Spatial-Temporal Marked Point Processes : A Spectrum of Stochastic Models

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Overview

- The construction and pattern analysis of spatial-temporal marked point processes has been fuelled by two separate fields of study.
- In biology plants are affected by others that compete for nutrient and natural resources.
- Whilst fundamental to the study of porous and granular material is the modelling and statistical analysis of random systems of hard particles.
- Renshaw and Särkkä (2001) and Särkkä and Renshaw (2006) construct a general packing algorithm that covers both situations in order to infer properties and generating mechanisms of space-time stochastic processes.

The Model

- Marks $m_i(t)$ $(i = 1, \ldots, n)$ have location x_i and change size through the *deterministic* incremental size change

$$m_i(t + dt) = m_i(t) + f(m_i(t))dt + \sum_{j \neq i} h(m_i(t), m_j(t); \|x_i - x_j\|)dt \; . \qquad (1)$$

- $f(\cdot)$ is the mark growth function in the absence of spatial interaction.
- $h(\cdot)$ is an appropriate spatial interaction function taken over all points $j \neq i$.
- Random variation can be induced in many ways, e.g. via the simple immigration-death or birth-death process.
- If $m_i(t + dt) \leq 0$ then point i dies 'interactively' and is deleted, as happens for natural death.

Huge number of potential forms for $f(\cdot)$ and $h(\cdot)$

- The simple birth function $f_1(m(t)) = \lambda m(t)$ is unbounded.
- So stable forms such as the linear and logistic processes $f_2(m(t)) = \lambda(1 - m(t))$ and $f_3(m(t)) = \lambda m(t)(1 - m(t)/K)$ are better.
- Both are special cases of the logistic power-law process

$$dm(t)/dt = am(t) - d[m(t)]^{p+1} \quad \Rightarrow \quad m(t) = K[1 + ce^{-apt}]^{-1/p}$$

for $K = (a/d)^{1/p}$ and $c = [K/m(0)]^p - 1$.

- This plays a major role in the modelling of tree growth via the Von Bertalanffy-Chapman-Richards (VBCR) growth function

$$f_5(m(t)) = a_0 m_i(t)^{a_1} - a_2 m_i(t)$$

where $a_0 = \beta K^v/v$, $a_1 = (1 - v)$ and $a_2 = \beta/v$: K is the tree-size carrying capacity, β scales the time axis, and v defines the curve shape.

- *Multiple Equilibria:* $f_6(m) = (170m^2 + 100000)/(m^2 + 8000) - m$

has locally stable equilibrium points at 20 ($0 \leq m < 50$) and 100 ($m > 50$); $m = 50$ is a locally unstable equilibrium point (Renshaw, 2009). So gives large and small marks.

Two particular forms for $h(\cdot)$ cover a wide range of situations

- Symmetric hard-core interaction function

$$h_1(m_i(t), m_j(t); \|x_i - x_j\|) = -bI(\|x_i - x_j\| < r(m_i(t) + m_j(t))) \ ,$$

where $I(F) = 1$ if F is true and $I(F) = 0$ otherwise.

- For an asymmetric soft-core form that takes account of the relative sizes of two interacting marks, let $D(x_i, s)$ denote the disk with centre x_i and radius s, and place

$$h_2(m_i(t), m_j(t); \|x_i - x_j\|) = -b \ \text{area}\{D(x_i, rm_i(t)) \cap D(x_j, rm_j(t))\}/(\pi r^2 m_i^2(t)) \ .$$

R&S use maximum pseudo-likelihood to estimate parameters for patterns that are sampled at a *fixed* time point, whilst S&R develop a least squares procedure for *successive* time points.

Forestry Application Comparing Two Proposed Thinning Regimes

(1) Single-thinning from below with 100% and 50% trees cut from small & medium diameter classes:

(2) Double-thinning with (1) followed by thinning from above which cuts 50% of trees from remaining medium and large diameter classes.

Figure 1 shows population size over 100 years, quadratic mean diameter & stand basal area.

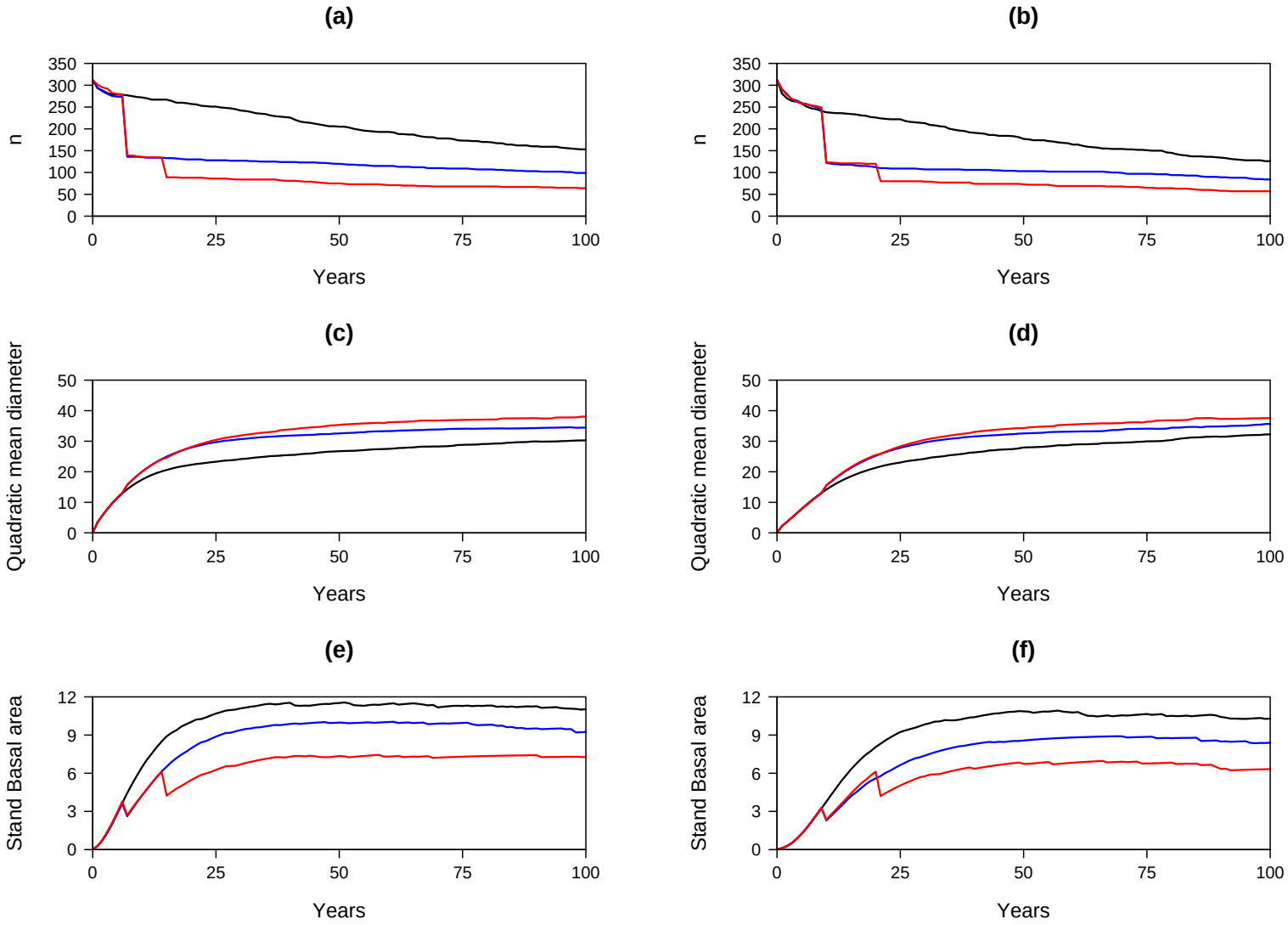


Fig. 1: $h_2(\cdot)$ with $r = 0.01$ and VBCR $f_5(\cdot)$ with $\beta = 0.052$, $K = 25$ and $b = 0.6$; $n = 312$ trees at $t = 0$ with $U(0.25, 0.75)$ radii. Cases (a), (c) and (e) relate to $v = 1$, and (b), (d) and (f) to $v = 0.7$.

Non-treated forest (—); single-thinning from below (—); from below & above (—).

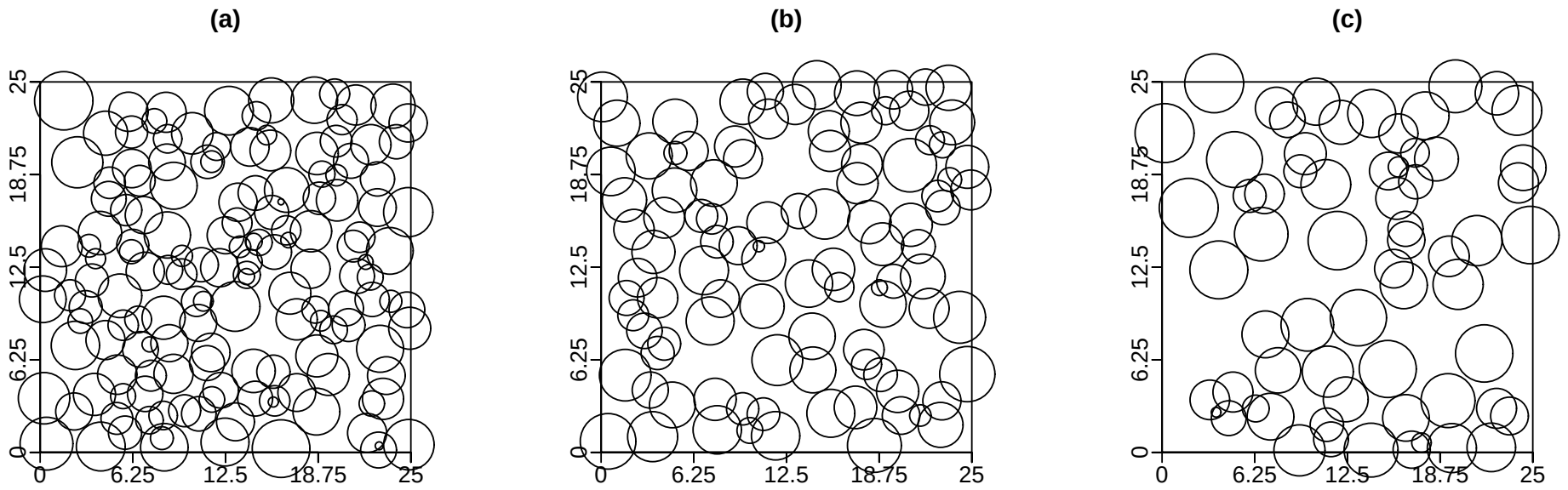


Fig. 2: Spatial structure at $t = 100$ under $v = 1$: (a) no thinning; (b) single-thinning from below; (c) thinning from below and then above (from Renshaw *et al.* 2008).

- Under linear growth ($v = 1$) pop size is larger than under sigmoid growth for both thinning regimes.
- This is in contrast to quadratic mean diameter.
- Thinning from below increases individual tree size: due to reduction in between-tree competition.
- Second thinning from above means increased individual tree size.
- Trees under linear growth have less initial spatial interaction so grow faster.

A Spectrum of Stochastic Modelling Strategies

- In some situations, e.g. materials science, immigration and death might not be appropriate, so how do we inject stochasticity into the system?

To set the scene first consider the non-spatial immigration-death process with $\{U\}$ a sequence of i.i.d. pseudo-random numbers.

Exact Algorithm A1: construct a complete set of event-time pairs $\{e_i, t_i\}$.

(i) set $t = 0$ and $n = n_0$

(ii) cycle over $i = 1, 2, \ldots$

if $U \leq \alpha/(\alpha + n\mu)$ then $e_i = 1$ (immigration) so $n \to n + 1$

else $e_i = -1$ (death) so $n \to n - 1$

place $t_i = t_{i-1} + s_i$ where $s_i = -\ln(U)/(\alpha + n\mu)$

Time-Increment Algorithm A2: In complex scenarios this may be too slow, so replace the variable s by small fixed dt. Then (ii) in A1 becomes

(ii)' cycle over $t = dt, 2dt, 3dt, \ldots$

if $U \leq \alpha dt$ then $n \to n + 1$

else if $U \leq (\alpha + n\mu)dt$ then $n \to n - 1$

else no change

If n varies a great deal, having $\max(n)[(\lambda+\mu)dt] \ll 1 \Longrightarrow$ most events are 'no change'. So could let dt vary with n, e.g. $dt = 0.01/[n(\lambda+\nu)]$.

Tau-Leaping Algorithm A3: Interest in large-scale chemical reaction systems led Dan Gillespie to investigate a more pragmatic approach. Replace dt by a larger τ. Then number of immigrants in $(t, t+\tau)$ is $B(t+\tau) = \text{Poisson}(\alpha\tau)$ etc. So population size is

$$x(t+\tau) = x(t) + B(t+\tau) - D(t+\tau) \qquad (t = 0, \tau, 2\tau, \ldots) \; .$$

For $\{Z_0, Z_1, \ldots\} \sim U(0,1)$, B is the largest integer j such that $\prod_{j=0}^{\infty} Z_j \leq e^{-\alpha\tau}$. So replace (ii)' in A2 by

(ii)" cycle over $t = \tau, 2\tau, \ldots$
evaluate $B \sim \text{Poisson}(\alpha\tau)$ and $D \sim \text{Poisson}(\mu\tau x(t))$
update $x(t)$ to $x(t) + B - D$ and t to $t + \tau$

This works well in any situation deemed to be stiff, i.e. transition rates do not change substantially over time, and no significant dependence between different event types.

Langevin Algorithm A4: Replace Poisson by Normal, then for rates $\{r(x(t))\}$ and $Z \sim N(0,1)$

$$x(t+\tau) = x(t) + \tau \sum_j \mathrm{E}[r_j(x(t))] + \sqrt{\tau} \sum_j \sqrt{\mathrm{E}[r_j(x(t))]} Z_j \; .$$

Chemical Reaction Rate Algorithm A5: Now take the reverse limit $\tau \to dt$, whence A4 becomes the chemical Langevin equation (s.d.e.)

$$x(t+\tau) = x(t) + \tau \sum_j \mathrm{E}[r_j(x(t))] + \sqrt{\tau} \sum_j \sqrt{\mathrm{E}[r_j(x(t))]} dW_j \ ,$$

where $\{dW_j(t)\}$ are independent Brownian motions.

Reaction Rate Algorithm A6: Finally, ignoring the stochastic part of A5 yields the reaction rate (i.e. deterministic) representation

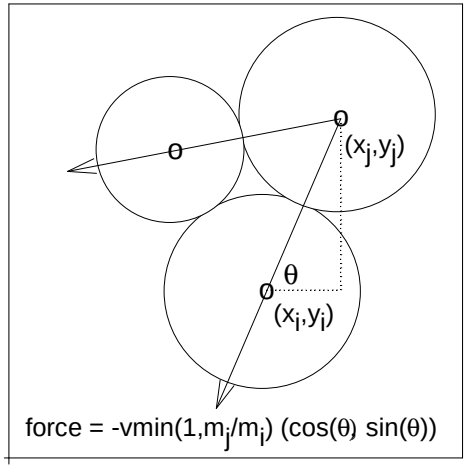
$$x(t+\tau) = x(t) + \tau \sum_j \mathrm{E}[r_j(x(t))] \ .$$

- See Higham(2008) for current challenges and short, downloadable MATLAB codes.

Extending These Ideas to Marked Point Processes

- Spatial-temporal processes may be far more computationally demanding and complex. For example, the construction of maximally packed patterns requires points to move under interaction pressure.

- Reasonable to assert that the relative interaction pressure is greater on the smaller mark than the larger, let the vector force on i from j be (for example) $v \min(1, m_j(t)/m_i(t))$. Then the force-field



shows that during $(t, t + dt)$, i's position is perturbed by

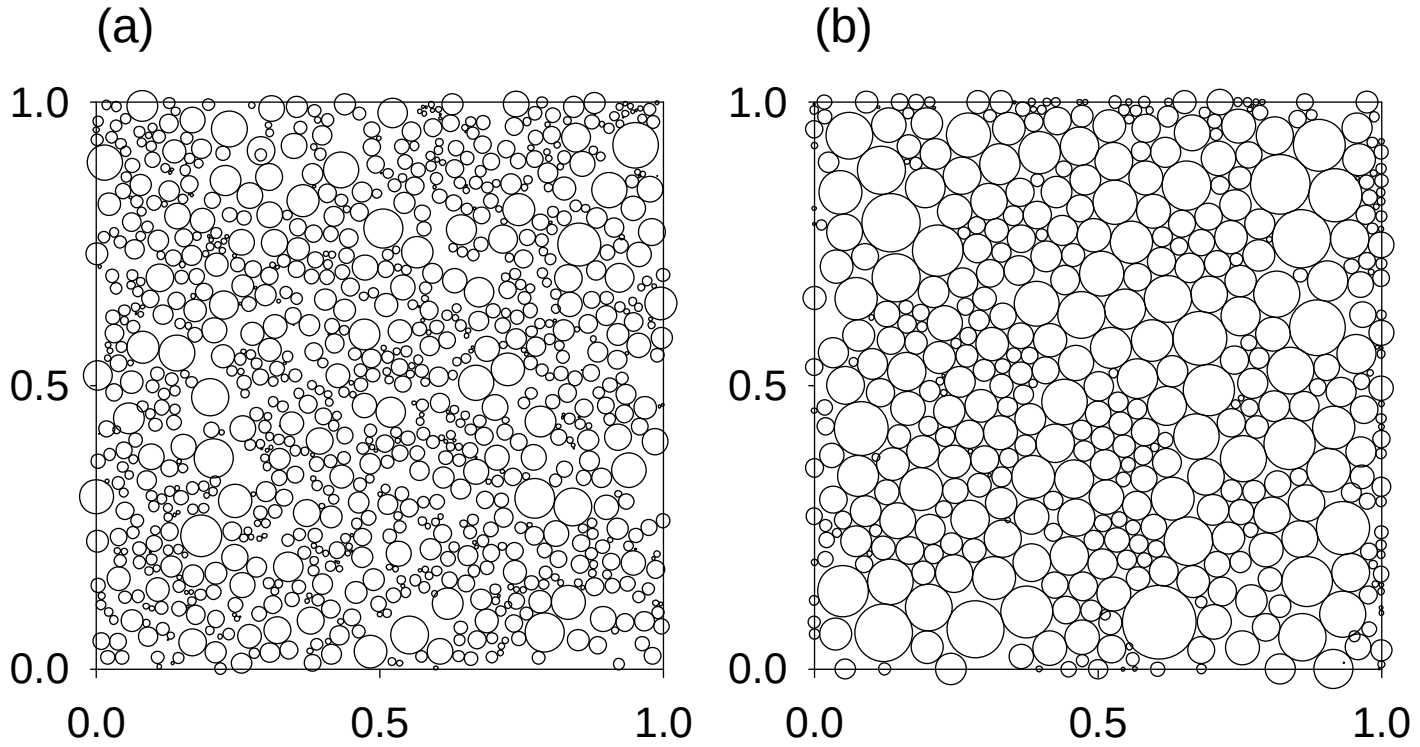
$$(dx_i, dy_i) = -v \min(1, m_j(t)/m_i(t))(\cos(\theta), \sin(\theta))$$

Let $r_{ij} = \sqrt{\{(x_i - x_j)^2 + (y_i - y_j)^2\}}$ be the smallest of the 8 inter-point distances.

Denote $\sum_{j\backslash i}$ to be the sum over all points j that interact with i. Then

$$x_i(t + dt) = x_i(t) + vdt \sum_{j\backslash i} \min(1, m_j(t)/m_i(t))(x_i - x_j)/r_{ij} \ , \quad \text{etc.}$$

Fig. 4: Pattern at $t = 200$ for linear-growth hard-core model (f_2, h_1) with $\alpha = 10$, $\lambda = 1 < b = 2$, $K = 20$, $r = 0.005$, $\tilde{m}_k = 0.01$: (a) $v = 0$ and (b) $v = 0.01$.



- Decompose the growth and interaction functions into general stochastic birth and death components:

$$\begin{aligned} f_i &= f(m_i(t)) && \to f_i^+ - f_i^- \\ h_{ij} &= h(m_i(t), m_j(t); ||i-j||) && \to h_{ij}^+ - h_{ij}^- \end{aligned}$$

where f_i^+ and f_i^- denote pure birth and death h_{ij}^+ and h_{ij}^- denote spatial enhancement and inhibition. Write

$$\lambda_i = f_i^+ + \sum_{j \neq i} h_{ij}^+ \,, \quad \mu_i = f_i^- + \sum_{j \neq i} h_{ij}^- \,, \quad rate = \alpha + \sum_{i=1}^{n} (\lambda_i + \mu_i) \,.$$

- As each marked point is affected differently, we have to use an individual-based approach. Thus for points $i = 1, \ldots, n$, event-time pairs $\{e_k, t_k\}$ $(k = 1, 2, \ldots)$, incremental mark size δ and new mark size $\tilde{m} = integer \times \delta$, A1 becomes:

Exact MPP Algorithm B1:

(i) set $t = 0$ and $n = n_0$

(ii) cycle over individuals $i = 1, 2, \ldots, n$
compute λ_i, μ_i and $rate$
if $U \times rate \leq \alpha$ then $m_{n+1} = \tilde{m}$ at location (U', U''), $n \to n + 1$
else if $U \times rate \leq \alpha + \lambda_1$ then $m_1 = m_1 + \delta$
$\ldots$
else if $U \times rate \leq \alpha + \sum_{i=1}^{n-1}(\lambda_i + \mu_i) + \lambda_n$ then $m_n = m_n + \delta$
else $m_n = m_n - \delta$

(iii) if $i = r$ is the altered mark then recalculate h_{rj} and h_{jr} $(j \neq r)$
if $m_r(t) = 0$ remove r, relabel $i \to i - 1$ for $i > r$, $n \to n - 1$

(iv) update time t to $t - \ln(U)/rate$ and return to (ii)

- Note the switch in mark size from continuous to discrete on $0, \delta, 2\delta, \ldots$.

Time-Increment Algorithm B2:

- Replacing the event times $t = 0, s_1, s_1 + s_2, \ldots$ by the incremental times $t = 0, dt, 2dt, \ldots$ carries through as for A1 to A2, with
- each mark acting independently of all others during $(t, t + dt)$.

Thus in B1 parts (ii) to (iv) are replaced by:

(ii) cycle over individuals $i = 1, 2, \ldots, n$
compute λ_i, μ_i and $rate$
if $U \times rate \leq \alpha dt$ then $m_{n+1}(t + dt) = \tilde{m}$ at (U', U''), $n \longrightarrow n + 1$
else if $U \times rate \leq (\alpha + \lambda_i)dt$ then $m_i(t + dt) = m_i(t) + \delta$
else if $U \times rate \leq (\alpha + \lambda_i + \mu_i)dt$ then $m_i(t + dt) = m_i(t) - \delta$
else $m_i(t + dt) = m_i(t)$

(iv) update time t to $t + dt$ and return to (ii)

Tau-Leaping Algorithm B3:

Switching to Tau-Leaping (A3) involves replacing dt by τ and the independent Bernoulli events by Poisson variables. So B2 is altered to:

(ii) cycle over individuals $i = 1, 2, \ldots, n$
compute λ_i, μ_i and $rate$
$m_i(t + \tau) = \text{Poisson}(\alpha\tau) + \text{Poisson}(\lambda_i\tau) - \text{Poisson}(\mu_i\tau)$

Langevin-Leaping Algorithm B4. Replace Poisson variables in B3 by Normal variables.

Chemical Langevin Algorithm B5. Apply the reverse limit $\tau \longrightarrow dt$ in B4.

Deterministic/Reaction Rate Algorithm B6: Hits problems if allow immigration since cannot allocate new locations deterministically.

Summary

- The R&S procedure, which is B6 and a stochastic 'driver' may be easily generalised to encompass the other approaches B1–B5 across a wide range of disciplines.
- If the exact algorithm B1 incurs too large a compute-time penalty, then analyse B2 to B5 in sequence in order to assess the trade-off between pattern structure and computational efficiency.
- Studies are currently being undertaken to generate models that accurately replicate three-dimensional packing structures for mixed-sized particle systems which previously could only be simulated by using 'sequential packing under gravity' and 'collective rearrangement strategies'.
- A further promising avenue would be to transfer methods recently developed for chemical reaction systems with a low to moderate number of molecules across to marked point processes.
- The scope for future development in this arena is enormous.

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