Increasing model efficiency by dynamically changing model representations

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Abstract

There are a number of strategies to deal with modelling large complex systems such as large marine ecosystems. These systems are often comprised of many submodels, each contributing to the overall trajectory of the system. The balance between the acceptable modelling error and the run-time often dictates the form of these 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 encounters a diffuse contaminant in a localised region as an example of such a system, and discusses the key issues that arise from the approach.

1. Introduction

There is a body of literature stretching back several decades which discusses individual-based modelling as a useful alternative to classical models. Early examples modelled forest canopy dynamics, notably JABOWA and its derivatives (Botkin et al. (1972a), Botkin et al. (1972b)). The number of significant papers and books has steadily increased since the 1980s. These works describe the use of individual-based models across a broad range of systems, and the relative strengths and weaknesses of the approach (such as Huston et al. (1988), DeAngelis and Gross (1992) and Grimm and Railsback (2005)). Classical models exploring populations and ecological systems are usually associated with modelling the dynamics of large groups and arguably appeared at the end of the eighteenth century with Malthus's ***An Essay on the Principle of Population*** (1798). The properties of these models are well understood and their state variables usually correspond to measurable quantities. Often, they are much faster than individual-based counterparts, and the analysis of model error may be much more straightforward. Classical and individual-based approaches represent the ends of a spectrum of aggregation in time, space and membership. Representations lying between these extrema, such as described by Scheffer et al. (1995), capitalise on the process-fidelity of an individual-based representation and gain some of the computational efficiency of a more aggregated classical approach, but an adaptive exploitation of the strengths of different representations is possible and worth exploring.

Ecosystem models are becoming broader in scope (Rose et al. (2010), DeAngelis et al. (1998), Harvey et al. (2003) Fulton et al. (2004), CSIRO (2007), CSIRO (2009)) and include more species with richer environments. The environmental response to climate change has also made anthropogenic pressure an important feature in many of these models. As this trend grows it seems less likely that a single model drawn from any particular region of this spectrum will be able to address all members and processes equally well. Simulation models often embed their subject in an "environment" comprised of primary data and other models and these components may occupy many places in the spectrum of representations. The model's actual implementation may be anything from a set of distinct models which are coupled together but retain their independence, to a corpus of code with the submodels so integrated that there is no real distinction between one "model" and the next.

The dynamics associated with biological and ecological systems can depend on the distributions and states of individuals in ways which are not amenable to equation-based modelling. The individual-based models described in Farolfi et al. (2010), and de Almeida et al. (2010) deal with systems of this sort. Versions of these models could be embedded in a common simulation environment in order to address more complex problems which span traditional domain boundaries, and such a model could address broader questions, such as how mosquito control strategies may best adapt to evolving agricultural practices and watershed conditions. Thiele and Grimm (2010) describes an

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extension to NetLogo which allows modellers to incorporate calls to R functions to aid in configuring the model to meet desirable mathematical conditions, to provide ongoing analysis, and to display the model's state through its run. This interface between R and NetLogo could be extended to support incorporating mathematical decision models written in R into the model's decision tree. The fusion of these three elements would form a system capable of simulating possible trajectories for the management of watersheds and human health in ways which would not be possible with a traditional monolithic modelling approach.

Models are including more functional groups and the interactions between components are becoming more detailed. It is costly in terms of computational load to address this increased demand for detail: individual-based models of populations may be very good at capturing vulnerability to exceptional events, but such simulations take a long time. Much of this time may be spent with the model in a largely unchallenging or uninteresting part of its state-space.

This paper explores the technique of changing the representation of a component of a model based on its location in its state-space. Modellers already do this to some degree: time-steps or spatial resolutions are changed, particular code paths may be by-passed to avoid pointless work, or additional calculations might be performed to reduce the error when the state is changing rapidly. These optimisations are largely optimisations of the *encoding* of the model or submodels, rather than an actual change in representation.

Vincenot et al. (2011) make a clear case for considering what the authors term "hybrid-models." They present four reference cases which they use to describe ways in which equation-based models and individual-based models might be coupled to increase their utility. Their categories of hybrid-models are: individual-based models interacting with a single system dynamics model, system dynamics models embedded in individual-based models, individual-based models interacting with a number of system dynamics models, and models in which the representation swaps between individual-based and an equation-based form. They argue that a hybrid approach may provide a means of increasing the speed and accuracy of our models and Lyne et al. (1994) and Gray et al. (2006) have demonstrated that large models of ecosystems can be modelled this way. Vincenot et al. note that they found relatively few models which use both individual-based and equation-based submodels, and they present no existing models representing their fourth reference case. This final case, where models swap from equation-based to individual-based, is briefly described in general terms and is clearly intended to encompass models like the model of this paper.

This "mutating" or "switching" approach to the problem of managing complex simulations was developed using the experience from making several large scale human-ecosystem interaction models (Lyne et al.; Gray et al.; and a current, larger study of Ningaloo coastal region (*work in progress*)). In each of these studies a significant component of the model focused on simulating the interaction between organisms and contaminant plumes, though there is nothing that inherently limits the techniques to these sorts of studies. Lyne et al. assessed the potential of contaminants originating in industrial waste percolating through the food chain into commercially exploited fish stocks. Gray et al. developed a regional model to assess managment strategies for human activity which interacts with the biological systems along the Northwest Shelf of Australia.

Simulating contaminant interactions in an ecosystem is expensive in terms of run-time and memory use. The models described by Gray et al. and Lyne et al. include contaminant transport, uptake and depuration modelling, with behavioural sensitivity to contaminants. In Gray et al., the time taken to run a simulation with contaminants increased by roughly an order of magnitude, and in both studies a large amount of time was spent in regions where no interaction with contaminant plumes was possible. Monte (2009) presents a lucid discussion of analytic *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 states 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.

It is unnecessary to run a complex model and carry the burden of maintaining its state when a simple model may perform better. If representations are switched appropriately, there is potential for improvements in run-time and accuracy. We need to consider four basic questions to do this:

1. What data need to persist across representations?
2. When should a model change representation?
3. How is the initial state for a new representation constructed?
4. How should the error associated with the loss of state information be managed?

The answer to these questions is specific to the set of submodels in question. Before expending resources and effort on a large scale model there needs to be a demonstration that the notion is worth pursuing, and some indication of how it might be accomplished. The aim of this paper is to

provide this demonstration rather than to develop a comprehensive body of techniques supporting the approach. Many systems may benefit from similar techniques; obvious candidates are models of marginal populations, and the population dynamics of animals with behaviour where short periods of time have a significant influence on population levels (Wolff (1994) and Elderd and Nott (2008), for example).

2. Overview: an *ODD* model description

The *ODD* protocol (Grimm et al., 2006) is used to describe the example model. We discuss the issues associated with making such a system, strategies and the reasons behind them in the Discussion section.

2.1. Purpose

This example model plays two roles. Its first is as an explicit demonstration, and the second is as a tool to explore the larger subject of changing a model's representation in response to its state. This example is overly simple, but it shares a number of features with plausible models and the analysis and development of the mutating model should be a reasonable template for other systems.

The model simulates organisms moving along a simple migratory path which intersects a region containing a field of fluctuating contamination (see Figure 2.1). This model exhibits fundamental attributes of larger studies of pollutant/ecosystem interactions (Lyne et al. and Gray et al.) and, while it is not intended to accurately represent any particular system, it might loosely correspond to some body of water influenced by contaminant loads associated with terrestrial runoff resulting from intense rainfalls.

Figure 1: Snapshots of individuals' locations at 28 day intervals superimposed on the migratory path. The plume's contact domain is marked by a grey ellipse near the position of individuals at day 28, with the track of a single individual approaching it. The domain of a population is is circumscribed around the individuals at day 196 for comparison.

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. In a *mutating* configuration, a trial will have different models take turns representing components of the system.

The population-based and individual-based submodels have been kept as similar as practicable in order to minimise the sources of divergence.

2.2. State variables and scales

There are essentially three distinct submodels in the simulation: an individual-based representation of the migrating group, population-based representation of the group, and a contaminant uptake-depuration model. We can think of the models which take the role of the group as candidates for filling a *niche*, which we can think of as the "sub-model shaped hole" in the middle of the program. Because the individual-based and population based models have fundamentally different spatial representations, each of these models include mechanisms to evaluate their contact with a plume as they move through their environment. The spatial domain of the whole model system is a circular region with an arbitrary radius of somewhat more than 100km which encompasses both the area influenced by the contaminant source and the annual migratory path of the organisms. The plume can be viewed as a forcing function in the model and it has a maximum footprint area of approximately $43km^2$ which may be circular or elliptical and is centered on a point of the migratory circle. Both the elliptic and circular variants of the plume have the same area, and their intensities are adjusted so that the integral of the contaminant concentration over the region is the same.

The individual-based representation maintains a contaminant load associated with contact with the plume, a location, a direction and the next time at which it is scheduled to run. The population-based representation treats the group as homogeneous with respect to all state variables other than the contaminant load, and maintains only a record of its next time-to-run and an indication of contaminant load in the population. In the straight population-based representation, this is a single value, but in the mutating system the submodel maintains a list of contaminant loads which correspond to the non-zero loads of individuals. The plume model is deterministic with respect to time and location and maintains no state variables.

2.3. Process overview and scheduling

Simulations were run with 90 minute timesteps for a period representing twelve years. At each time-step, each instance of a submodel is rostered in a priority queue sorted on the "time-to-run" state variable, and when it comes to the top of the queue it executes.

Populations operate in a straightforward way: their path is deterministic, exposure to contaminants is calculated, and the resulting values are fed through the uptake-depuration equation. Individuals calculate their path (a segment of a directed random walk which follows the path of migration) and contact for the timestep and an apply the uptake-depuration equation. At the end of a timestep in non-mutating configurations, data is accumulated for output and each submodel reinserts itself in the priority queue. Otherwise, a heuristic is used to choose an appropriate representation for the niche in next timestep and that is inserted into the queue. Randomisation within a time-step is unnecessary, since the individual's or the population's contaminant updates are resolved for the contaminant contact across their time-step and are not dependent on the state of any other agents.

3. Design concepts

The central reason for the model is the mutability of the representation of the simulated organisms. Individuals and populations in the model are profoundly simple: no real scope is present for any of the trait categories mentioned in Grimm et al. (2006), apart from their interaction with the contaminant plume, though this interaction is completely deterministic with respect to their path through the plume. In place of these traits, we have the basic heuristics associated with triggering a change from a population-based representation to individuals and a corresponding heuristic which indicates when an individual should join (or become) a population. The actual mechanism which turns a population into individuals or its converse is not necessarily a property of those models. Since the objective is to examine the impact of changing model representation in a fairly narrow situation, no attempt is made to optimise the submodels in the "non-contact" areas which constitute most of the model domain.

4. Details

4.1. Initialisation

Individuals and populations initially begin with no contaminant load, and individuals are positioned according to the two-dimensional normal distribution which characterises the population's assumed distribution. When a population mutates into an appropriate set of individuals, the individuals are positioned in the same fashion (centered on the centre of the population) with their corresponding contaminant loads either taken from the list of non-zero contaminant loads maintained by the population or initialised to be zero should the population's list fall short.

4.2. Input

Several characteristic features of the model are determined by the time and location represented. The contaminant intensity (and hence extent) at any point, $\mathbf{r}$, relative to the centroid of the plume, $\mathbf{m}_{plume}$, at a time, t, by the equation

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

where p is the period of 34 days, $\psi = 0.05$ is a decay exponent. We take ϕ to be a distance function, either $\phi(\mathbf{a}, \mathbf{b}) = |\mathbf{a} - \mathbf{b}|$, for a circular plume, or $\phi(\mathbf{a}, \mathbf{b}) = \sqrt{(\mathbf{a} - \mathbf{b}) \cdot (\sqrt{2}, \sqrt{1/2})}$, for an elliptical plume. The effective radius of the circular plume in the model is about 3.7% of the circular migratory path of the populations and individuals. The intensity of the elliptical plume is adjusted by scalar multiplication so that the integral of I for the two plumes over their domain is the same.

The individual-based and population-based models follow a circular migratory path about the origin. The path is traced annually and its location at any given time follows the equation $\mathbf{l}(t) = 10^5 (\cos(2t\pi/365.25), \sin(2t\pi/365.25))$.

4.3. Submodels

4.3.1. Individual-based representation

Individuals follow a directed random walk around the migratory circle described in the previous section. At each time-step the stride the individual takes is calculated according to its proximity to the "target" on the migratory path. There are a number of parameters associated with the movement of the individuals presented in Table 1.

Table 1: Parameters associated with individual movemement

Parameter	Value	Description
$\overline{V}$	4	A "variability" parameter associated with a Poisson-like process
q	0.5	A magnitude control parameter on directional change
μ_δ	1 day	Notional interval over which we calibrate individual's movement
μ	20km	Indicates the radius which is likely in a period of μ_δ
s	4ms^{-1}	nominal speed of the individuals

If we take δ to be the length of the current time step, and v to be a realisation of an event in a Poisson-like process with a mean of $\overline{V}$, we can take

$$Q = \left[1 - \exp\left(\frac{v}{\overline{V}} \log(1 - q)\right)\right]$$

to be a "variation" scalar which we use to evaluate an effective radial speed,

$$\nu_s = \left| -1 + \sqrt{1 + 4sQ^2 \frac{\delta}{\overline{V}}} \right| / 2Q^2.$$

Large values of Q correspond to long stretches of time without a change in direction, so we include Q in the calculation of α, the partial change in the individual's direction vector, by setting it to $\alpha = \pi rnd(-Q, Q)$. We can take their effective displacement over the 90 minute interval to be determined by a weighted sum of the normalised vector which joins them to their "target" location on the migratory path and a direction vector of length ν_s which is deflected by α.

4.3.2. Population-based representation

The population-based model assumes that a radially symmetric, normal distribution of individuals is an appropriate representation. Trials using the movement model of the individual-based model were run, and the positions of individuals relative to their "target" on the migratory circle at each time-step closely matched a 2D-normal distribution with a $\sigma^2 = 3136.25^2$. Using this value, we define the density of the population at the point $\mathbf{p} = (p_x, p_y)$, relative to the population's centre, to be

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

$S_L = 1.015$ is a scaling parameter chosen so that the integral over the population's effective disk, $\mathbf{D} = \left\{\mathbf{q} \in Domain\,(\rho) : |\mathbf{q}| \leqslant 3\sigma^2\right\}$, gives

$$\int_{\mathbf{D}} \rho\,(\mathbf{p})\, d\mathbf{p} = 1.$$

4.3.3. Contaminant handling

Initially a contact value is calculated for the time step. For an individual, this value is the integral of the contaminant level over its path. Population contact is calculated in an analogous way over the domain of the population and it represents the average contact of the members of the population.

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

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

where our variable $\mathbf{p}$ is a vector with time and location and we assume that the motion from $\mathbf{P}_t$ to $\mathbf{P}_{t+\delta}$ is along a straight line segment. We take $\|\mathbf{p}\|$ to be the speed at which the individual is moving.

Population's contact occurs across its domain and we calculate the definite integral

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

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 $\mathbf{p}$. The contact equations are solved using a simple adaptive quadrature routine. This value corresponds to the most likely mean contact in the population.

For both models of our organisms, uptake and depuration is modelled by the ordinary differential equation

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

where $u = 0.02$ is the uptake rate, a decay rate which is approximately λ =0.0059. The equation 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

4.3.4. Mutating sub-models

The individual-based representation requires no change to run in a mutating configuration, but the population-based representation must maintain a list of contaminant loads which are processed in exactly the same way a scalar might be processed in one of the simple configurations. In the mutating configuration, each instance of a model is assessed at the end of its timestep to determine whether a change in representation is appropriate.

When a population disaggregates into individuals, the set of individuals with contaminant loads corresponding to the entries in the list are created. Their locations are normally distributed within the population disk. Any shortfall in numbers is handled by creating individuals which have no contaminant load and positioning them in the same fashion. Once the individuals are created, the population model is allowed to terminate.

An individual joins a population by having its contaminant load added to the list the population maintains. The first step in the process is to determine if there is a population close enough to the individual. If not, an empty population is created. Once a population's contaminant load has been inserted into the population the individual is allowed to terminate. The population model itself does not really play a part in this transaction: the "import" call is never used directly by the population, rather it is the supervising scheduler which organises the transfer to and from individuals and populations.

5. Results

The data presented in section 5.1 are based on two sets of simulations representing forty individuals. The first set uses a circular plume and the second an elliptical plume. These data sets allow a comparison of run-times, the equivalence (or lack of equivalence) amongst the submodels, and thet provide data to examine the robustness of the representations to changes in the configuration of the plume. To ensure that run-time comparisons are meaningful all of the simulations in the first set of trials were run on the same computer.

The first set is comprised of forty trials of the homogeneous individual-based model, corresponding trials of the mutating model, and a single run of the population-based model. The second set is comprised of eighty trials of the mutating model and a single run of the population-based model. The data in the first set of trials establishes the equivalence of the homogeneous individual-based model and the mutating model. We pool the data from the mutating and homogeneous individual-based runs from the first set to match the eighty runs in the second to compare the effect of the plume's configuration. The results with an elliptical plume were not consistent across the model representations.

The individual-based representation produces a time series of contaminant levels for each individual, while the

population submodel produces a "mean load" across a group of entities. 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 contaminant load at t in time series, C, associated with individual j in trial k of representation r, $C_{rk}(t)$ is the mean at a time t over all the groups simulated 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. 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 $C_{mk}(t)$. We are careful to generate 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 the mean time series, $C_{rk}(t)$, corresponds to the mean contaminant load of the population, $C_p(t)$, produced by the population submodel; averaging them, that is 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,

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

5.1. Contaminant load correspondence between representations

Both sets, $\bar{C}_r$ and $\hat{C}_r$, are presented in Table 2.

Table 2: 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.

5.2. 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 will 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 variability are presented in Table 3.

Table 3: 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

The data here indicate that the variability about the mean is consistent in the two representations which use simulated individuals to estimate 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 this model does not perform in quite the same way.

5.3. Sensitivity to the shape of the plume

We will use the same notation as Section 5.2 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 4 and 5 respectively.

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

Table 4: 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 5: 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

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.

5.4. Run-time

Each run collected data regarding the amount of time spent in different parts of the submodel; 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 submodel (about 3%). It 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; 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.

6. Discussion

In the example our objective is to produce time-series data associated with the contaminant load of the group. Our individual-based model is taken as the best model for capturing the contact that real organisms have with an intermittent plume, and the population based representation has a computational efficiency that the individuals lack. The case for swapping in the example model is reasonably clear: there is a distinct improvement in run-time with no apparent deterioration in the fidelity of the dynamics. It seems likely that the naïve population distribution may be introducing a systematic divergence from what we see as an accurate, but computationally intense, individual-based model.

The general case is not limited to the polar extremes of switching between individual-based models and populations. A niche may have many representations, each of which has a particular set of strengths and weaknesses. This adaptive approach would present the same scope for improvement in purely equation-based models, where rules of thumb might be replaced by first-order approximations, or by complex systems of differential equations. In a purely individual-based example, the depth of the representation of the individual might vary from a simple mass and location through to a level of detail which included the individual's metabolic rates and breeding characteristics.

6.1. State spaces

To make our population-based model compatible with the individual-based model we have to extend the population's state space and maintain additional information to preserve the essential parts of the individual representation that makes it valuable to us. This is basically posing the first of the enumerated question from section 1. The *significant* information which the individual-based representation possesses is embodied in the contaminant loads amongst the individuals which comprise the group. We assume that the role of their relative locations about the population's centre is not important over a large portion of the global state-space and that we can discard it when we move from individuals to populations.

The union of submodels' state-spaces can generally be decomposed into *processing sets* of state-variables. Partitioning the state variables in this way – particularly in advance – makes it easier to analyse and minimise the boundary effects associated with the transition from one representation to another. Within a representation, the state variables which are unique to it form a special subset. The subset can be divided into the variables which need to be maintained by other representations, which we call V_r, and the variables which do not which we will call U_r. In principle, the variables in V_r might be maintained by a routine which is common to them all. The variables in U_r are more complex: when some other representation is mutating to representation r, the values assigned to the variables in U_r should reflect the state implied by the state of the old representation.

In the example model, an individual's relative location is a member of this set. Variables which are maintained and used by more than one representation are the third major group. This group can be divided into the set which is used consistently across the submodels (W_r), and the group of variables which have different dynamics in the various representations (X_r). In our example case, the

contaminant load level of an individual would belong to the set V_{ind}. Its location and velocity would be in U_{ind}, the current time for both individuals and populations belongs to W_r, and a list of contaminant loads for populations belongs to V_{pop}.

6.2. Heuristics

The example model has very simple dynamics: the plumes are always in the same place, the migration is very predictable, and the spatial domain an individual may explore is well contained. Implementing a heuristic for the model which efficiently decides when to move from one representation to another is very straightforward: *If we are close enough that an individual might encounter the plume if the plume were at its maximum, switch a population to a group of individuals. Conversely, if there is no chance that an individual heading straight toward the plume (backwards) will encounter it, move the individual to a "close enough" population, or create a new population to accomodate the individual.* The model was constructed so that any number of populations could be run, and the heuristic was framed so that there were no assumptions about the number of population agents and the size of the groups they represented.

In this model, the decision process was shared between the representations themselves and the controlling scheduler. The representations reported their "robustness" to the scheduler which would then decide how to act on the advice, either triggering a change in representation or not.

The goal is to have a complex ensemble of niches which will change representations under the aegis of the scheduler to optimise the global outcome. For this more general approach additional information is needed: the scheduler would incorporate information about what properties each of the current representations required from other niches in order to decide what the mix of submodels filling the niches ought to be.

6.3. Transitions

The transition from individuals to population and population to individuals involves the loss and reconstruction of fine-scale position data, which may be a source of error. In our example, we assume that we can reconstruct a plausible position for each individual from the population's distribution function because we know the typical distribution of individuals and there is no behavioural change associated with contaminant load. A contaminant that made an organism sluggish would skew the distributions of both the population as a whole and the distribution of intoxicated organisms within the population. In the example model, individuals were randomly located in this way with enough time to randomise their velocities and blur any artifacts resulting from the selection of their locations. This corresponds to the perception that the velocities and relative locations of the individuals are comparatively unimportant except as they related to the distribution of the population. When values of state variables are generated in the process of changing to another representation, they need to conform to the distributions of the representation they are leaving. If for some strange reason (like behavioural change) the distribution of individuals, for example, does *not* conform to the distribution associated with a coherent population, then additional steps need to be taken accomodate this when changing to a population-based representation.

In section 6.2, transitions between representations in the example model are mediated by the scheduler. Decisions to change representation must be based, in part, on whether the transition will increase or decrease the efficacy of the suite of representations as a whole. If the example model were more than a pedagogic tool, it would have been useful to assess the mean error introduced in the transition from population to individual and individual to population. Our simulation was aimed at producing contaminant load results, but in this context our aim would be to track the mean position, variance and extrema of the distribution of individuals relative to the population. To do this we would perform a comparison similar to that of section 5 but using positional data rather than contaminant load. The results would indicate if there might be significant transition effects associated with the change in representation. This sort of testing should ideally be performed at a number of scales (temporal or spatial, for example) since the knowledge of how long it takes for the transition boundary effects to settle (if they do) should feed into the high-level managing scheduler. In a sophisticated system, a representation might be spun up in advance so that the boundary effects have settled before it takes over from a less efficient representation.

6.4. Errors

Estimating error and confidence is extremely hard in complex models. Not only are the abstract processes deeply connected, but there may be hundreds of thousands of lines of code[1] which may introduce error of their own. Confronted with the code of a large-scale marine ecosystem model, one might turn around and contemplate joining a monastery rather than try and track the error propagation through the system. When we look at making an aggregate model out of niches, we can make the set of each of the representations which fill the niche simpler than some chimera which tries to take the best bits of each of the candidate representations. With well isolated transition mechanisms, we side-step nests of conditional code-paths and can contain the potential sources of error we must analyse. Since transitions can be recorded (like other useful data), we can generate an indication of the likely level of confidence based on our understanding of the representations used in a simulation.

[1] Ningaloo-InVitro is currently more than 233000 lines of C++, NWS-InVitro is slightly more than 118000 lines of C++ and Atlantis is more than 145000.

7. Conclusion

Interesting and unanticipated results have come from this experiment. The discrepancy between the data concerning elliptical and circular plumes suggests that, at least in contaminant work, we need to pay closer attention to the movement dynamics of individuals and the density functions of populations. More predictably, the run-times show that mutating configurations provide a reasonable means of increasing computational speed without sacrificing fidelity in appropriate situations. The simple example demonstrated that a model which changes the representation of the system according to its location in its state space could provide much better computational efficiency than a model with a constant representation with no loss of accuracy.

Increasing population and resource use often reduce our environment's resilience and there is a growing need to model larger, more complex parts of the system we live in. Techniques for this have been iteratively moving toward a more systematic approach: many models will optimise their run-time and accuracy by suppressing unnecessary calculation, models will split their timesteps according to what they are simulating, or perhaps even adaptively set an appropriate timestep or spatial scale.

This paper proposes that actually changing the representations to suit the different regions of the state space of the model could provide a better balance between computational efficiency and error.

In our experience of large scale marine ecosystem modelling, the size of the system considered is growing much faster than 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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