

## 7.1 Formal notation

We can consider many simulation models to be the repeated application of a chain of function compositions, and indeed adherents of the functional-programming paradigm would regard this as the natural approach. Each application takes the model from the state associated with time $t$ to its next state at $t + \delta t$. Many of the approaches to modelling ecosystems can be dealt with in this way (cellular automata, variable speed splitting models, and classical individual-based models to name a few). One of the aspects which makes formalising the mutating model more complex is that not only may the number of functions in our chain change, but the functions themselves may change, but we are fortunate that we can choose to consider only finite systems, such as computer based models.

Let us consider the aggregate model and its domain: in principle this corresponds to what happens (or might happen) in some patch of the real world. So, we let $G$ be a function on the state-space $\boldsymbol{S}$ where $G(\boldsymbol{s}_t) = \boldsymbol{s}_{t+\delta t} \, \forall \boldsymbol{s} \in \boldsymbol{S}$. Already we find that our notation is too sparse: just a moment ago we indicated that the form of $G$ changes with respect to its location in the state space. So, we refine things just a little. Let $\boldsymbol{F}$ be the set of all functions which map elements of $\boldsymbol{S}$ onto another element of $\boldsymbol{S}$, and let $\Gamma(\boldsymbol{s}, g) = h$ for $g, h \in \boldsymbol{F}, \boldsymbol{s} \in \boldsymbol{S}$.

Then in a straightforward model we might write a typical update step as

$$G(\boldsymbol{s}_t) = \left( \bigodot_{i=1}^{n} g_i \right) = \boldsymbol{s}_{t+\delta t}$$

where $n$ is the number of entities in the aggregate model, and $g_i \in \boldsymbol{F}$ which is (probably) associated with the ordinates of the state space associated with one submodel, though it ought to be noted that the an entity may represent more than one individual or facet of the simulation. With this notion in place, we can recast it as

$$(\Gamma(\boldsymbol{s}_t, G_{t-\delta t}))(\boldsymbol{s}_t) = G_t(\boldsymbol{s}_t) = \left( \bigodot_{i=1}^{n} g_i \right) = \boldsymbol{s}_{t+\delta t}.$$

This version makes explicit the dependence of $G_t$ on the state, $\boldsymbol{s}_t$, and the representation in the previous step, and it should be observed that the value of $n$ depends largely on where $\Gamma$ maps $(\boldsymbol{s}_t, G_{t-\delta t})$.

if we know that the composition of these functions, denoted by $\odot$, is commutative. In order to preserve the commutativity of the component mappings, we introduce the mutation step as a mapping $\mathcal{M}(\boldsymbol{s}_t, \mathcal{A}_t) = \mathcal{A}_{t+\delta t}$ where $\mathcal{M}$ is a function used to map a set of submodels which spans the the state space of the simulation to another spanning set of submodels based on both the present state of the model as a whole and on the collection of submodels in $\mathcal{A}_t$. This mapping corresponds to the activity of the scheduler in the model.

In our simple example of motion above, both models require the same data: the object's mass, location, velocity and acceleration. This set of variables is adequate to represent any state in either model: a non-trivial model should consider a system which has model representations with different state spaces. The transition from one state-space to another which is associated with the change in representation may be introduce error either from the loss of particular attributes or from the assumption of some "default" value for an attribute which was not previously present.

# 8 Conclusion

The mutating model can be viewed from either direction – as a population model which converts itself to an individual-based representation when contaminants are encountered, or as an individual-based model which changes into a population when the specific locations of the individuals become irrelevant. The most challenging parts of the task are to determine what information must be maintained in each of the representations to ensure that the migration from one formulation to another doesn't introduce unreasonable error, and to control the migration between forms with a minimum of overhead.

This simple model demonstrated that changing the representation of a system from one form to another can provide a mechanism for increasing the efficiency or accuracy with only a little extra effort. A more challenging avenue for study would be a similar model which included population recruitment and mortality – particularly if there were sub-lethal effects associated with the contaminant load which changed the behaviour or fecundity of the simulated organisms.