Increasing model efficiency by dynamically changing model representations

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Abstract

We use one model,

but many may be more deft.

Is it worth trying?

There are a number of strategies to dealing with modelling large complex systems – in our case, large marine ecosystems. These systems are often comprised of many submodels, each representing a particular process or participant in a way which tries to capture the dynamics which contribute to the overall trajectory of the system. The balance between the acceptable modelling error and the run-time often dictates the form of submodels. There may be scope to improve the position of this balance point in both regards by structuring models so that submodels may change their algorithmic representation and state space in response to their local state and the state of the model as a whole.

This paper uses an example system consisting of a single population of animals which periodically encounter a diffuse contaminant in a localised region. We compare the performance of a population-based representation, an individual-based representation, and a *mutating model* which allows the representation to change from population-based to individual-based and vice versa depending on the likelihood of contaminant contact. The resulting run-times and contaminant dynamics associated with each of the strategies suggest that such a mutating model approach may be an avenue to gain accuracy within time constraints, time within accuracy constraints, or both.

Keywords: Model structure, model efficiency, equation-based model, individual-based model, integrated model, contaminant uptake

1. Introduction

In modeling the effects of human interactions with the environment and with animal and plant populations, researchers and modellers are often faced with the dilemma of choosing an appropriate scale for these interactions. Population level effects are likely to be modelled with an analytic approach, but an agent-based or individual-based approach may be more appropriate if our system exhibits behaviour which isn't compatible with mean-field assumptions.

There is a body of literature stretching back several decades which discusses individual-based modelling as an effective approach when individual variability is perceived

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to be an important driver of the system's dynamics, notably JABOWA and its derivatives (Botkin et al. (1972a), Botkin et al. (1972b)). Since the early 1980s, a rapidly increasing number of significant papers and books have appeared which address the use of individual-based models across a broad and with discussion of the relative strengths and weaknesses of the approach (such as Huston et al. (1988), DeAngelis and Gross (1992) and Grimm and Railsback (2005)). The use of classical (equation based) models to explore populations and ecological systems goes back much further, arguably to the end of the eighteenth century with Malthus's ***An Essay on the Principle of Population*** (1798).

In some sense these approaches represent extrema in a spectrum which exhibits, through its range, varying degrees of aggregation and resolution in time, space, and membership. Models at the boundaries of this spectrum are obvious representatives of a "choice of paradigm," but there are a large number of models which incorporate representatives from the extrema, and indeed adopt intermediate representations, such as described by Scheffer et al. (1995). Each of these representations has advantages: perhaps in the mathematical power of the technique, the speed of simulation or the sensitivity to the life-history of individuals. Many systems operate in a number of different "modes" which may be associated with distinct spatial or temporal scales. Examples of this include the difference in a plant or animal's diurnal activity, seasonal changes such as hibernation, and the very dramatic difference in the scales associated with grazing and with flight from predators. Perhaps a better approach is to dynamically adopt a model representation appropriate to the "mode" of the system and make use of the strengths of the alternative approaches.

As ecosystem models become broader in scope, including more species and richer environments, the notion that a single model can be identified within some particular region of this spectrum addresses all members and processes equally well starts to break down. Simulation models often embed the subject of study within an "environment" comprised of primary data and other interacting models within the system. The components of the environment may simultaneously lie in quite a number of places on the spectrum of representations. The actual implementation may be anything from a set of quite distinct submodels which are coupled together but retain their independence and, in some sense, stand as models in their own right, to a corpus of code where the submodels are integrated to the point where there is no real distinction between one "model" and the next.

As the climate changes and the environment we live in and use drifts further from its familiar state, there is a corresponding need to manage human interaction with ecosystems more carefully. The scope of ecosystem models is steadily increasing (DeAngelis et al. (1998), Harvey et al. (2003), Fulton et al. (2004), Gray et al. (2006)). Models are including more functional groups within their modeled ecosystems and the interactions between components are becoming more detailed. Addressing the increased demand for detail is costly in terms of computational load: individual-based models of populations may be very good at capturing the vulnerability to exceptional events, but such simulations take a long time. Worse still, much of this time may be spent with the model in a largely unchallenging or uninteresting part of its state-space.

As a simple example, we might consider the motion of a mass capable of acceleration; perhaps a rocket or a taxi. The rules of Newtonian motion make a good model as long as the mass doesn't move too quickly, and, while relativistic motion is much more accurate at high speeds, it is more expensive to calculate. A simulation of a spacecraft (or taxi) 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.

The notion we explore in this paper is that we might change the *representation* of a submodel based on its location in its state-space, and that by doing so we may actually be able to simulate the system more effectively. To some degree modellers do this anyway: time-steps or spatial resolutions are changed, particular code paths may be by-passed according to local conditions within the simulation, or additional calculations might be performed to reduce the error when the state is changing rapidly; but these optimisations are largely optimisations of the *encoding* of the model or submodels, rather than an actual change in representation. This sort of optimisation increases the model's complexity. In contrast, moving from a population modelled by a set of differential equations to a model tracking the life-history of a large number of individuals involves a change of domain, state-space and changed assumptions concerning the homogeneity of the constituent members of the population being modelled, but neither the population-based nor the individual-based models are made more complex. There must be additional code to map the state of each representation to the domain of the other, but these mapping functions are discrete and not really part of the models at all.

This approach to the problem of managing complex simulations was developed in light of experiences with several large scale human-ecosystem interaction models (Lyne et al. (1994), Gray et al. (2006), and modelling similar interactions in a larger study of the region containing the Ningaloo Marine Park (*work in progress*)). In each of these studies a significant component of the model focused on simulate the interaction between organisms and contaminant plumes. The focus in Lyne *et al.* was the potential for the percolation of contaminants originating in industrial waste up through the food chain into commercially exploited fish stocks. Gray *et al.* developed a regional model focused on assessing ways of managing the impact of human activity on the biological systems along the Northwest Shelf of Australia, one component of which was the effects on commercial prawn fisheries of flushing bitterns from salt production into the surrounding environment.

Monte (2009) presents a lucid discussion of *contaminant migration-population effects* models. These models incorporate the movement of populations and their internal distribution, the transport of contaminants through the system via biotic and abiotic pathways, and the changes in behaviour and population dynamics associated with contamination. Monte discusses a method of coupling the equations which govern contaminant dispersion with the equations for population dynamics and migration. The technique depends on the equations of the location and the dispersion of members of a population satisfying an independence condition with respect to time and location which must hold. He summarises the implications of the conditions, stating that the class of systems where the "movement of animals, the death and birthrates of individuals in $\mathbf{x}$ [location] at instant t [time] depend on previously occupied positions" is not generally amenable to the approach, and suggests that repeated simulations of many individuals is an appropriate way of dealing with this situation.

The treatment of contaminants is expensive in terms of run-time and memory use. The model described by Gray et al. (2006) contaminant modelling increased the time taken by roughly an order of magnitude, and in all of these studies a considerable amount of time was spent in regions where no interaction with contaminant plumes was possible.

Running a complex model and maintaining its state in a region where a simple model may perform better, or just as well, imposes a burden which is unnecessary. There is potential for significant improvements by reducing run-time and modelling error if representations are switched appropriately. In doing this, there are four basic questions that arise: "When should a model change represen-

tation?", "What data needs to persist across representations?", "How is the initial state for a new representation constructed?" and "How should the error associated with the loss of state information be managed?" In general, the answer to these questions is specific to the ensemble of submodels in question. Before expending the resources and effort required to implement such a strategy in a large scale model there needs to be, *prima facie*, a demonstration that the notion is worth pursuing. The aim of this paper is to provide this demonstration rather than to develop a body of techniques supporting the approach.

We present a model of organisms moving along a simple migratory path which intersects a region with a field of contamination with varying levels. This model exhibits fundamental attributes of larger studies of pollutant/ecosystem interactions (Lyne et al. (1994) and Gray et al. (2006)), and while it isn't intended to accurately represent any particular system, it might loosely correspond, for example, to some body of water influenced by contaminant loads associated with terrestrial runoff resulting from intense rainfalls. 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.

Our strategy uses two basic representations of the group of organisms; the first uses a single submodel to represent the whole group in a simple population-based submodel, the second uses an instance of an individual-based submodel to represent each organism in the group. The mutating submodel is derived from these two basic representations, and it switches between them when appropriate. The population model requires the assumption that the likelihood of an individual being at any given location within its ambit is represented by its distribution function and that the population's contact with the contaminant can be distributed through its members according to this function.

2. The models

The test models are composed of one or more submodels which run within a simple time-sharing system. Each submodel runs for a nominated period of time and passes control to the next submodel, very much like tasks running in many modern computer operating systems.

The population-based and individual-based submodels have been kept as similar as practicable in order to minimise the sources of divergence. Both representations are used to model a group of organisms which proceed around a common circular migratory path, $\mathbf{m}(t)$, on an annual basis. While both submodels use the same uptake-depuration equation to calculate their contaminant load, the calculation of the contact with the contaminant differs since the interactions of an individual moving through a 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.

The individual-based representation models the group as a set of individuals (agents, or instances of submodels) which move in a directed random walk. 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 maintains its own contaminant load, position and velocity, and these attributes are independent of the state of the other agents.

Our population-based approach models the organisms with a radially symmetric distribution whose centroid lies on the migratory path. In the individual-based test model, the density of the individuals around their target location arising from their movement model closely follows the probability density function of a 2d normal distribution. From this representation of the individuals' density, we define the population's density, $\rho(\mathbf{p})$, to be the value of the standard 2d normal distribution with a mean of zero in each ordinate and a variance. So our population's density

at $\mathbf{p}$ is given by

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

where $\mathbf{p} = (p_x, p_y)$ 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, ρ, integrated over the finite disk with a radius, τ, is one, and σ^2 is the variance for the distribution. The effective radius of the population, τ, was taken to be three times the variance in the distance of the individuals from $\mathbf{m}(t)$. If the distribution of individuals around the point $\mathbf{m}(t)$ and the distribution of the population around $\mathbf{m}(t)$were not consistent, then the contaminant exposure of the two submodels would be incompatible and the sort of mutation error discussed in the introduction becomes significant.

In contrast to individuals, populations do not need to maintain position or velocity since both are determined by $\mathbf{m}(t)$. They do, however, maintain the number of organisms they represent and, in order to make mutation simpler, populations maintain a list of contaminants. In the homogeneous population model the length of this list never exceeds one, since the population has only one mean, but in a mutating submodel, the contaminant loads of the individuals are carried along and decayed as described in section 2.1.

2.1. The migratory circle and the plume

The migratory path is the circular periodic function $\mathbf{m}(t)$ which has a radius of R and a period Y. This path is used for all the variant submodels of the system.

The plume is modelled as a circular or elliptical cloud of some contaminant which intersects this path and has an intensity which varies sinusoidally at a frequency which is relatively prime to the annual migration cycle.

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, $\mathbf{r}$, within the plume at time t is given by

$$I(t, \mathbf{r}) = \frac{1}{2}(1 + \cos(2\pi t/p)) \exp(-\psi\phi(\mathbf{r}, \mathbf{m}_{plume})),$$

where p is the period of the plume, $\mathbf{m}_{plume}$ is the centroid of the plume, ψ is a decay exponent, and for a circular plume the distance function ϕ is taken to be $\phi(\mathbf{a}, \mathbf{b}) = |\mathbf{a} - \mathbf{b}|$. The intensity is made elliptical by instead taking $\phi(\mathbf{a}, \mathbf{b}) = \sqrt{(\mathbf{a} - \mathbf{b}) \cdot (\sqrt{2}, \sqrt{1/2})}$ since this transformation preserves the area of the plume. The effective radius of the circular plume in the model is about 3.7% of R.

2.2. Contaminant load and contact

The equation for 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 a standard uptake-depuration equation

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

which is solved numerically with a fourth order Runge-Kutta algorithm for the value of C given a contact mass, M, and an initial contaminant value or vector of values for C.

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

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

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

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

where $\mathbf{\Omega}$ is an area over which we assess the effective area of the population and $\mathbf{p}+\omega$ denotes the area $\mathbf{\Omega}$ translated so

that its centroid corresponds to **p**. The contact equations are solved using a simple adaptive quadrature routine.

3. The mutating submodel

The mutating submodel is formed by interleaving the population representation and the individual-based representation. The transitions between a submodel and its alternate representation are dictated by its proximity to the contaminant plume. Initially the test model begins with the group of organisms represented as a population. The starting location is far enough away from the plume that there is no chance of any interaction between organisms represented by the population and the contaminant field. As the population moves about the circle it reaches a point at which there is a likelihood that sometime in the next few time steps an individual within its disk could conceivably encounter contaminants, and at this point the population is disaggregated into submodels representing individuals. Similarly, an individual-based submodel switches to a population submodel when there is no possibility that it will encounter the plume. These decisions obviously rely on knowledge of the system; specifically the static location of the plume, the rates of movement and the length of time steps.

The scenario presented exhibits traits that are common to a number of situations which may pertain to broad class of contaminant uptake models. Many contaminant sources, such as storm water outfalls and agricultural crops, are relatively stationary and in some regards their "plumes" are reasonably well bounded and predictable. The migratory path is a simple equivalent to some periodic behaviour that brings our simulated animals into contact with the area of the plume, such as the seasonal movement from one foraging ground to another, migration for breeding purposes, and even the long, isolated intervals underground exhibited by cicadas.

The contaminant levels of the individual-based submodels subsumed by the population representation are maintained and updated every step by the application of the uptake-depuration equation. No relative location information is maintained.

4. Experimentation

The comparison of the three modelling schemes is based on the following:

1. the correspondence between the total contaminant loads across the biomass through time
2. a comparison of variability in contaminant load through time amongst the representations
3. the run-times for each representation
4. and the sensitivity to variability in the nature of the plume.

Our strategy is to first establish the equivalence of the results from the mutating submodel representation and the individual-based representation. 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 twelve years in each of the two individual-based representations using a circular contaminant field. The homogeneous population model is deterministic and so one run is sufficient.

A second set of trials is used to compare the performance of the mutating test model against the homogeneous population model when the contaminant plume is elliptical. Ideally, the results with an elliptical plume would be consistent across the model representations, though the results will show this is not the case.

The analysis in this section is based on two sets of simulations. The purpose of each of these sets is to provide data for a comparison of run-times, the equivalence (or lack of equivalence) amongst the submodels, and to examine the robustness of the representations to changes in the configuration of the plume.

The first set is comprised of forty trials of each of the homogeneous representations (individual-based and population-based) and the mutating model. Each of these trials tracked either forty individuals or a population which represented forty individuals or a mixed system. In this set of runs the contaminant plume was circular 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 equivalence which ought to exist between the purely individual-based submodel and the mutating submodel.

A set of trials with an elliptical plume were run to generate a set of data for comparison against the the data from the trials with a circular plume. Our analysis in these trials is based on the data from the first series of trials and from eighty trials of forty individuals with a mutating representation and a corresponding population-based trial with each trial covering twelve years. The elliptical plume has a major axis which is tangential to the migratory path and covers the same area as the circular plume. The integral over the area of the plumes are the same, up to the numerical error in the quadrature. Our initial analysis will only consider the trials in the first set of runs; a comparison of the responses to the elliptical plume will be treated separately.

Both population-based and individual-based representations suppress 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.

4.1. 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 submodel produces a "mean load" across the whole group of entities it is representing. The mutating submodel sits between the two, sometimes producing individual time series and sometimes mean time series for varying parts of the population. We denote representations by a subscript $r \in \{i, m, p\}$, so that $C_{rkj}(t)$ is the time series associated with individual j in trial k of representation r, $C_{rk}(t)$ is the mean over all the individuals in the indicated representation and trial, and $C_r(t)$ denotes the mean of $C_{rk}(t)$ across the k trials for the indicated representation. 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 submodel from time steps which have a mixture of individual trajectories and mean trajectories from population-based representations. Each of mean time series, $C_{rk}(t)$, correspond to the mean contaminant load of the population, $C_p(t)$, produced by the population submodel; averaging them – constructing

$$C_r(t) = \frac{1}{k} \sum_{j=1}^{k} C_{rj}(t),$$

where r is one of 'i' or 'm' – is equivalent to running many stochastic trials and averaging to fit the population submodel.

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,

$$\bar{C}_r = \frac{1}{T} \sum_{t \in T} C_r(t)$$

These data are presented in Table 1.

Table 1: Maxima and Means

$Series_r$	$\hat{C}_r$	$\bar{C}_r$
C_i	0.1787	0.0390
C_m	0.1821	0.0392
C_p	0.1387	0.0350

These data suggest that the mutating representation is consistent with the homogeneous individual-based representation. The population-based representation seems to present markedly different mean and maximum values.

4.2. Contaminant load variability

We calculated measures of variability in the time series using the aggregated time series $C_{ik}(t)$ and $C_{mk}(t)$ and their respective means across the k trials, $C_i(t)$ and $C_m(t)$. We'll take T to be the total number of time steps taken, and we take

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

and

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

to be the maximum root mean square error and the average root mean square error. Clearly we can write $\bar{\sigma}_{rr}$ as $\bar{\sigma}_r$ without introducing ambiguity, and similarly for $\hat{\sigma}_r$. The values for these measure of of variability are presented in Table 2.

The data here indicate that the variability about the mean is consistent in the two representations which use simulated individuals as an avenue for estimating contact and uptake. This is what we would expect since the mechanisms of uptake and contact are the same. In contrast, the population's values suggest that the contact and uptake are quite different, and that the model does not perform in quite the same way.

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

r.m.s.e.	$r = i$	$r = m$	$r = p$
$\widehat{\sigma}_{ir}$	0.0083	0.0084	0.0534
$\bar{\sigma}_{ir}$	0.0024	0.0024	0.0096
$\widehat{\sigma}_{mr}$	0.0090	0.0090	0.0538
$\bar{\sigma}_{mr}$	0.0024	0.0024	0.0096

4.3. Sensitivity to the shape of the plume

We will use the same notation as Section 4.2 for the data derived from the circular plumes, while we will add a prime symbol to the data derived from the elliptical plumes. Thus, the mean value time series for the mutating submodel with elliptical plumes would be denoted C'_m and the mean value of that time series is $\bar{C}'$.

There is a good correspondence between the means and deviations associated with the mutating model in the circular and elliptical plume scenarios, but there is much poorer correspondence in the population based results in the two scenarios. The data for the circular plume and for the elliptical plume are presented in Tables 3 and 4 respectively.

Table 3: Circular plume results

$Series_r$	$\hat{C}_r$	$\bar{C}_r$	StdDev	$r = m$	$r = p$
C_m	0.1738	0.0392	$\widehat{\sigma}_{mr}$	0.0088	0.0535
C_p	0.1387	0.0350	$\bar{\sigma}_{mr}$	0.0024	0.0098

Table 4: Elliptical plume results

$Series_r$	$\widehat{C'}_r$	$\overline{C'}_r$	StdDev	$r = m$	$r = p$
C'_m	0.1856	0.0394	$\widehat{\sigma}'_{mr}$	0.0087	0.0616
C'_p	0.1763	0.0445	$\bar{\sigma}'_{mr}$	0.0025	0.0092

The population based model is clearly more sensitive to the shape of the plume than the mutating model. It seems likely that the major driver of this difference is that the long axis of the plume (a region where the net contact will be higher) remains in close proximity to the centroid of population where the population density is greatest.

4.4. Run-time

Each run collected data regarding the amount of time spent in different parts of the submodel. 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 provides illumination into just where the effort is concentrated. Predictably, most of the effort is in calculating contact and updating contaminant loads.

The optimisation of suppressing 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 submodel (of the order of 3%), and seems unlikely to make a great deal of difference to the mutating submodel. In the case of the purely individual-based submodel, this sort of optimisation is likely to play a much bigger role in that any penalty would be multiplied by the number of animals simulated.

The population submodel ran for 98.7 cpu seconds. This submodel 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 submodels took just over a mean time of 4205 cpu seconds with a standard deviation of approximately 16 seconds and the mean of the mutating submodel's run time was 1157 cpu seconds with a standard deviation of slightly over 11 cpu seconds.

5. Discussion

The data establish the relative speeds of the three approaches and support the assertion that the mutating submodel 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 runtime with the mutating submodel when compared to the individual-based submodel. The population submodel, while fastest by several orders of magnitude, showed responses to the two distinct contaminant plumes which were significantly different to those of the other two submodels.

The divergence between the population's density function and the observed distribution of individuals in the individual-based representation is potentially a source of model mismatch or bias. Though the actual distribution of individuals is slightly skewed by their motion along the migratory circle, it was very close to a two dimensional normal distribution and a standard 2d normal distribution was chosen to represent the density function of population with its variance taken from the observed individuals. Such a distribution corresponds to an ideal situation – in practice there may be a number of environmental influences which make a such a simple population distribution unrealistic: in the case of a coastal population, exceptions might include mud-flats, sand bars or islands.

5.1. Mutating models

The mutating model tests whether it may be more efficient in terms of time or representational accuracy to change the representation of components of the model in response to the local states of its submodels. The specific

example we are dealing with is very simple, 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 tests for coincidence, generating a random walks, and evaluating the uptake and decay of contaminant loads. 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 between animals and the plume. This strategy of changing representation is fundamentally about managing the often competing demands of representational accuracy, mathematical tractability, and run-time.

The mutating submodel is an ensemble of cooperating submodels working together like a team in a relay race. Each of the representations has its own strengths and passes the baton to another at an appropriate time. So each of the submodels must have mappings between other representations which preserve as much information as possible without imposing excessive burden. As a first step in construction we must determine what information should be maintained in each of the representations to ensure that the migration from one formulation to another doesn't introduce unreasonable error and how that information should be maintained. In our example, the *significant* information which the individual-based representation possesses (which the population representation does not) is the variation in contaminants amongst the individuals within the group. We assume that the role of the individual locations of these individuals in this model is not important over 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 their relative position.

The state spaces of our base-line representations differ, in contrast to the example of Newtonian and Relativistic motion. The natural state space of the individual based submodel must incorporate position information lacking in the population's state space, since the population's movement is determined wholly by $\mathbf{m}(t)$ and the individuals each have their own path. This is quite different to adaptive models where scales or step sizes are adjusted to improve the efficiency of the algorithm. Not only does the algorithm change in this model, but the domain and range of the system changes as well, and the mapping between these state spaces should be considered carefully.

The initial premise was that an individual's trajectory through its environment plays a significant role in its contact with contaminants, and that the population model doesn't capture this contamination load as well. The implication is that the contaminant loads of the individuals must be preserved through model transitions, so in this regard the state space should remain the same, though our implementation of the uptake and decay of the contaminant load of populations has to operate on a list of contaminants.

The transition from individuals to population and population to individuals involves the loss and reconstruction of this fine-scale position data. The assumption that we can reconstruct a plausible position for each individual from the population's distribution function is tenable because there is no behavioural change associated with contaminant load – a contaminant that made an organism sluggish would obviously skew the distributions of both the population as a whole and the distribution of intoxicated organisms within the population. This is an important point: if the data we glean from the individual-based representations is valuable, we don't want to lose it or corrupt it by an inappropriate treatment of the data. Any systematic behaviour arising from the interaction with the plume must be accounted for when we transfer from one representation to another.

In the presented model, individuals are mapped into a population by adding their contaminant level to the contaminant list of an appropriate population after their movement and contaminant decay have been calcu-

lated. When a population submodel is mapped back to an individual-based representation, new individual-based submodels are created with appropriate contaminant levels and random locations which 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 submodels 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.

This illustrates the two basic ways of managing the transitions between state spaces: by adjusting the algorithmic representation of a submodel to maintain essential data, or by dynamically generating missing data at the point of transition. In our example model both of these mechanisms are relatively straightforward, but it is easy to see greater complexity may arise. The state information which may be required by an alternative representation may not be easy to synthesise, as may be the case where there are strong interactions between individuals; or alternatively the update step may require a much larger contextual environment.

5.2. Transition heuristics

When do we swap from one representation to another? More fundamentally, *how* do we decide to swap? The constraints we impose on this example model are quite stringent so the heuristics we can use to decide when to change representation may 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 consistently encounter contaminants for some non-trivial period, and a mapping is called for.

The test 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 accommodate it. This spatial constraint is stringent enough, when combined with the movement constraints, that the system hasn't needed to create more than one population in any of the annual cycles in the trials.

The transition rules in this submodel, 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 instantiated sources, when the sources of contamination could be determined at the beginning of a time-step. This particular submodel 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.

5.3. Means, maxima and variation

In terms of the formulation of the mutating submodel, it is difficult to see how there could be a significant difference between its contaminant loads and those of the the purely individual-based submodel. The means, maxima and the various calculations of deviation between the individual-based and mutating submodels were very close and this supports the belief that they can be treated as essentially equivalent models of the contaminant load in the group of simulated organisms. Both of these representations, however, differed noticeably from the population submodel; 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 statistics on the variation between representations ($\bar{\sigma}_{ab}$, and $\hat{\sigma}_{ab}$) indicate that there is very little difference between the data produced by either the base-line individual-based model and the data produced by a mutating model. The population model, in contrast, produces means and maximum values which are significantly lower (11% and 22%) than those of the individual-based model.

The discrepancy between the population-based uptake and individual-based uptake is enough to suggest the following three possibilities:

- the (normal) distribution of the population around its centroid was not consistent with the individual's spatial dynamics,
- the extent of the population submodel was not adequately tuned with respect to the individuals,
- interactions between the plume and the population or the plume and the individuals was not modelled appropriately

This is the sort of situation discussed in section 5.4. The fundamental submodels 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.

5.4. Representational sensitivity to plume distribution

The issue of whether the configuration of the plume has an 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 representation affords, but this may not be a good idea if there is poor correspondence between the two submodels over their domain.

The data from the mutating model in the set of trials with elliptical plumes had means, maxima and standard deviations which were consistent with the set of trials which used circular contaminant fields. This matches our expectations since the total areas covered and the total contaminant load over the area are the same for the two representations, and the speed of the agents through the plume is relatively slow. In contrast, the circular and elliptical trials of the population submodel 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 submodel may have systematic problems with the population wide sampling of the plume – the increase in mean and maximum levels when the plume was elliptical 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 normal distribution about a centroid may not behave well with respect to plume dynamics.

Set against this, the numeric modelling of populations is well established. It is quite likely that the individual-based submodel would have failed to adequately capture recruitment and mortality dynamics if they had been included in the study. In such a situation, the mutating submodel would have performed best overall – largely maintaining the fidelity of each of the representations across the state-space.

5.5. Run-time

The population submodel 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 vastly outweigh benefits of individual-based representations. In situations where mean-field assumptions occasionally fail to hold it is similarly clear that there are benefits to using mutating submodels. Purely individual-based submodels 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 submodel's 'non-productive' overhead may be competitive with the overheads associated with the management and transition of mutating submodels.

It is difficult to decide what an optimal representation of a system is – not only is the trade-off between run-time and resolution a dilemma, but we then have to consider (at least in the case of stochastic models) whether to go for minimal error, or to maximise the number of trials in the time at hand. In the case of error versus number of trials, we can make an informed decision on where that balance lies if we have a good estimate of how closely the model tracks the "truth" but this is often not possible, particularly when the subject of the study is poorly observed.

6. Conclusion

The case for considering modelling schemes where the representation of a system changes in response to its local state seems to have merit. There are clear advantages in run-time relative to homogeneous individual-based simulations. In contrast there would seem to be little to gain in run-time with a shift from population-based representations to individual-based representations, but in situations where there are behavioural changes – particularly changes which affect the distribution of individuals – the scope for increasing the accuracy of the models is attractive.

The principle source of extra overhead in this modelling structure is in the scheduler which manages the multiple submodels. In the homogeneous population model, there is only one submodel running, and the extra cost of the more general scheduler over a simple iterative loop is negligible. Similarly the overhead in the homogeneous individual-based model is comparable to an additional iterative loop over the agents. Neither contribute a significant amount to the total time spent running a trial; both the solution of the uptake-depuration equation and the calculation of the contact dominated the run-time in both homogeneous models.

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.

Even if we can count on the regular doubling of computational capacity which we've enjoyed for so long, the mag-

nitude of the problems we consider seems likely to grow as fast as our capacity and possibly faster. In our experience of large scale marine ecosystem modelling, the size of the system considered is growing much faster than the computational capacity. Even for small systems the possibility of adjusting the representation of submodels to optimise the accuracy of the model as a whole has great appeal. Mutating models may provide an effective means of concentrating the use of computational capacity where it is most needed.

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