Supplementary Information for 'Going from microscopic to macroscopic on non-uniform growing domains'

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S.1. THE NECESSITY OF THE VORONOI PARTITION

Recall equations (20)-(22) of Section III B of the main manuscript, relating the mean particle density in the stochastic model:

$$\begin{aligned}
\frac{\mathrm{d}u_1}{\mathrm{d}t} &= \frac{1}{l_1}\left(T_2^- u_2 l_2 - T_1^+ u_1 l_1\right), \\
\frac{\mathrm{d}u_i}{\mathrm{d}t} &= \frac{1}{l_i}\left(T_{i-1}^+ u_{i-1} l_{i-1} - \left(T_i^+ + T_i^-\right) u_i l_i + T_{i+1}^- u_{i+1} l_{i+1}\right), \qquad i = 2, \ldots, k-1, \\
\frac{\mathrm{d}u_k}{\mathrm{d}t} &= \frac{1}{l_k}\left(T_{k-1}^+ u_{k-1} l_{k-1} - T_k^- u_k l_k\right),
\end{aligned} \tag{S.1}$$

where u_i is the density of particles in interval i and l_i is its length. Upon Taylor expansion (recalling the definitions of the distances between domain points: $h_i = x_i - x_{i-1}$, $h_{i+1} = x_{i+1} - x_i$, $h_1 = 2x_1$ and $h_k = 2(y_k - x_k)$) of the density terms in equation (S.1) about x_i we are left with a system of three equations which must be satisfied in order for the particle densities in the stochastic model to recapitulate the diffusion equation in the continuum model:

$$T_{i-1}^+ l_{i-1} h_i - \left(T_i^+ + T_i^-\right), l_i + T_{i+1}^+ l_{i+1} = 0, \tag{S.2}$$

$$T_{i-1}^+ l_{i-1} h_i = T_{i+1}^- l_{i+1} h_{i+1}, \tag{S.3}$$

$$T_{i-1}^+ h_i^2 l_{i-1} + T_{i+1}^- h_{i+1}^2 l_{i+1} = 2 l_i D. \tag{S.4}$$

These equations (valid for $i = 2, \ldots, k$) come from equating coefficients of u_i, $\partial u_i/\partial x$ and $\partial^2 u_i/\partial x^2$, respectively, in the right-hand side of equation (S.1) (once Taylor expansions have been carried out) and the right-hand side of the diffusion equation. Equations (S.3) and (S.4) can be used to find the transition probabilities T_{i-1}^+ and T_{i+1}^- in terms of interval lengths:

$$T_{i-1}^+ = \frac{2Dl_i}{l_{i-1} h_i \left(h_i + h_{i+1}\right)}, \tag{S.5}$$

$$T_{i+1}^- = \frac{2Dl_i}{l_{i+1} h_{i+1} \left(h_i + h_{i+1}\right)}. \tag{S.6}$$

These in turn determine the transition rates T_i^+ and T_i^- by a simple relabeling of indices:

$$T_i^+ = \frac{2Dl_{i+1}}{l_i h_{i+1} \left(h_{i+1} + h_{i+2}\right)}, \tag{S.7}$$

$$T_i^- = \frac{2Dl_{i-1}}{l_i h_i \left(h_{i-1} + h_i\right)}. \tag{S.8}$$

Substituting these expressions for the transition probabilities into equation (S.2) leaves us with the relationship:

$$\frac{l_i}{h_i\left(h_i+h_{i+1}\right)}+\frac{l_i}{h_{i+1}\left(h_i+h_{i+1}\right)}-\frac{l_{i+1}}{h_{i+1}\left(h_{i+1}+h_{i+2}\right)}-\frac{l_{i-1}}{h_i\left(h_{i-1}+h_i\right)}=0. \quad \text{(S.9)}$$

In order to satisfy this equation the length of interval i must be chosen to be proportional to the distance between the neighboring interval definition points of interval i:

$$l_i=\alpha\left(h_i+h_{i+1}\right), \quad \text{(S.10)}$$

for some constant α. The additional constraint that the intervals must be contiguous, covering the domain without any overlaps or gaps between intervals, $\sum_{i=1}^{k} l_i = y_k$, provides us with a value for the constant of proportionality: $\alpha = 1/2$. With this value of α the relationship (S.10) defines the Voronoi domain partition. It is of comfort to note that these choices of l_i, in combination with equations (S.7) and (S.8), recapitulate the transition rates that were given in Section III B of the main manuscript.

S.2. FURTHER ANALYSIS OF THE INTERVAL-CENTERED PARTITION ON THE STATIONARY DOMAIN

Our aim in this section is to test whether the effects of different domain partitions for each repeat of the simulation can lead to a better correspondence between the PDE and the stochastic simulations on the interval-centered partition. In order to test this we ran similar stochastic simulations to those described in Section III D of the main manuscript with the alteration that the non-uniform partition was different for each repeat of the simulation. In order to take an average particle density from each simulation we mapped the particle density of each repeat onto a uniform domain partition, and averaged the density on this partition, as in Section VI of the main manuscript. Fig. S.1 shows the results of these simulations for the simple diffusion process. Clearly the stochastic particle density profile matches the PDE density profile much better than in Fig. 4 of the main manuscript where the domain partition is the same for each simulation. This is demonstrated qualitatively by the lower histogram distance error in Fig. S.1 (f).

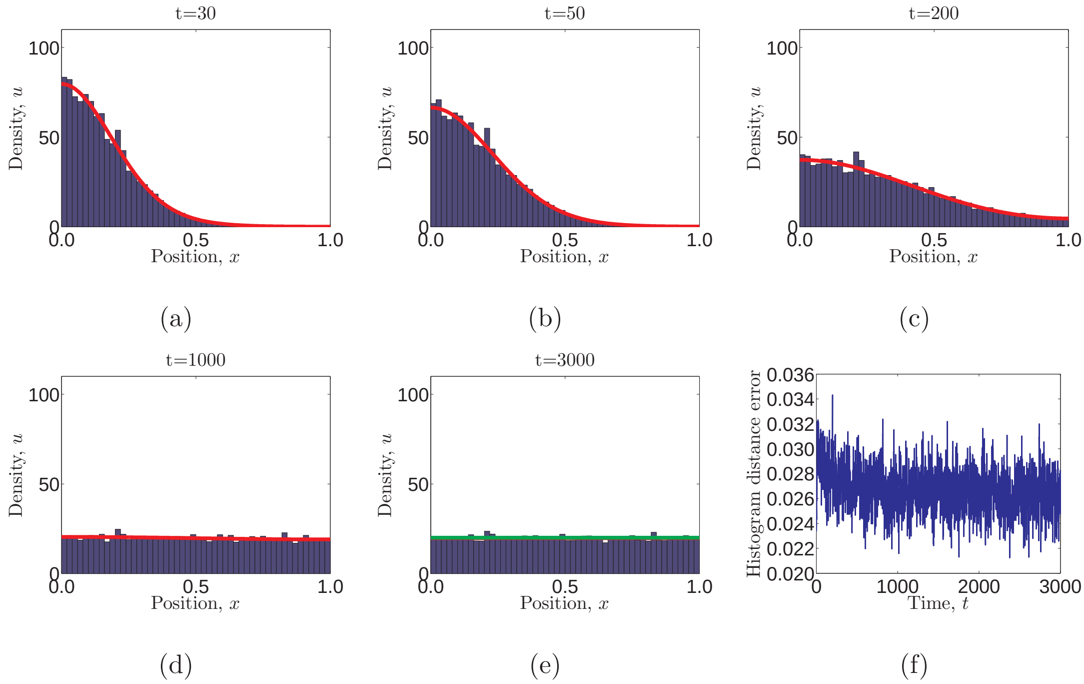

FIG. S.1. *Particles undergoing simple diffusion on an interval-centered domain partition, different for every repeat, at several time points. (a)-(e) Histograms represent an average of 40 stochastic realizations. The solid lines exhibit the result of numerical simulation of the corresponding diffusion equation and the green curve in (e) represents the stationary solution derived analytically. (f) The histogram distance error between the stochastic simulations and the PDE. The boundaries are assumed to be reflecting. Initially particle density has an exponentially decaying profile across the domain. Parameters are as follows:* $k = 50$, $\Delta x = 1/k$, $D = \Delta x^2$. *For a video of the evolution of particle density please see movie FigS2.avi of the supplementary materials.*

It is possible that this improved correspondence between the stochastic simulations and the PDE is an artifact of the regularized repartitioning carried out in order to take averages of the stochastic simulations. In order to test this hypothesis we re-ran the simulations with the same domain partition for each repeat, as in Section III D of the main manuscript, but instead of using these particle densities to compare the stochastic simulation to the PDE we redistribute the particle density onto a regular domain partition as we did in Fig. S.1. The results of these simulations are shown in Fig. S.2. Although the repartitioning improves the qualitative and quantitative comparison between the stochastic simulations and the PDE it is clear that it is by no means the only contributing factor. Repartitioning alone reduces the histogram distance error by half, but repartitioning in combination with random initial domains for each repeat reduces the histogram distance error by an order of magnitude in comparison with the original simulations. This suggests that randomizing the domain for each repeat may be a viable method of obtaining a good approximation to the PDE from the stochastic simulations on the interval-centered domain.

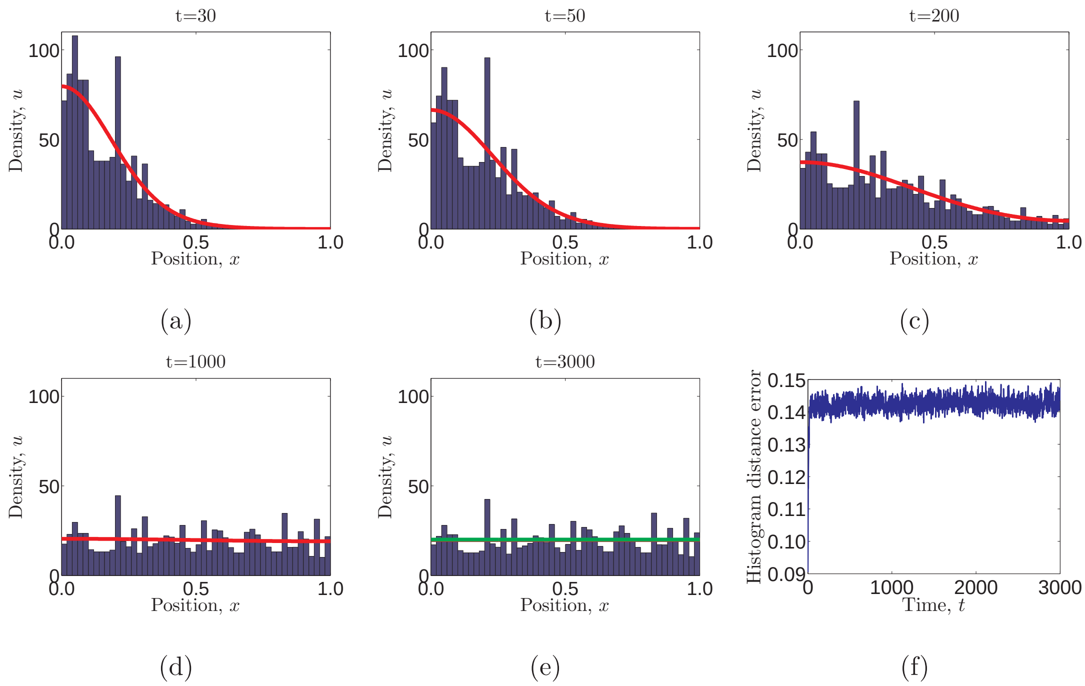

FIG. S.2. *Particles undergoing simple diffusion on the same interval-centered domain partition for every repeat, at several time points. (a)-(e) Histograms represent an average of 40 stochastic realizations. The solid lines exhibit the result of numerical simulation of the corresponding diffusion equation and the green curve in (e) represents the stationary solution derived analytically. (f) The histogram distance error between the stochastic simulations and the PDE. The boundaries are assumed to be reflecting. Initially particle density has an exponentially decaying profile across the domain. Parameters are as in Fig. S.1. For a video of the evolution of particle density please see movie FigS3.avi of the supplementary materials.*

S.3. DERIVATION OF A PDE FOR MEAN PARTICLE NUMBERS DIVIDED BY MEAN INTERVAL LENGTH FOR THE INTERVAL-CENTERED DOMAIN PARTITION

As noted previously, instead of deriving a PDE for density it is possible (and indeed simpler) to derive, as a proxy for particle density, a PDE for average particle numbers divided by average interval length. We begin by assuming average exponential domain growth of each interval, as proved in Section IV C of the main manuscript or as assumed in Section IV A of the main manuscript:

$$\langle l_j \rangle (t) = l_j(0) \exp(r\Delta l t) \quad \text{for} \quad j = 1, \dots, k, \tag{S.11}$$

where $l_j(0)$ is the initial size of interval j. We define $x_j(t)$ as the mean position of the left-hand edge of interval j:

$$x_j(t) = \sum_{i=1}^{j-1} \langle l_i(t) \rangle = \left(\sum_{i=1}^{j-1} l_i(0) \right) \exp(r\Delta l t) = x_j(0) \exp(r\Delta l t), \tag{S.12}$$

where $x_j(0) = \sum_{i=1}^{j-1} l_i(0)$ is the initial position of the left-hand edge of interval j. Consider a continuum level approximation to the density of particles across the domain,

$$\rho(x_j, t) = \frac{N_j}{\langle l_j(t) \rangle}, \tag{S.13}$$

where N_j is the number of particles in interval j at time t which does not change during an interval growth event. Then

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\rho(x_j, t) &= \frac{\partial \rho}{\partial t} + \frac{\partial \rho}{\partial x}\frac{\mathrm{d}x_j}{\mathrm{d}t}, \\ &= \frac{\partial \rho}{\partial t} + r\Delta l x \frac{\partial \rho}{\partial x}. \end{aligned} \tag{S.14}$$

However,

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{N_j}{l_j} \right) &= -\frac{N_j}{l_j^2}\frac{\mathrm{d}l_j}{\mathrm{d}t}, \\ &= -\rho r \Delta l. \end{aligned} \tag{S.15}$$

Equating equations (S.14) and (S.15) for the time derivative of particle density leads us to a PDE for particle density:

$$\frac{\partial \rho}{\partial t} + r\Delta l x \frac{\partial \rho}{\partial x} = -\rho r \Delta l, \tag{S.16}$$

which can be re-written as

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho r \Delta l x) = 0. \tag{S.17}$$

In the absence of particle movement between intervals, this is exactly the equation we would expect for the evolution of particle density (see equation (2) of the main manuscript).

S.4. NUMERICAL SOLUTION OF THE PDE FOR DENSITY-DEPENDENT DOMAIN GROWTH.

In this case we use a Lagrangian formulation, making a transformation of coordinates of the form [1–4]

$$x = \Gamma(X, \tau) \quad \text{and} \quad t = \tau, \tag{S.18}$$

where the advection due to domain growth is defined by the strain rate, $\sigma = u_x$ satisfying

$$\sigma = f(c(x,t)) = \frac{\Gamma_{X\tau}}{\Gamma_X}, \tag{S.19}$$

and the subscripts denote partial derivatives. This leads to the system of PDEs:

$$c_\tau = \frac{D}{\Gamma_X}\left(\frac{c_X}{\Gamma_X}\right)_X - \sigma c, \tag{S.20}$$

$$\Gamma_{X\tau} = \sigma \Gamma_X, \tag{S.21}$$

where $\Gamma(X,0) = X$, $\Gamma(0,t) = 0$ and the usual zero flux boundary conditions apply.

We transform the system to one of first order and employ the NAG library routine D03PE and the NAG Matlab toolbox in order to solve the system numerically.

S.5. HISTOGRAM DISTANCE ERROR FOR INSTANTANEOUS INTERVAL DOUBLING AND SPLITTING DOMAIN GROWTH METHOD

Fig. S.3 shows the histogram distance error for an exponentially growing domain using the interval doubling and splitting method of Baker et al. [5]. The improved correspondence between our new growth method and the mean-field PDE in comparison to the old interval splitting method is demonstrated by a lower histogram distance error (*c.f.* Figs. 9 and 10 in the main manuscript). The difference is particularly stark later in the simulations. Our incremental growth method tends to have a smaller variance in domain length and hence fewer contributions to the histogram distance error from intervals which have grown beyond the region for which we have a PDE solution. These contributions add significantly to the histogram distance error.

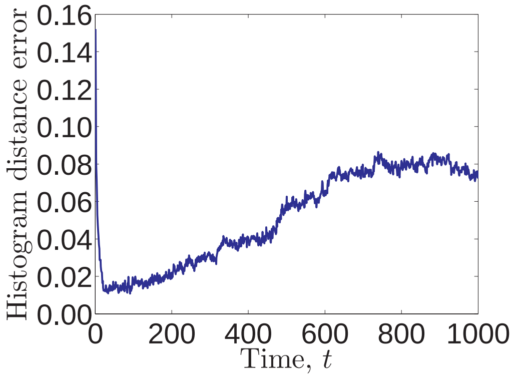

FIG. S.3. *Histogram distance errors for a diffusion simulation using the growth method of Baker et al. [5]. All the particles are initialized in the first interval. Parameters are as follows:* $k_0 = 50$, $\Delta x = 1/k_0$, $D = \Delta x^2$, $r = 0.0001$.

S.6. FURTHER ANALYSIS OF THE INTERVAL-CENTERED PARTITION ON THE GROWING DOMAIN

Fig. S.4 shows the evolution of the average particle density for an initially non-uniform, interval-centered domain partition. The initial partition is different for each repeat of the simulation. The particle density from the discrete model is closer to the density in the PDE model than in the case when all repeats were initialized with the same domain partition (see Fig. 11 in the main manuscript). This is evidenced by the smaller histogram distance error throughout the duration of the simulation shown in Fig. S.4 (f).

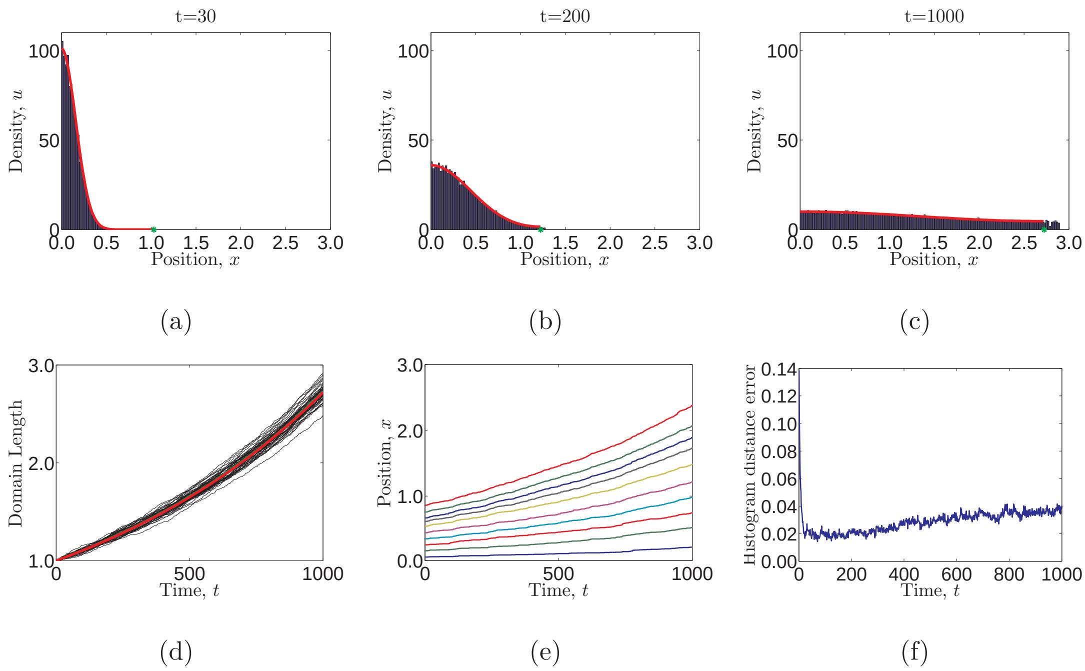

FIG. S.4. *Particles undergoing diffusion at several time points. The underlying stochastic model has an initially non-uniform, interval-centered domain partition (different for each repeat) and undergoes stochastic interval growth. Figure descriptions are as in Figs. 9 and 10 in the main manuscript. All particles are initialized in the first interval. Parameters are as follows:* $k_0 = 50$, $\Delta x = 1/k_0$, $D = \Delta x^2$, $r = 0.0001$, $\Delta l = 0.1 \times \Delta x = 0.002$, $\Delta x_{split} = 2\Delta x = 0.04$. *For a video of the evolution of particle density and domain length please see movie FigS5.avi of the supplementary materials.*

S.7. CONSIDERING MASTER EQUATIONS ON THE VORONOI DOMAIN PARTITION

A. A master equation for interval length on the Voronoi domain partition

Consider a time interval small enough that the probability of more than one growth event occurring in $[t, t + \delta t)$ is $O(\delta t)$ and ignore, for the meantime, the movement of particles. We can express the evolution of the probability that the random variable representing the length of each interval of the domain, L_j, takes the value l_j at time t via the following master equation:

$$
\begin{aligned}
\frac{\mathrm{d}\Pr(\boldsymbol{L}=\boldsymbol{l},t)}{\mathrm{d}t} = r\Bigg\{ & \sum_{i=1}^{k-1} \Pr\left(\boldsymbol{L}=(l_1,\ldots,l_i-\Delta l/2, l_{i+1}-\Delta l/2,\ldots,l_k)\right)(l_i-\Delta l/2) \\
& + \Pr\left(\boldsymbol{L}=(l_1,\ldots,l_k-\Delta l)\right)(l_k-\Delta l)\Bigg\} \\
& - r\sum_{i=1}^{k} l_i \Pr(\boldsymbol{L}=\boldsymbol{l},t),
\end{aligned}
\tag{S.22}
$$

where $\boldsymbol{L}=(L_1,\ldots,L_k)$ is the vector of interval lengths and $\boldsymbol{l}=(l_1,\ldots,l_k)$ is the current state of this vector. Note that we have to treat the end interval as a special case, since when selected to grow it can grow on its own by Δl without the need to make a partner interval grow. In order to find the mean length of interval j we multiply through by l_j and sum over all the (finite number of) possible values that $\boldsymbol{l}$ can take. Upon simplification we arrive at three ODEs which describe how the intervals grow:

$$\frac{\mathrm{d}\langle l_1\rangle}{\mathrm{d}t} = \frac{r\Delta l}{2}\langle l_1\rangle, \tag{S.23}$$

$$\frac{\mathrm{d}\langle l_j\rangle}{\mathrm{d}t} = \frac{r\Delta l}{2}\left(\langle l_{j-1}\rangle + \langle l_j\rangle\right) \quad \text{for} \quad j=2,\ldots,k-1, \tag{S.24}$$

$$\frac{\mathrm{d}\langle l_k\rangle}{\mathrm{d}t} = r\Delta l\left(\frac{\langle l_{k-1}\rangle}{2} + \langle l_k\rangle\right). \tag{S.25}$$

Summing these ODEs for $j=1,\ldots,k$ gives us an ODE for the total domain length:

$$\frac{\mathrm{d}\langle L\rangle}{\mathrm{d}t} = r\Delta l\,\langle L\rangle. \tag{S.26}$$

$$\Rightarrow \langle L(t)\rangle = L_0\exp(r\Delta l t). \tag{S.27}$$

Although we can show that the domain length will increase exponentially, it is clear, from equations (S.23)-(S.25), that individual intervals do not. This means that, on the Voronoi domain, we should not expect to derive a PDE which is completely consistent with uniform exponential growth across the domain as we did with the interval-centered partition.

B. Derivation of the partial differential equation for growth from the master equation on the Voronoi domain partition

Using the same notation as in Section V of the main manuscript (see Table I) we can write down the pre-growth densities on the post-growth domain partition. For all $j < i$ we have

$$q_j = \frac{N_j}{l_j} = \rho_j. \tag{S.28}$$

However, things are more complicated for $j \geq i$ since the post-growth boundaries of the intervals to the right of and including interval i (the interval that splits) no longer correspond to their pre-growth counterparts. For $j = i$:

$$q_i = \frac{N_i + N_{i+1}\left(\Delta l/\left(2\left(l_{i+1} - \Delta l/2\right)\right)\right)}{l_i} = \rho_i + \frac{\rho_{i+1} l_{i+1} \Delta l/2}{l_i\left(l_{i+1} - \Delta l/2\right)}. \tag{S.29}$$

For $j = i + 1$:

$$q_{i+1} = \frac{N_{i+1}\left(1 - \Delta l/2\left(l_{i+1} - \Delta l/2\right)\right) + \left(\Delta l/l_{i+2}\right) N_{i+2}}{l_{i+1}} = \rho_{i+1}\left(\frac{l_{i+1} - \Delta l}{l_{i+1} - \Delta l/2}\right) + \frac{\Delta l \rho_{i+2}}{l_{i+1}}. \tag{S.30}$$

If $i + 1 < j < k$ then we can write the pre-growth densities on the post-growth domain, q_j, associated with interval j as

$$q_j = \frac{N_j\left(1 - \Delta l/l_j\right) + \left(\Delta l/l_{j+1}\right) N_{j+1}}{l_j} = \rho_j\left(1 - \Delta l/l_j\right) + \frac{\Delta l \rho_{j+1}}{l_j}. \tag{S.31}$$

Finally for the last interval, k, the density will become

$$q_k = \frac{N_k\left(1 - \Delta l/l_k\right)}{l_k} = \rho_k\left(1 - \Delta l/l_k\right). \tag{S.32}$$

Now that we have formulated the pre-growth densities on the post-growth domain partition we are in a position to consider the master equation for domain growth (as in the main manuscript),

$$\begin{aligned}\frac{\partial \Pr(\boldsymbol{\rho}, \boldsymbol{l}, t)}{\partial t} &= r \sum_{i=1}^{k} \Pr(q_1, \ldots, q_i, q_{i+1}, \ldots, q_k, l_1, \ldots, l_i - \Delta l/2, l_{i+1} - \Delta l/2, \ldots, l_k, t)\left(l_i - \Delta l/2\right) \\ &\quad - r \sum_{i=1}^{k} \Pr(\boldsymbol{\rho}, \boldsymbol{l}, t) l_i.\end{aligned} \tag{S.33}$$

Multiplying through by the particle density in interval j, ρ_j, and summing over all the possible values that particle density can take (again using the shorthand notation, $\sum_{\boldsymbol{\rho}}$, to represent the double sum over all possible particle numbers and all possible interval widths, $\sum_{\boldsymbol{N}}\sum_{\boldsymbol{l}}$) we arrive at

$$\frac{\partial\langle\rho_j\rangle}{\partial t} = r\sum_{i=1}^{k}\sum_{\boldsymbol{\rho}}\rho_j\,\mathrm{Pr}(q_1,\ldots,q_i,q_{i+1},\ldots,q_k,l_1,\ldots,l_i-\Delta l/2,l_{i+1}-\Delta l/2,\ldots,l_k,t)\,(l_i-\Delta l/2)$$
$$-\,r\sum_{i=1}^{k}\langle\rho_j l_i\rangle\,, \tag{S.34}$$

where $\langle\rho_j\rangle = \sum_{\boldsymbol{\rho}}\rho_j\,\mathrm{Pr}(\boldsymbol{\rho},\boldsymbol{l},t)$ represents the mean particle density in interval j and $\langle\rho_j l_i\rangle = \sum_{\boldsymbol{\rho}}\rho_j l_i\,\mathrm{Pr}(\boldsymbol{\rho},\boldsymbol{l},t)$. For the first sum on the right-hand side we must carefully consider each value of i. For $i > j$ the terms are of the form

$$r\sum_{\boldsymbol{\rho}}\rho_j\,\mathrm{Pr}(q_1,\ldots,q_i,q_{i+1},\ldots,q_k,l_1,\ldots,l_i-\Delta l/2,l_{i+1}-\Delta l/2,\ldots,l_k,t)\,(l_i-\Delta l/2) = r\,\langle\rho_j l_i\rangle\,, \tag{S.35}$$

since $q_j = \rho_j$ for $i > j$. However, if $i \leq j$ then the growth event occurs at, or to the left of, interval j and things are not so simple.

For $j = i$:

$$r\sum_{\boldsymbol{\rho}}\rho_j\,\mathrm{Pr}\Bigg(\rho_1,\ldots,\rho_{i-1},\rho_j+\frac{\rho_{j+1}l_{j+1}\Delta l/2}{l_j\,(l_{j+1}-\Delta l/2)},\rho_{j+1}\left(\frac{l_{j+1}-\Delta l}{l_{j+1}-\Delta l/2}\right)+\frac{\Delta l\rho_{j+2}}{l_{j+1}},\ldots,$$
$$\rho_k\,(1-\Delta l/l_k)\,,l_1,\ldots,l_j-\Delta l/2,l_{j+1}-\Delta l/2,\ldots,l_k,t\Bigg)(l_j-\Delta l/2)\,,$$
$$= r\sum_{\boldsymbol{\rho}}\left(\rho_j+\frac{\rho_{j+1}l_{j+1}\Delta l/2}{l_j\,(l_{j+1}-\Delta l/2)}\right)\mathrm{Pr}\Bigg(\rho_1,\ldots,\rho_{i-1},\rho_j+\frac{\rho_{j+1}l_{j+1}\Delta l/2}{l_j\,(l_{j+1}-\Delta l/2)},\rho_{j+1}\left(\frac{l_{j+1}-\Delta l}{l_{j+1}-\Delta l/2}\right)$$
$$+\frac{\Delta l\rho_{j+2}}{l_{j+1}},\ldots,\rho_k\,(1-\Delta l/l_k)\,,l_1,\ldots,l_j-\Delta l/2,l_{j+1}-\Delta l/2,\ldots,l_k,t\Bigg)(l_j-\Delta l/2)$$
$$-\,r\sum_{\boldsymbol{\rho}}\frac{\rho_{j+1}l_{j+1}\Delta l/2}{l_j\,(l_{j+1}-\Delta l/2)}\mathrm{Pr}\Bigg(\rho_1,\ldots,\rho_{i-1},\rho_j+\frac{\rho_{j+1}l_{j+1}\Delta l/2}{l_j\,(l_{j+1}-\Delta l/2)},\rho_{j+1}\left(\frac{l_{j+1}-\Delta l}{l_{j+1}-\Delta l/2}\right)$$
$$+\frac{\Delta l\rho_{j+2}}{l_{j+1}},\ldots,\rho_k\,(1-\Delta l/l_k)\,,l_1,\ldots,l_j-\Delta l/2,l_{j+1}-\Delta l/2,\ldots,l_k,t\Bigg)(l_j-\Delta l/2)\,,$$
$$= r\,\langle\rho_j l_j\rangle - r\frac{\Delta l}{2}\,\langle\rho_{j+1}\rangle + O(\Delta l^2). \tag{S.36}$$

For $i = j-1$:

$$r\sum_{\boldsymbol{\rho}}\rho_j\,\mathrm{Pr}\Bigg(\rho_1,\ldots,\rho_j\left(\frac{l_j-\Delta l}{l_j-\Delta l/2}\right)+\frac{\Delta l\rho_{j+1}}{l_j},\rho_{j+1}\,(1-\Delta l/l_{j+1})+\frac{\Delta l\rho_{j+2}}{l_{j+1}},\ldots,$$
$$\rho_k\,(1-\Delta l/l_k)\,,l_1,\ldots,l_{j-1}-\Delta l/2,l_j-\Delta l/2,\ldots,l_k,t\Bigg)(l_{j-1}-\Delta l/2)\,,$$

$$= r\sum_{\boldsymbol{\rho}} \left(\frac{l_j - \Delta l/2}{l_j - \Delta l}\right) \left(\left(\frac{l_j - \Delta l}{l_j - \Delta l/2}\right)\rho_j + \frac{\Delta l}{l_j}\rho_{j+1}\right) \Pr\Bigg(\rho_1, \ldots, \rho_{i-1}, \rho_j\left(\frac{l_j - \Delta l}{l_j - \Delta l/2}\right) + \frac{\Delta l \rho_{j+1}}{l_j},$$

$$\rho_{j+1}\left(1 - \Delta l/l_{j+1}\right) + \frac{\Delta l \rho_{j+2}}{l_{j+1}}, \ldots, \rho_k\left(1 - \Delta l/l_k\right), l_1, \ldots, l_{j-1} - \Delta l/2, l_j - \Delta l/2, \ldots, l_k, t\Bigg)(l_{j-1} - \Delta l/2)$$

$$- r\sum_{\boldsymbol{\rho}} \left(\frac{l_j - \Delta l/2}{l_j - \Delta l}\right)\frac{\Delta l}{l_j}\rho_{j+1} \Pr\Bigg(\rho_1, \ldots, \rho_{i-1}, \rho_j\left(\frac{l_j - \Delta l}{l_j - \Delta l/2}\right) + \frac{\Delta l \rho_{j+1}}{l_j}, \rho_{j+1}\left(1 - \Delta l/l_{j+1}\right)$$

$$+ \frac{\Delta l \rho_{j+2}}{l_{j+1}}, \ldots, \rho_k\left(1 - \Delta l/l_k\right), l_1, \ldots, l_{j-1} - \Delta l/2, l_j - \Delta l/2, \ldots, l_k, t\Bigg)(l_{j-1} - \Delta l/2),$$

$$= r\sum_{\boldsymbol{\rho}} \left(1 + \frac{\Delta l}{2(l_j - \Delta l)}\right) \left(\left(\frac{l_j - \Delta l}{l_j - \Delta l/2}\right)\rho_j + \frac{\Delta l}{l_j}\rho_{j+1}\right) \Pr\Bigg(\rho_1, \ldots, \rho_{i-1}, \rho_j\left(\frac{l_j - \Delta l}{l_j - \Delta l/2}\right) + \frac{\Delta l \rho_{j+1}}{l_j},$$

$$\rho_{j+1}\left(1 - \Delta l/l_{j+1}\right) + \frac{\Delta l \rho_{j+2}}{l_{j+1}}, \ldots, \rho_k\left(1 - \Delta l/l_k\right), l_1, \ldots, l_{j-1} - \Delta l/2, l_j - \Delta l/2, \ldots, l_k, t\Bigg)(l_{j-1} - \Delta l/2)$$

$$- r\sum_{\boldsymbol{\rho}} \frac{\Delta l}{l_j - \Delta l}\rho_{j+1} \Pr\Bigg(\rho_1, \ldots, \rho_{i-1}, \rho_j\left(\frac{l_j - \Delta l}{l_j - \Delta l/2}\right) + \frac{\Delta l \rho_{j+1}}{l_j}, \rho_{j+1}\left(1 - \Delta l/l_{j+1}\right) + \frac{\Delta l \rho_{j+2}}{l_{j+1}},$$

$$\ldots, \rho_k\left(1 - \Delta l/l_k\right), l_1, \ldots, l_{j-1} - \Delta l/2, l_j - \Delta l/2, \ldots, l_k, t\Bigg)(l_{j-1} - \Delta l/2) + O(\Delta l),$$

$$= r\left\langle \rho_j l_{j-1}\right\rangle + r\frac{\Delta l}{2}\left\langle \frac{\rho_j l_{j-1}}{l_j}\right\rangle - r\Delta l\left\langle \frac{\rho_{j+1} l_{j-1}}{l_j}\right\rangle + O(\Delta l^2). \tag{S.37}$$

To go between the first and second equality in this statement we have added and subtracted terms that are $O(\Delta l^2)$. Similarly to go between the second and third equalities we have used the Taylor expansion of $1/(l_j - \Delta l)$ and grouped all $O(\Delta l^2)$ terms together:

$$\frac{1}{l_j - \Delta l} = \frac{1}{l_j - \Delta l/2} + \frac{\Delta l}{2}\frac{1}{(l_j - \Delta l/2)^2} + O(\Delta l^2). \tag{S.38}$$

In general for $1 < i < j - 1$ all terms will take a similar form (the same as in equation (61) for interval-centered domain growth in the main manuscript):

$$r\sum_{\boldsymbol{\rho}} \rho_j \Pr\Bigg(q_1, \ldots, q_{j-1}, \rho_j\left(1 - \Delta l/l_j\right) + \frac{\Delta l \rho_{j+1}}{l_j}, \rho_{j+1}\left(1 - \Delta l/l_{j+1}\right) + \frac{\Delta l \rho_{j+2}}{l_{j+1}}, \ldots,$$

$$\rho_k\left(1 - \Delta l/l_k\right), l_1, \ldots, l_i - \Delta l/2, \ldots, l_k, t\Bigg)(l_i - \Delta l/2),$$

$$= r\sum_{\boldsymbol{\rho}} \left(\frac{l_j}{l_j - \Delta l}\right)\left(\rho_j\left(1 - \Delta l/l_j\right) + \frac{\Delta l \rho_{j+1}}{l_j}\right) \Pr\Bigg(q_1, \ldots, q_{j-1}, \rho_j\left(1 - \Delta l/l_j\right) + \frac{\Delta l \rho_{j+1}}{l_j},$$

$$\rho_{j+1}\left(1 - \Delta l/l_{j+1}\right) + \frac{\Delta l \rho_{j+2}}{l_{j+1}}, \ldots, \rho_k\left(1 - \Delta l/l_k\right), l_1, \ldots, l_i - \Delta l/2, \ldots, l_k, t\Bigg)(l_i - \Delta l/2)$$

$$- r\sum_{\boldsymbol{\rho}} \left(\frac{\Delta l}{l_j - \Delta l}\right)\rho_{j+1} \Pr\Bigg(q_1, \ldots, q_{j-1}, \rho_j\left(1 - \Delta l/l_j\right) + \frac{\Delta l \rho_{j+1}}{l_j}, \rho_{j+1}\left(1 - \Delta l/l_{j+1}\right) + \frac{\Delta l \rho_{j+2}}{l_{j+1}},$$

$$
\begin{aligned}
&\quad \ldots, \rho_k\left(1-\Delta l/l_k\right), l_1, \ldots, l_i-\Delta l/2, \ldots, l_k, t\Big)\left(l_i-\Delta l/2\right),\\
&= r\sum_{\boldsymbol{\rho}}\left(1+\frac{\Delta l}{l_j-\Delta l}\right)\left(\rho_j\left(1-\Delta l/l_j\right)+\frac{\Delta l\rho_{j+1}}{l_j}\right)\Pr\Big(q_1, \ldots, q_{j-1}, \rho_j\left(1-\Delta l/l_j\right)+\frac{\Delta l\rho_{j+1}}{l_j},\\
&\quad \rho_{j+1}\left(1-\Delta l/l_{j+1}\right)+\frac{\Delta l\rho_{j+2}}{l_{j+1}}, \ldots, \rho_k\left(1-\Delta l/l_k\right), l_1, \ldots, l_i-\Delta l/2, \ldots, l_k, t\Big)\left(l_i-\Delta l/2\right)\\
&- r\sum_{\boldsymbol{\rho}}\left(\frac{\Delta l}{l_j-\Delta l}\right)\rho_{j+1}\Pr\Big(q_1, \ldots, q_{j-1}, \rho_j\left(1-\Delta l/l_j\right)+\frac{\Delta l\rho_{j+1}}{l_j}, \rho_{j+1}\left(1-\Delta l/l_{j+1}\right)+\frac{\Delta l\rho_{j+2}}{l_{j+1}},\\
&\quad \ldots, \rho_k\left(1-\Delta l/l_k\right), l_1, \ldots, l_i-\Delta l/2, \ldots, l_k, t\Big)\left(l_i-\Delta l/2\right),\\
&= r\left\langle\rho_j l_i\right\rangle + r\Delta l\left\langle\frac{\rho_j l_i}{l_j}\right\rangle - r\Delta l\left\langle\frac{\rho_{j+1} l_i}{l_j}\right\rangle + O(\Delta l^2).
\end{aligned}
\tag{S.39}
$$

Again to arrive at the last equality we have used a Taylor expansion of $1/(l_j-\Delta l)$:

$$
\frac{1}{l_j-\Delta l}=\frac{1}{l_j}+\Delta l\frac{1}{l_j^2}+O(\Delta l^2).
\tag{S.40}
$$

Substituting the expressions from equations (S.36)-(S.39) into the right-hand side of master equation (S.34):

$$
\begin{aligned}
\frac{\partial\left\langle\rho_j\right\rangle}{\partial t} &= r\sum_{i=1}^{k}\left\langle\rho_j l_i\right\rangle - r\sum_{i=1}^{k}\left\langle\rho_j l_i\right\rangle\\
&+ r\Delta l\sum_{i=1}^{j-2}\left\langle\frac{\rho_j l_i}{l_j}\right\rangle - \left\langle\frac{\rho_{j+1} l_i}{l_j}\right\rangle\\
&+ r\Delta l\left(\frac{1}{2}\left\langle\frac{\rho_j l_{j-1}}{l_j}\right\rangle - \left\langle\frac{\rho_{j+1} l_{j-1}}{l_j}\right\rangle\right)\\
&+ r\Delta l\left(\left\langle l_j\right\rangle\frac{\left\langle\rho_j\right\rangle-\left\langle\rho_{j+1}\right\rangle/2}{\left\langle l_j\right\rangle}\right) - r\Delta l\left\langle\rho_j\right\rangle + O(\Delta l^2).
\end{aligned}
\tag{S.41}
$$

We make the moment closure approximation

$$
\left\langle\frac{\rho_j l_i}{l_j}\right\rangle = \frac{\left\langle\rho_j\right\rangle\left\langle l_i\right\rangle}{\left\langle l_j\right\rangle},
\tag{S.42}
$$

in order to derive a PDE for particle density. We have already noted that because each interval does not grow proportionally to its own size domain growth will not be exponential uniformly across the domain. This means that we should not expect to derive the particle density PDE (see equation (67) of the main manuscript) with exponential domain growth, that we derived for the interval-centered domain partition in the main manuscript. In order to be able to compare the stochastic simulations with a deterministic formulation, in which the domain grows exponentially, we need to make an assumption about the relationship between the number of particles in intervals j and $j+1$ to ensure that the final two lines of equation (S.41) can be approximated by partial derivatives in the limit $\Delta l \to 0$. We assume that

$$\frac{r\Delta l}{2}\left(\langle l_{j-1}\rangle \langle \rho_j\rangle - \langle l_j\rangle \langle \rho_{j+1}\rangle\right) = O(\Delta l^2). \tag{S.43}$$

The accuracy of this approximation should determine how well the stochastic simulations correspond to the PDE. Applying these approximations to equation (S.41) gives

$$\frac{\partial \langle \rho_j\rangle}{\partial t} = -r\Delta l \langle \rho_j\rangle - r\Delta l \sum_{i=1}^{j} \langle l_i\rangle \left(\frac{\langle \rho_{j+1}\rangle - \langle \rho_j\rangle}{\langle l_j\rangle}\right) + O(\Delta l^2). \tag{S.44}$$

Taylor expanding the term ρ_{j+1} and neglecting terms of magnitude $O(l_j^2)$ (and hence neglecting $O(\Delta l^2)$ terms since $\Delta l \ll l_j$) we arrive at the final PDE for particle density $u(x,t)$:

$$\frac{\partial u}{\partial t} = -r\Delta l u - r\Delta l x \frac{\partial u}{\partial x}. \tag{S.45}$$

S.8. DOMAIN GROWTH ON THE INTERVAL-CENTERED DOMAIN PARTITION WITH DENSITIES GIVEN BY THE VORONOI PARTITION.

As mentioned in the discussion in the main manuscript, it might be possible to implement exponential domain growth on the interval-centered domain partition, in order to ensure the correct interval growth rates, but to use the Voronoi domain partition when considering particle densities. As a test case we consider the same principle on the stationary domain. The definition of the edges of the intervals are irrelevant to the simulation of particle numbers. It is only when we come to finding particle densities that the interval edges become important. It seems feasible, therefore, that we could implement a particle migration simulation on an interval-centered domain partition and map to the Voronoi domain partition only when we are interested in particle densities. Fig. S.5 shows this to be the case. Qualitatively, in Fig. S.5 (a)-(e) the stochastic particle density profiles match the PDE much better than in Fig. 4 of the main manuscript, and the histogram distance error in Fig. S.5

(f) is over an order of magnitude lower than when densities are calculated on the interval-centered domain partition.

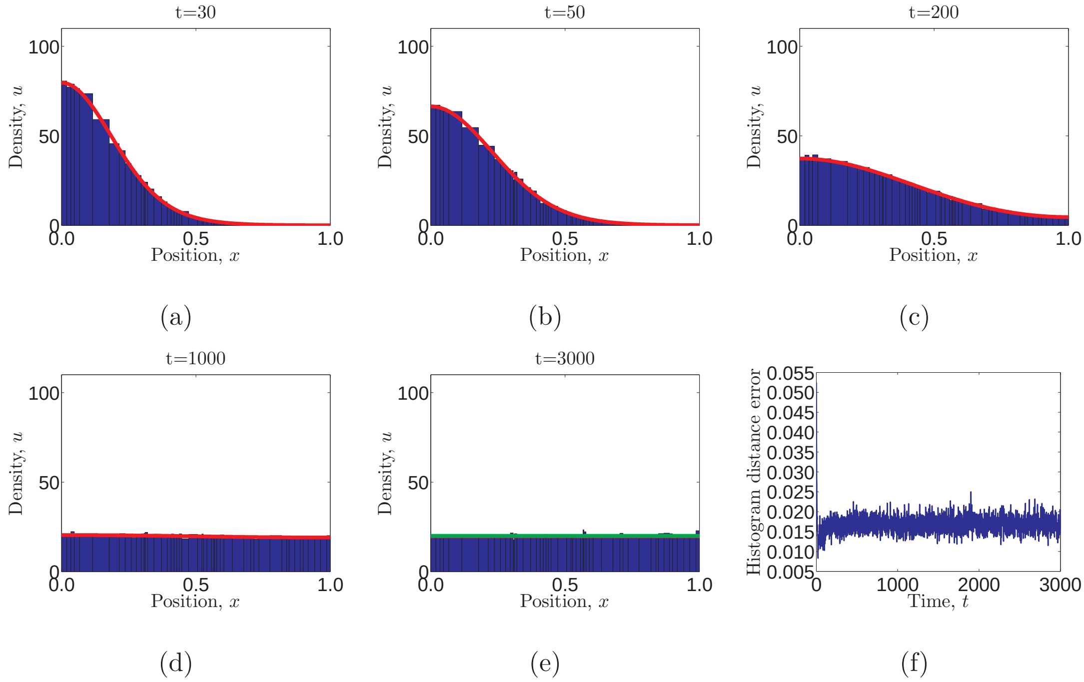

FIG. S.5. *Particles undergoing simple diffusion on an interval-centered domain partition, the same for every repeat, at several time points. Densities are calculated on the Voronoi domain partition. Details are as in Fig. S.1. The boundaries are assumed to be reflecting. All particles are initialized in the first interval. Parameters are as follows:* $k = 50$, $\Delta x = 1/k$, $D = \Delta x^2$. *For a video of the evolution of particle density please see movie FigS6.avi of the supplementary materials.*

The case for growing domains is somewhat different in that the lengths of intervals (and therefore the positions of interval edges) are important when determining the propensity of each interval to grow. It is not immediately clear whether using the interval-centered domain partition to implement domain growth and the Voronoi domain partition when considering densities will improve our results.

By implementing the Voronoi domain partition in order to find densities, Fig. S.6 demonstrates both a qualitative and quantitative improvement over the case when the interval-centered domain partition is used to implement growth *and* calculate particle densities (*c.f.* Fig. 11 of the main manuscript). It also appears to be at least as accurate as using the Voronoi domain partition for implementing growth and calculating particle densities (results not shown).

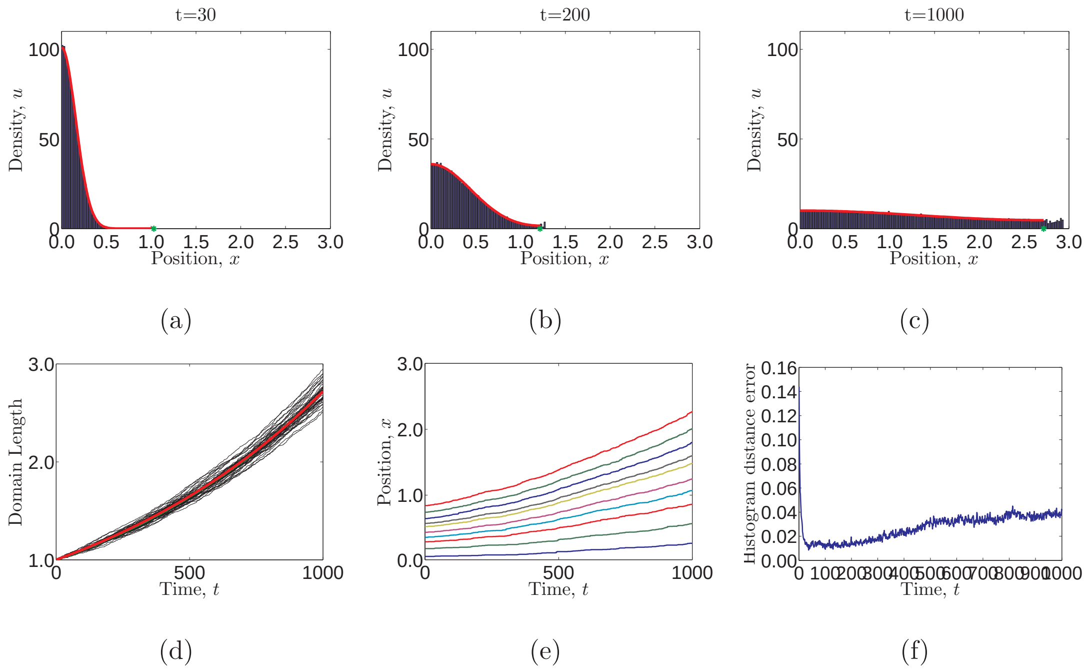

FIG. S.6. *Particles undergoing diffusion at several time points. The underlying stochastic model has an initially non-uniform, interval-centered domain partition (the same for each repeat) and undergoes stochastic interval growth. Densities are calculated on the Voronoi domain partition. Figure descriptions are as in Fig. 9 in the main manuscript. All particles are initialized in the first interval. Parameters are as follows:* $k_0 = 50$, $\Delta x = 1/k_0$, $D = \Delta x^2$, $r = 0.0001$, $\Delta l = 0.1 \times \Delta x = 0.002$, $\Delta x_{split} = 2\Delta x = 0.04$. *For a video of the evolution of particle density and domain length please see movie FigS7.avi of the supplementary materials.*

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