The auxiliary region method for coupling PDE and Brownian-based dynamics for reaction-diffusion systems
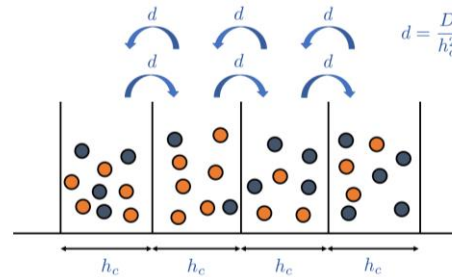
Cameron Smith
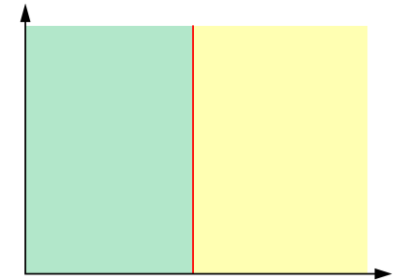
University of Bath

ECMTB, Lisbon 2018

Joint work with Christian (Kit) Yates
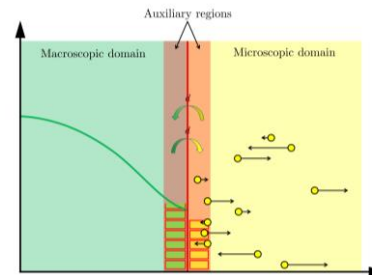
Outline

Reaction-diffusion systems

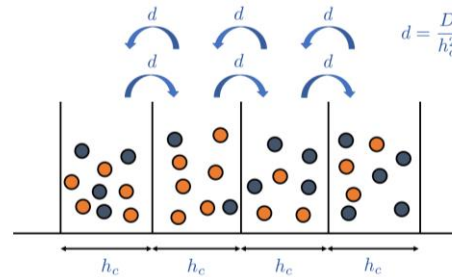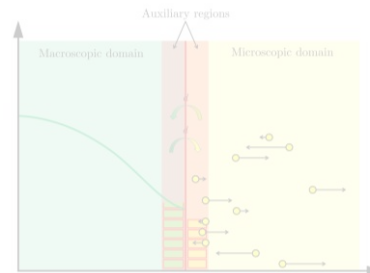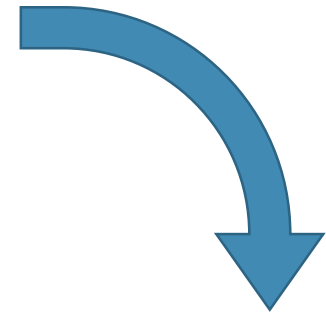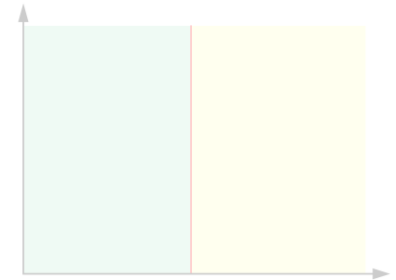
Spatially-extended hybrid methods

The auxiliary region method (ARM)

Outline

Reaction-diffusion systems

$d = \dfrac{D}{h_c^2}$

Spatially-extended hybrid methods

The auxiliary region method (ARM)

Auxiliary regions

Macroscopic domain   Microscopic domain

Reaction-diffusion

The auxiliary region method - Cameron Smith
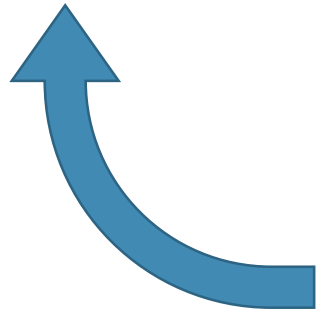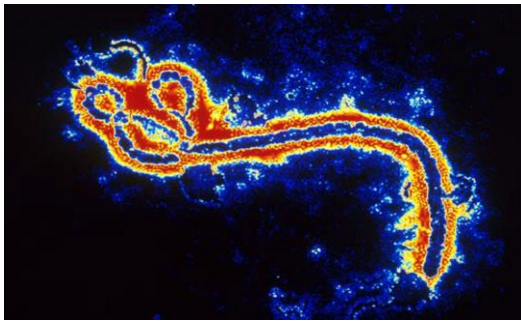
Reaction-diffusion systems

We look at modelling at three levels:

Macroscale – PDEs or SPDEs

$$\frac{\partial u}{\partial t} = D\nabla u + \mathcal{R}(u)$$

Mesoscale – Compartment-based modelling

Gillespie (1977)

$$d = \frac{D}{h_c^2}$$
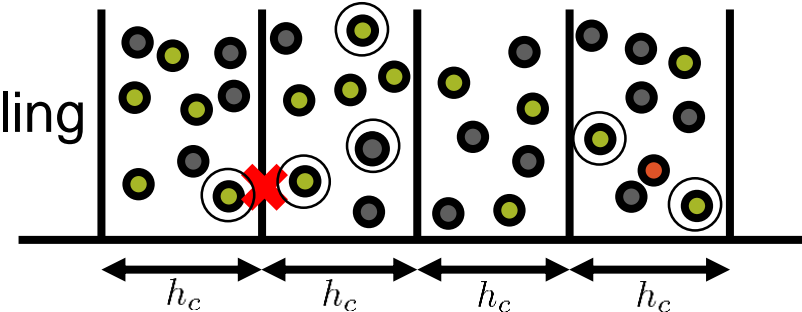
Microscale – Brownian-based dynamics

Erban and Chapman (2009)
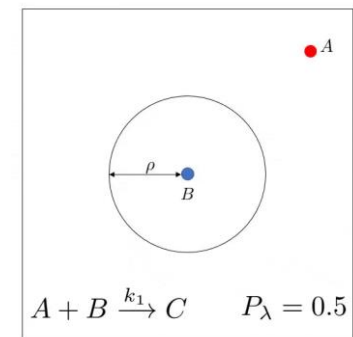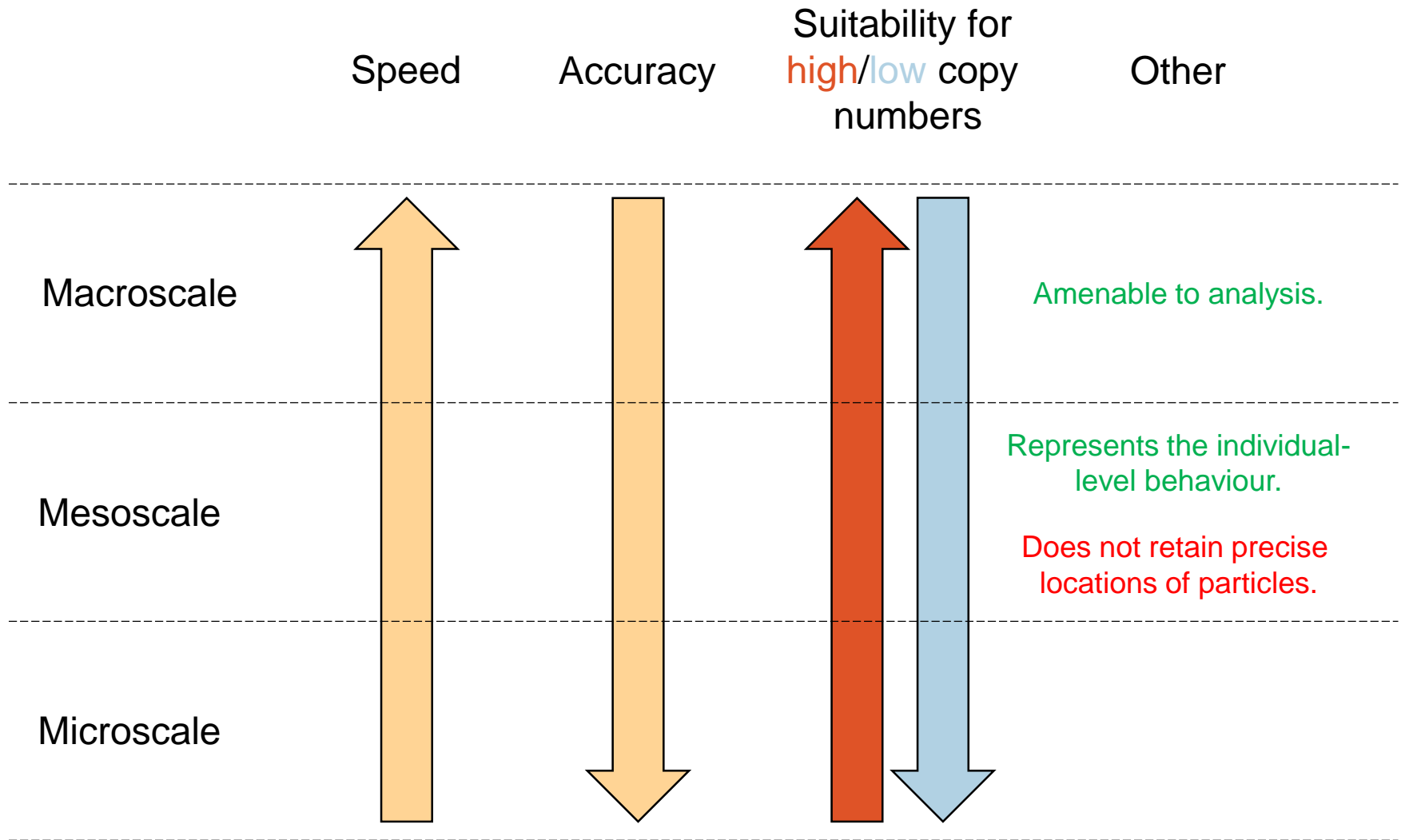
$$A + B \xrightarrow{k_1} C \qquad P_\lambda = 0.5$$

Summary of models

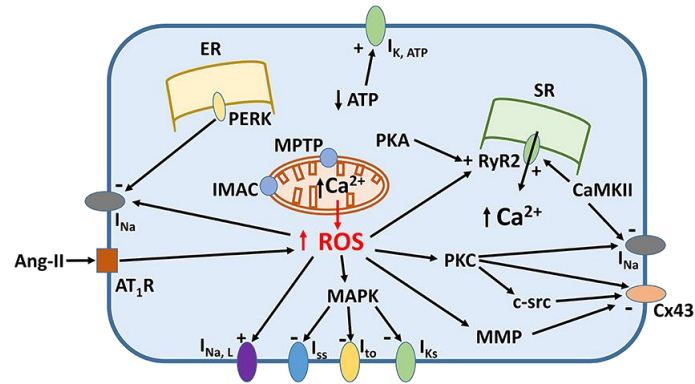|	Speed	Accuracy	Suitability for high/low copy numbers	Other
Macroscale				Amenable to analysis.
Mesoscale				Represents the individual-level behaviour. Does not retain precise locations of particles.
Microscale				

Outline

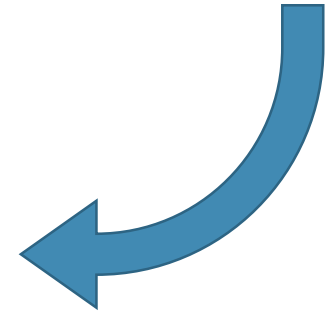Reaction-diffusion systems
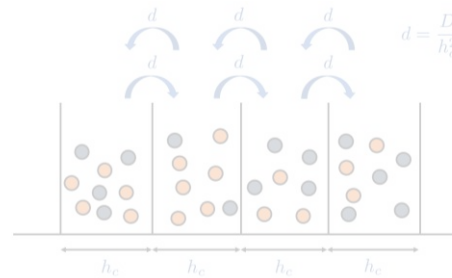
Spatially-extended hybrid methods

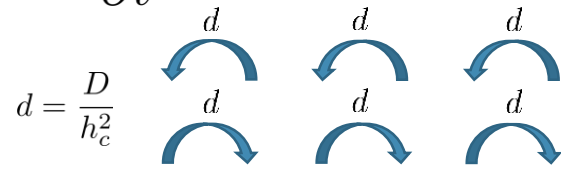The auxiliary region method (ARM)

Spatially-extended hybrid methods

Smith and Yates (2018a)
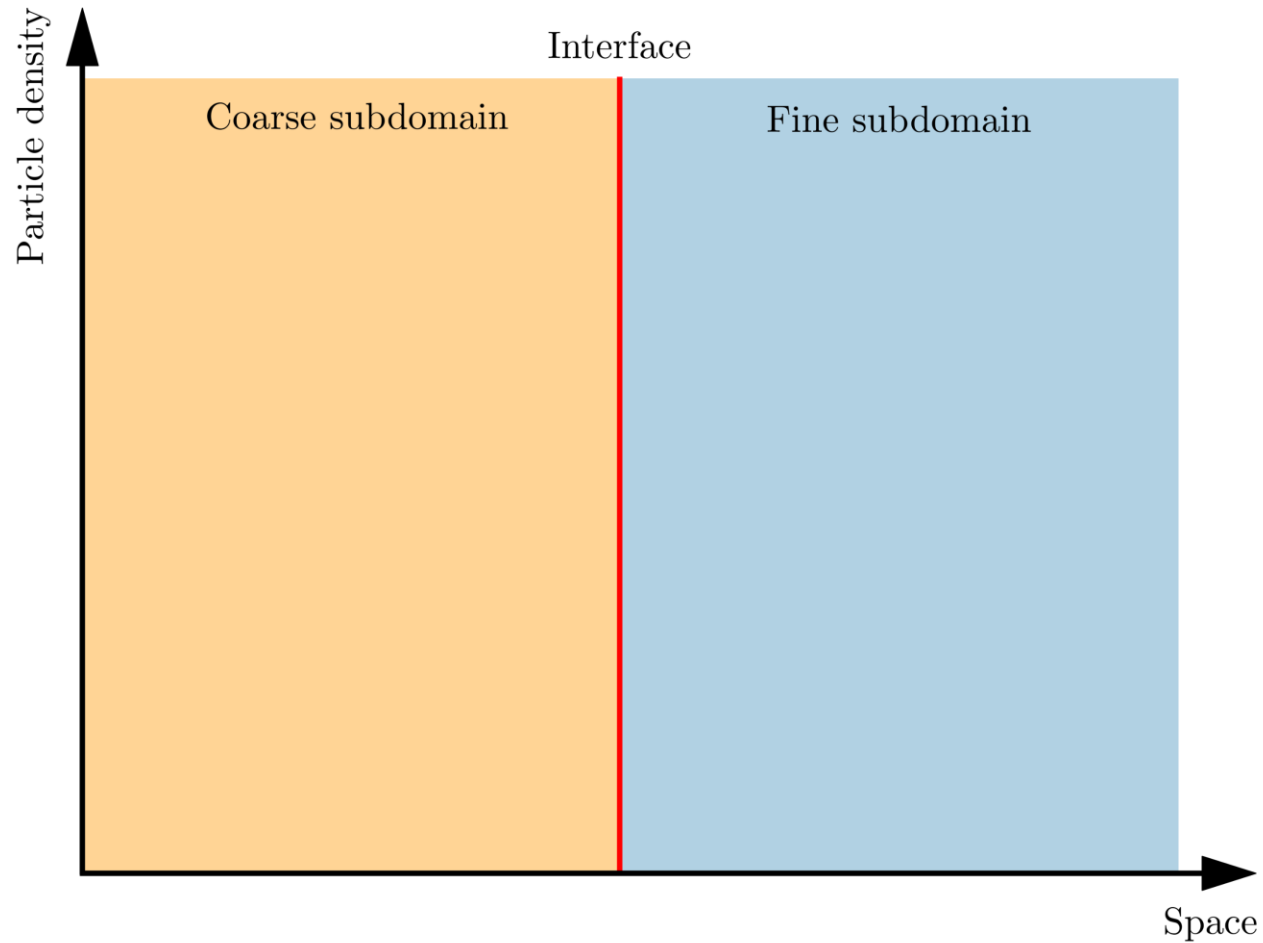
Examples – pseudo-compartment method

Yates and Flegg (2015)

The auxiliary region method - Cameron Smith
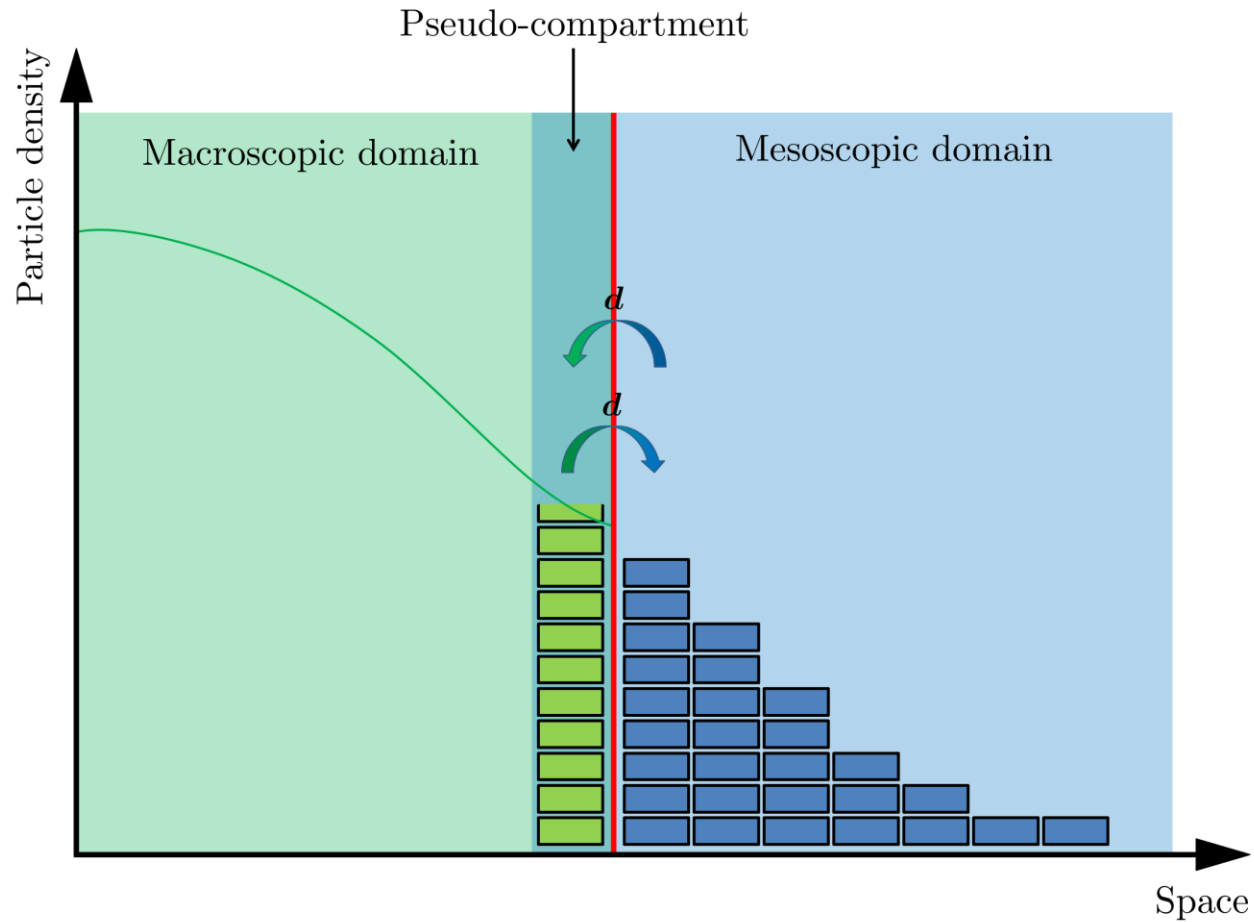
Examples – ghost cell method
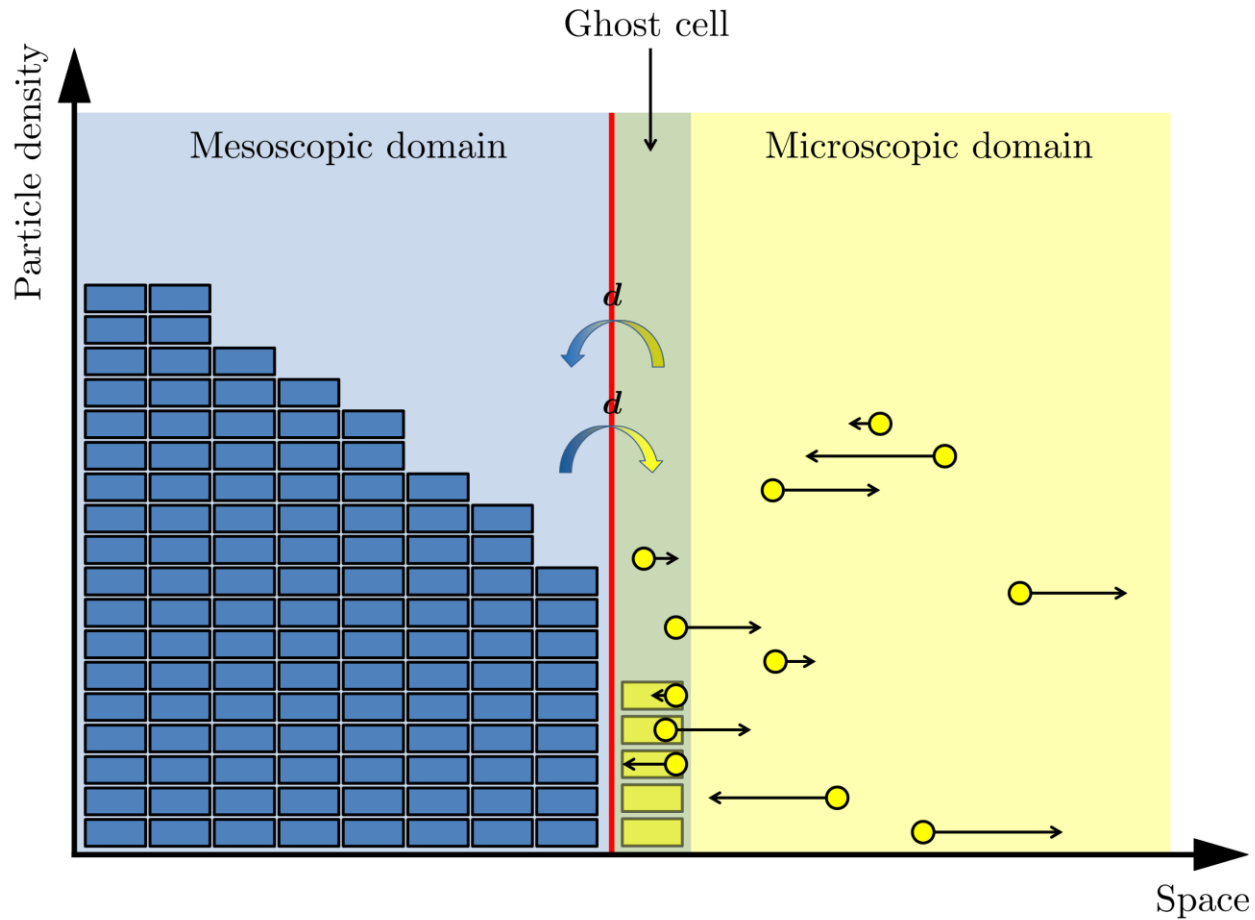
Flegg et al. (2015)

Outline

Reaction-diffusion systems
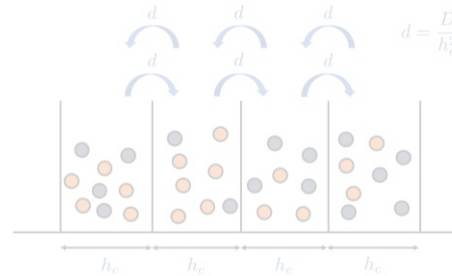
Spatially-extended hybrid
methods

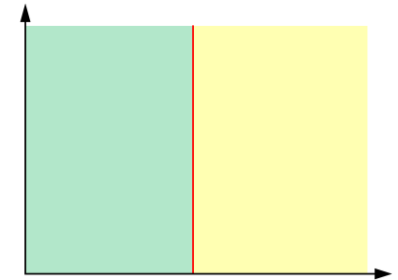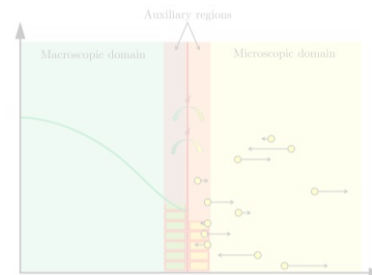The auxiliary region method
(ARM)

The auxiliary region method (ARM)

Smith and Yates (2018b)
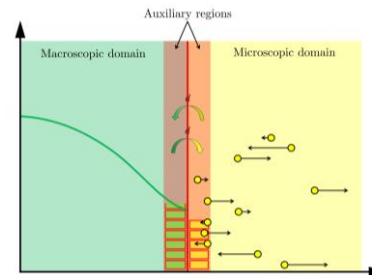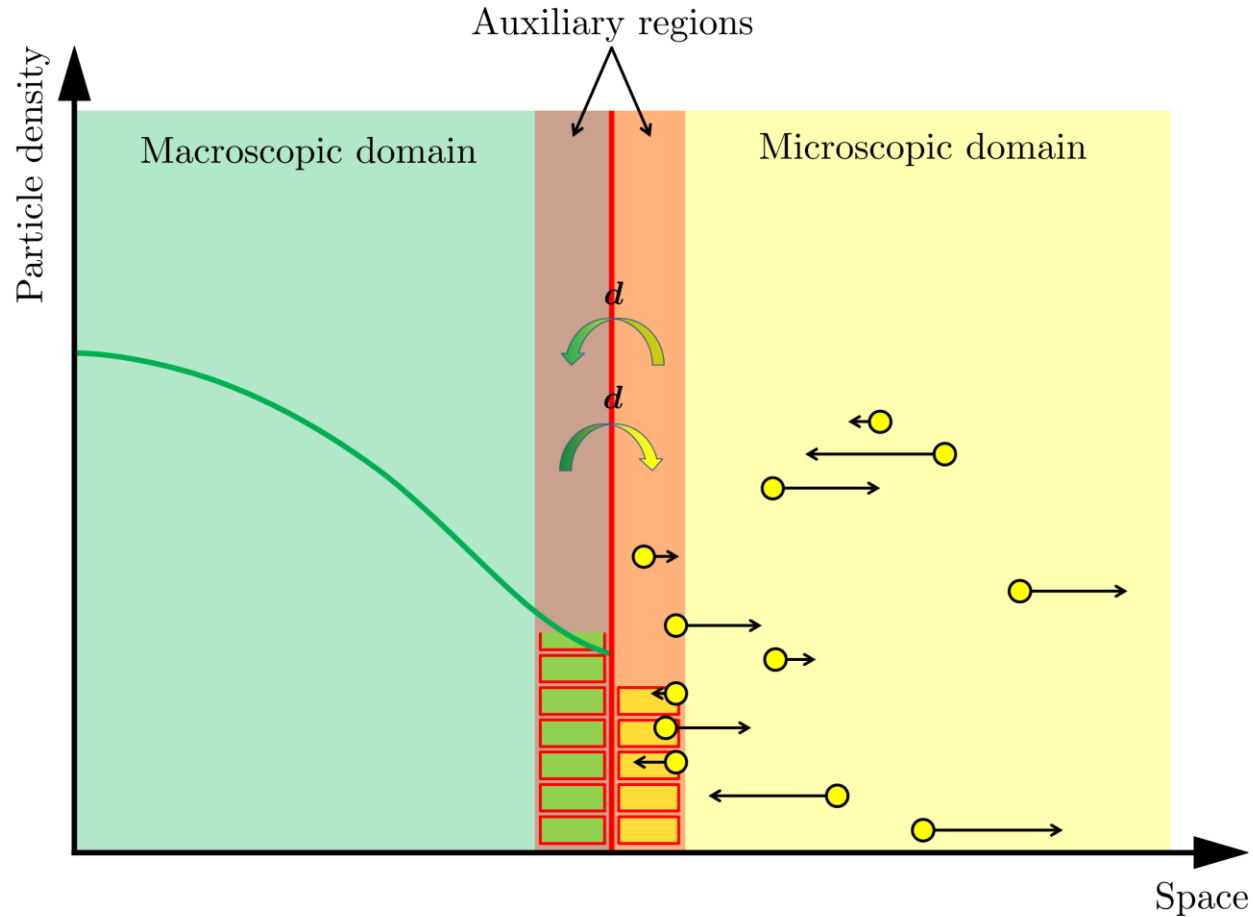
Basic algorithm

1) Find the time until the next event within the auxiliary regions occurs.

2) If this is less than the time until the next PDE/Brownian update, find the corresponding event and enact it.

3) Otherwise, evolve the PDE and Brownian domains.

4) Update time and return to step 1.

Results

Pure diffusion

Morphogen gradient

The auxiliary region method - Cameron Smith
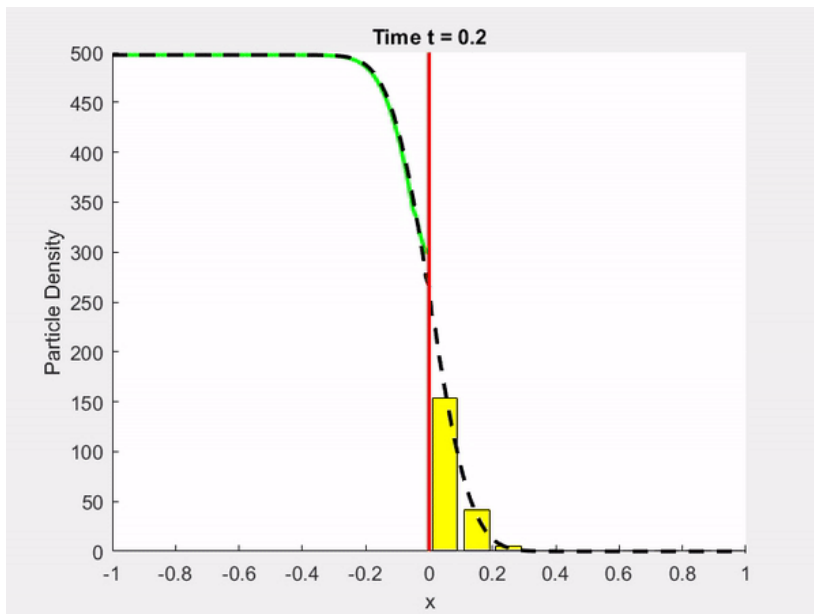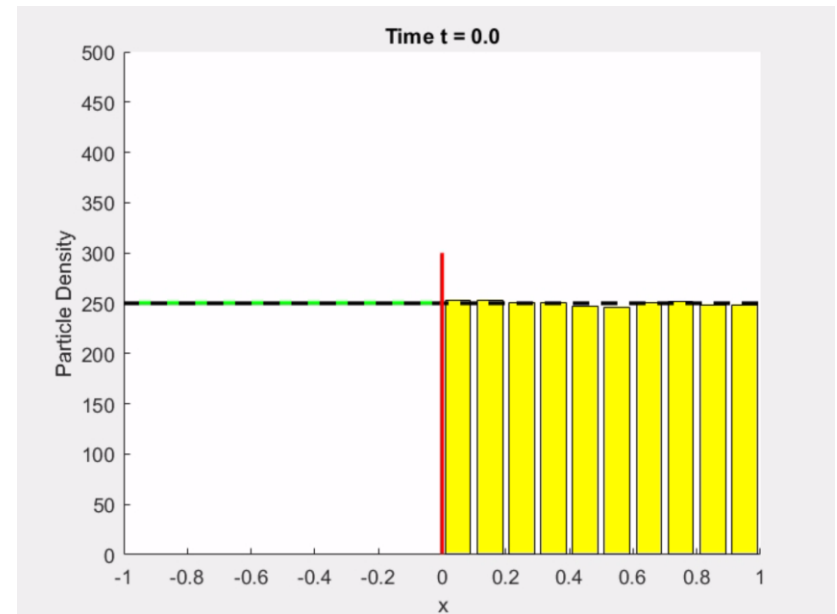
Results

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The auxiliary region method - Cameron Smith
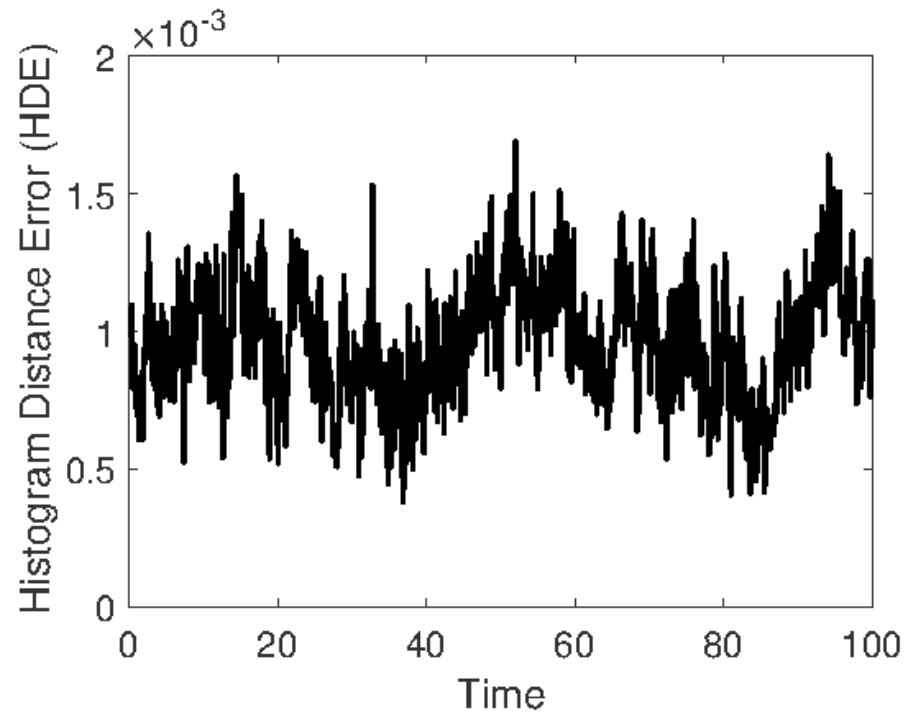
Conclusions

Reaction-diffusion systems have many representations – each with associated advantages and disadvantages.

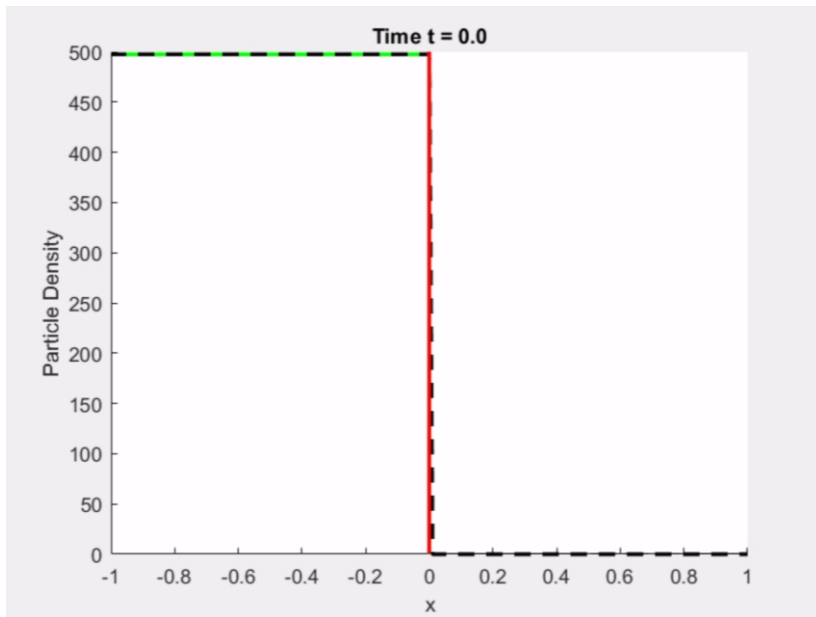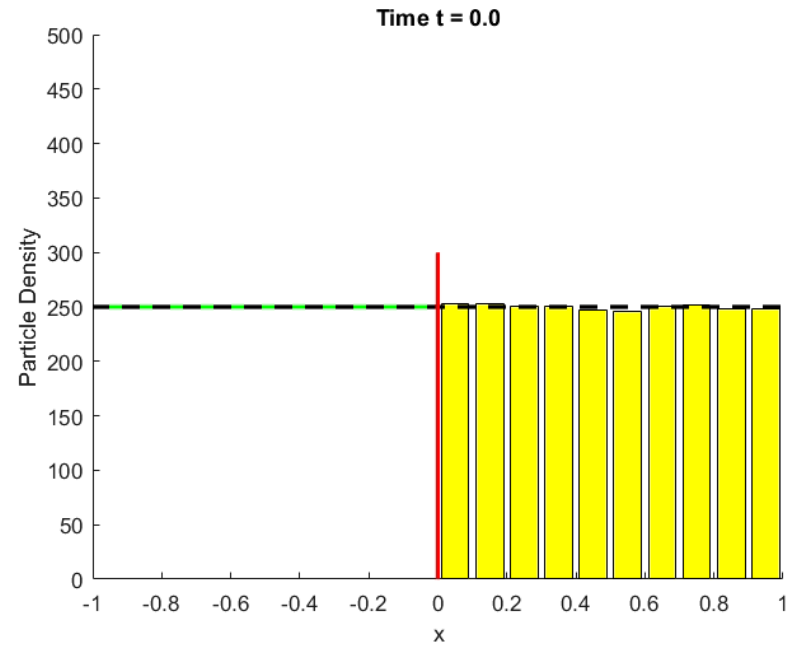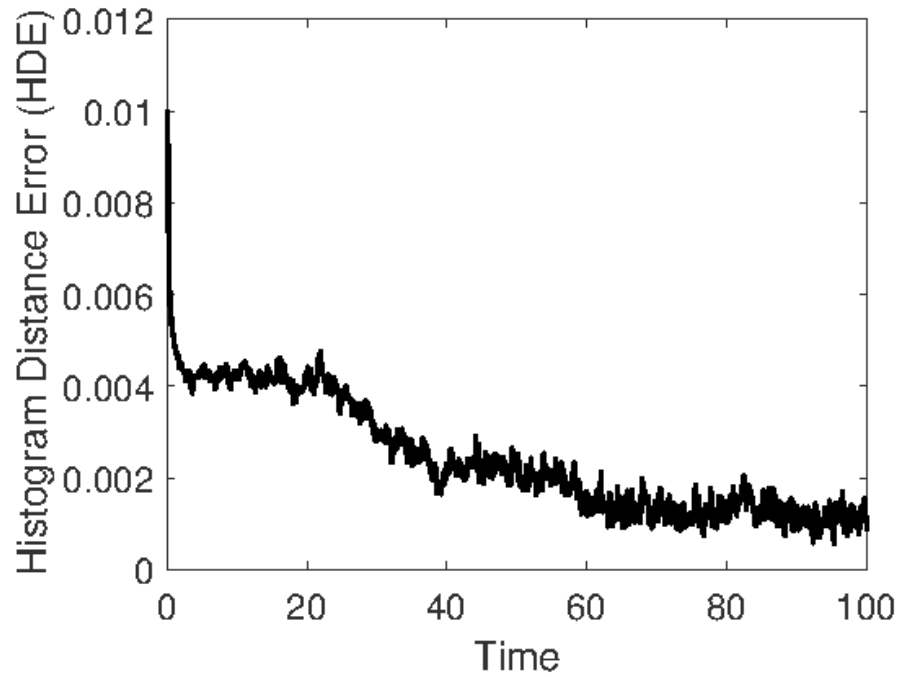| Scale	Advantages	Disadvantages
Macroscopic (Mean-field)	Fast to compute solutions. Suitable for high copy numbers. Amenable to analysis.	Inaccurate for low particle numbers. Mean-field dynamics diverge from individual-level behaviour for high-order reactions.
Mesoscopic (Compartments)	Fast for low copy numbers. Represents the individual-level behaviour.	Can be slow for large copy numbers. Does not retain precise locations of particles or particle identity.
Microscopic (Brownian-based)	Most accurate representation of the three. Can be used for low copy numbers.	Slow to compute reactions. Impractical for large numbers of particles.

Spatially extended hybrid methods try to complement the strengths and negate the weaknesses of these representations.
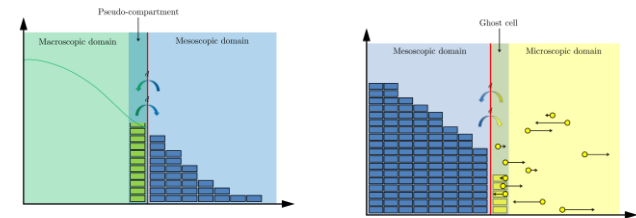
The ARM is a new macroscopic-to-microscopic method for simulating reaction-diffusion systems.

The auxiliary region method - Cameron Smith
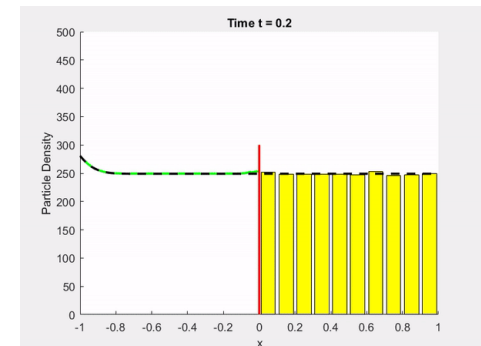
Image credits
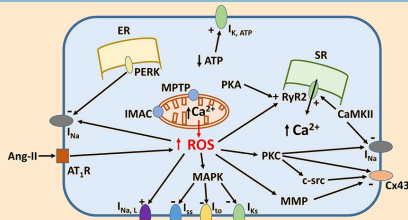
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References

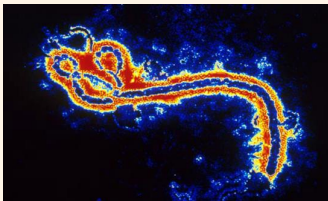- Gillespie D., **Exact stochastic simulation of coupled chemical reactions**, *J. Phys. Chem.*, 1977.

- Erban R. and Chapman S.J., **Stochastic modelling of reaction-diffusion processes: algorithms for bimolecular reactions**, *Phys. Biol.*, 2009.

- Yates C.A. and Flegg M., **The pseudo-compartment method for coupling partial differential equation and compartment-based models of diffusion**, *J. Roy. Soc. Interface,* 2015.

- Flegg M., Hellander S. and Erban R., **Convergence of methods for coupling of microscopic and mesoscopic reaction-diffusion simulations**, *J. Comput. Phys.*, 2015.

- Smith C.A., Yates C.A., **Spatially extended hybrid methods: a review**, *J. Roy. Soc. Interface*, 2018a.

- Smith C.A., Yates C.A., **The auxiliary region method: A hybrid method for coupling PDE- and Brownian-based dynamics for reaction-diffusion systems**, *(accepted by) Royal Soc. Open Sci.*, 2018b.

Thank you for your attention

Summary of models

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Reactions in the Brownian AR