Spatial Representations and Analysis Techniques Part II: Analysis

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COOPERATION

Outline

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1. Large discrete space models
2. SIR in space
3. Spatial moment closure
4. Going to the (spatial) limit

Large discrete space models

Large spatial models

- large: at least 100 distinct locations if not more
- regular: convenient to work with grid
- connectivity: full, von Neumann neighbourhood, Moore neighbourhood
- spatial homogeneity to heterogeneity
  - full connectivity, homogeneous parameters and initial values
  - smaller neighbourhood, homogeneous parameters and initial values
  - smaller neighbourhood, homogeneous parameters, varying initial values
  - smaller neighbourhood, heterogeneous parameters, varying initial values
- PDE analysis: step size of grid tends to zero

Recap of notation

Assuming n subpopulations and p locations, then $X_i^{(j)}$ is the size of the subpopulation i at location j.

$$\begin{aligned}
\mathbf{X}_i &= (X_i^{(1)}, \ldots, X_i^{(p)}) & X_i &= \textstyle\sum_{j=1}^{p} X_i^{(j)} \\
\mathbf{X}^{(j)} &= (X_1^{(j)}, \ldots, X_n^{(j)}) & X^{(j)} &= \textstyle\sum_{i=1}^{n} X_i^{(j)} \\
\mathbf{X} &= (\mathbf{X}_1, \ldots, \mathbf{X}_n) & X &= \textstyle\sum_{i=1}^{n} \sum_{j=1}^{p} X_i^{(j)} \\
 & & &= \textstyle\sum_{j=1}^{p} \sum_{i=1}^{n} X_i^{(j)}
\end{aligned}$$

$$\langle X_i \rangle = 1/p \textstyle\sum_{j=1}^{p} X_i^{(j)}$$

In the case of the $n \times m$ grid, $p = n \times m$ and

$$\langle X_i \rangle = 1/p \textstyle\sum_{j=1}^{n} \sum_{k=1}^{m} X_i^{(j,k)}$$

SIR model

- non-spatial model

$$\begin{array}{rclll} S+I & \to & I+I & & rate : kSI \\ I & \to & R & & rate : rI \end{array}$$

- spatial model with movement, assuming full connectivity

$$\begin{array}{rclll} S^{(i)}+I^{(i)} & \to & I^{(i)}+I^{(i)} & & rate : k^{(i)}S^{(i)}I^{(i)} \\ I^{(i)} & \to & R^{(i)} & & rate : r^{(i)}I^{(i)} \\ \hline S^{(i)} & \to & S^{(j)} & i \neq j & rate : {m_s}^{(ij)}S^{(i)} \\ I^{(i)} & \to & I^{(j)} & i \neq j & rate : {m_i}^{(ij)}I^{(i)} \end{array}$$

- defines a population CTMC with locations
- smaller neighbourhoods: $X^{(i)} \to X^{(j)}$ for $j \in \mathcal{N}(i)$

SIR model

- deterministic fluid approximation with assumption of parameter homogeneity across locations and full connectivity between locations

$$
\begin{aligned}
\frac{dS^{(i)}}{dt} &= -kS^{(i)}I^{(i)} && - \sum_{j=1}^{p} m_s S^{(i)} + \sum_{j=1}^{p} m_s S^{(j)} \\
\frac{dI^{(i)}}{dt} &= kS^{(i)}I^{(i)} - rI^{(i)} && - \sum_{j=1}^{p} m_i I^{(i)} + \sum_{j=1}^{p} m_i I^{(j)} \\
\frac{dR^{(i)}}{dt} &= rI^{(i)} &&
\end{aligned}
$$

- equivalent to adding location attribute to each subpopulation
- increases number of ODEs from 3 to $3p$

SIR model

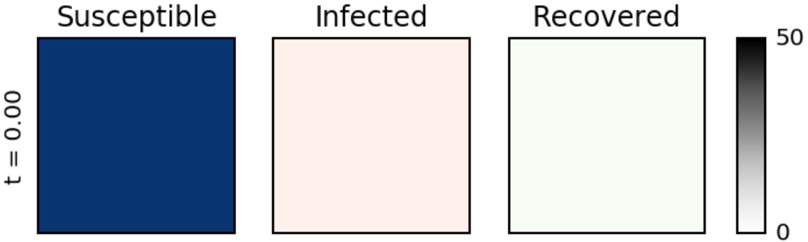
- deterministic fluid approximation with assumption of parameter homogeneity across locations and specified neighbourhood

$$
\begin{aligned}
\frac{dS^{(i)}}{dt} &= -kS^{(i)}I^{(i)} \qquad\qquad - \sum_{j\in\mathcal{N}(i)} m_s S^{(i)} + \sum_{j\in\mathcal{N}(i)} m_s S^{(j)} \\
\frac{dI^{(i)}}{dt} &= kS^{(i)}I^{(i)} - rI^{(i)} - \sum_{j\in\mathcal{N}(i)} m_i I^{(i)} + \sum_{j\in\mathcal{N}(i)} m_i I^{(j)} \\
\frac{dR^{(i)}}{dt} &= rI^{(i)}
\end{aligned}
$$

- same number of ODEs but fewer terms in each

SIR model on 12x12 grid
Stochastic: no connectivity

Initial values: $S^{(i)}(0) = 49, I^{(i)}(0) = 1, R^{(i)}(0) = 0$
Parameters: $k = 0.011$, $r = 0.1$, $m_s = m_i = 0.00001$



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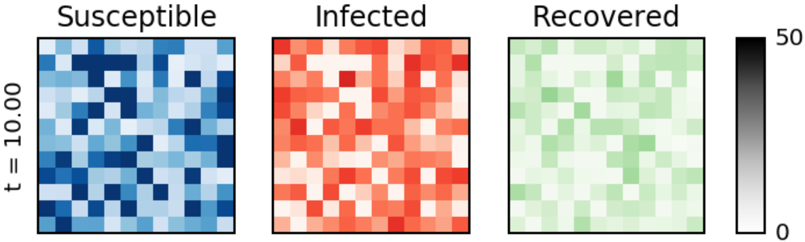

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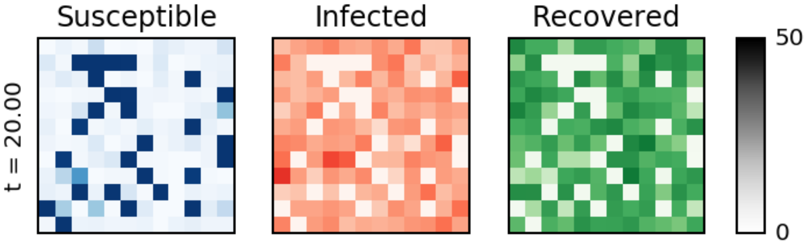

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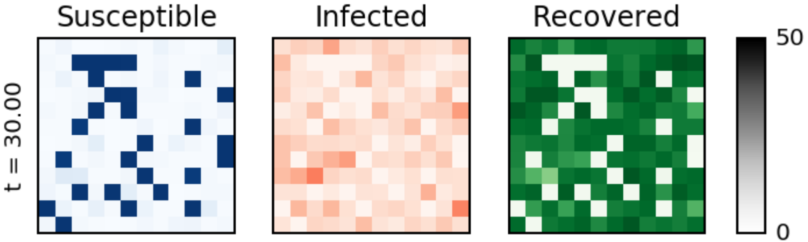

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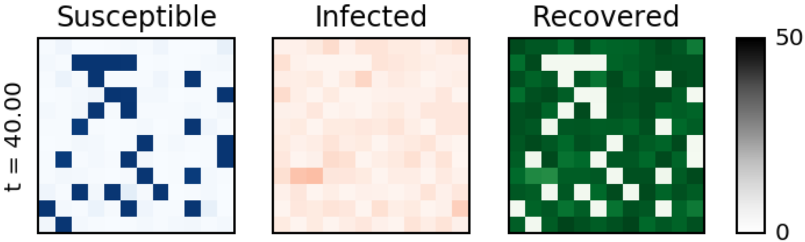

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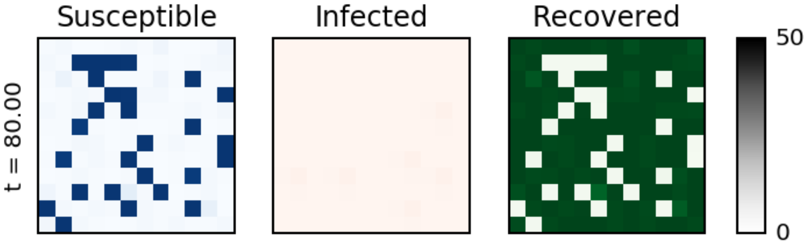

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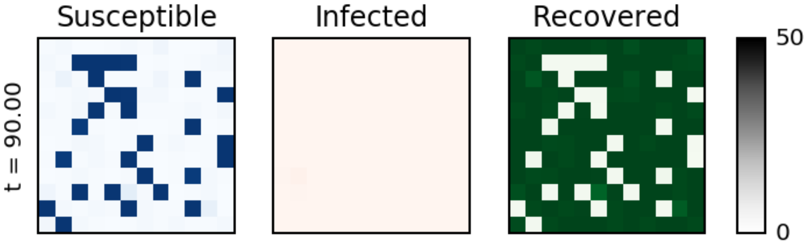

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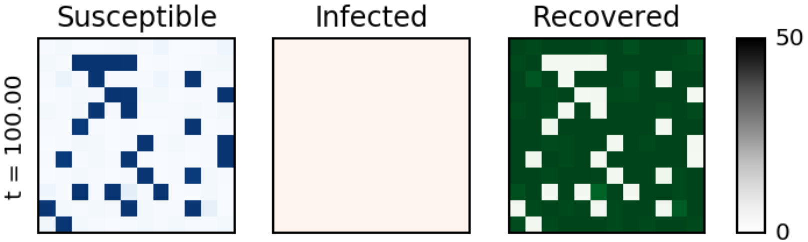

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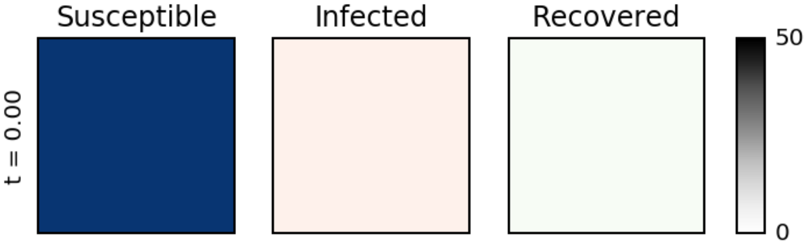

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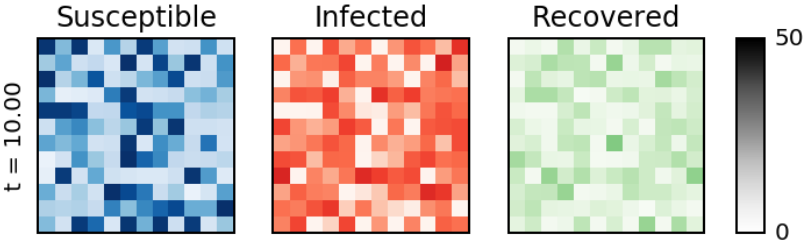

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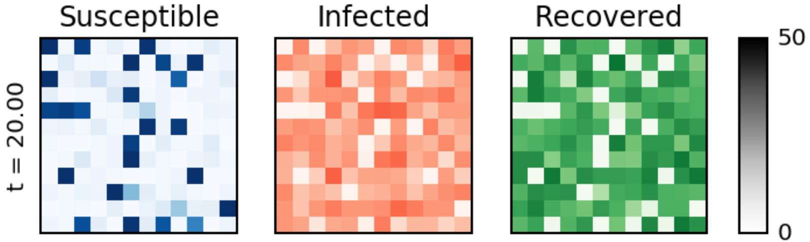

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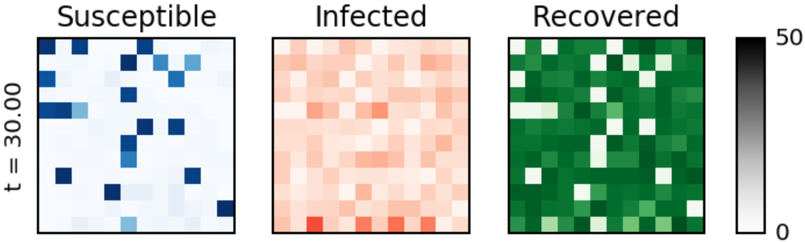

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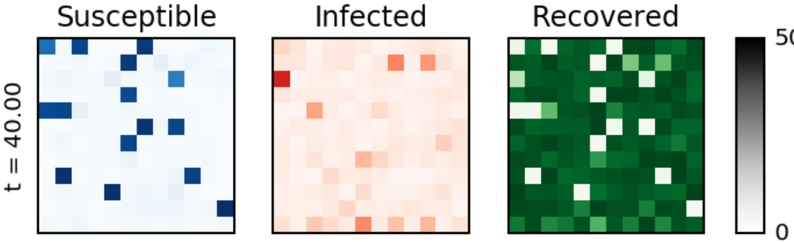

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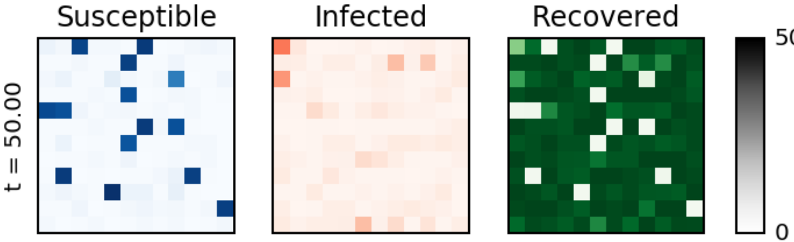

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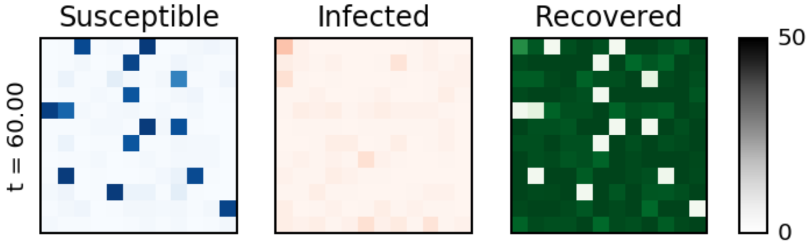

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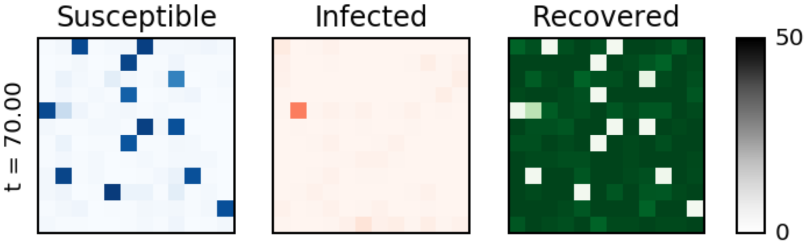

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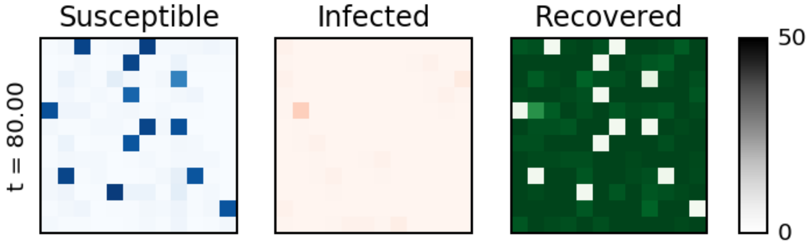

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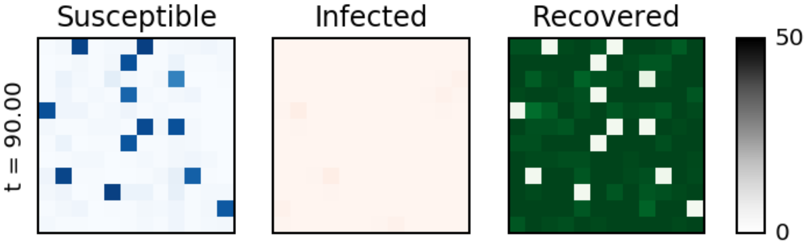

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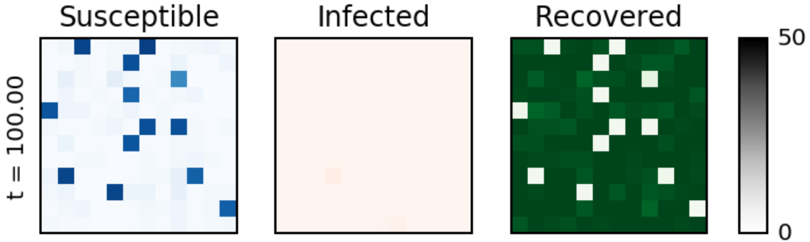

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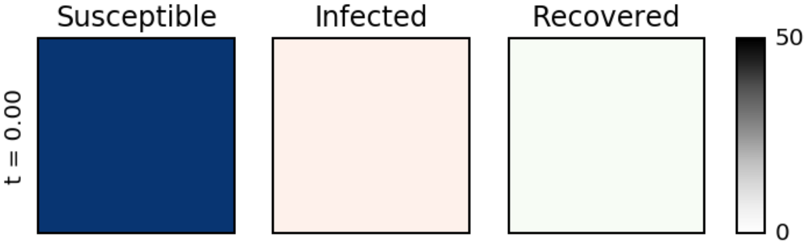

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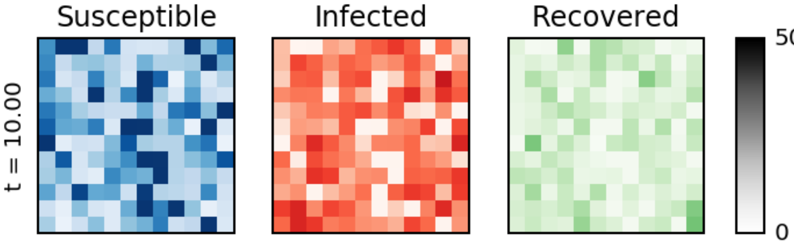

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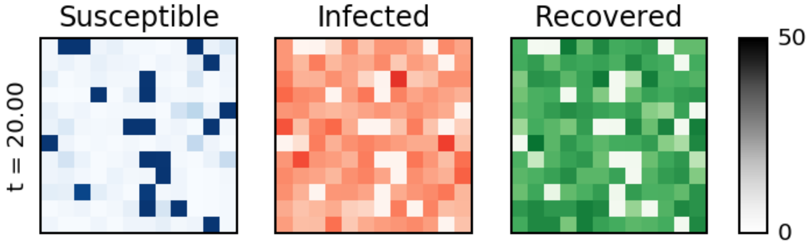

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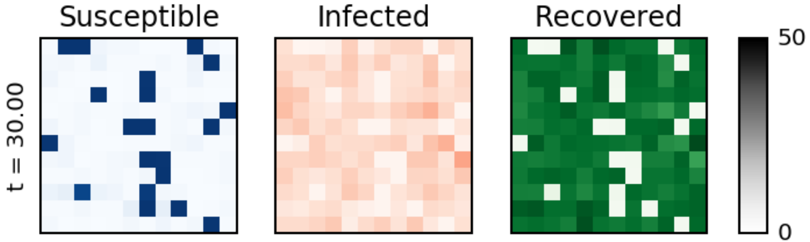

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Stochastic: von Neumann neighbourhood

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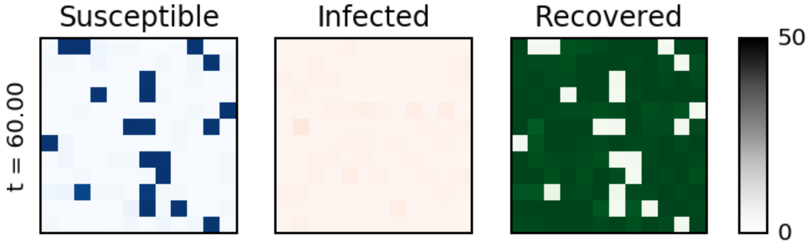

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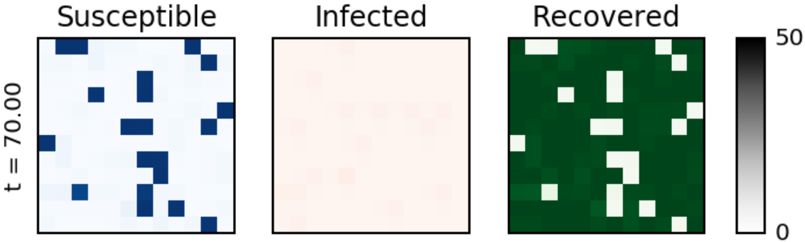

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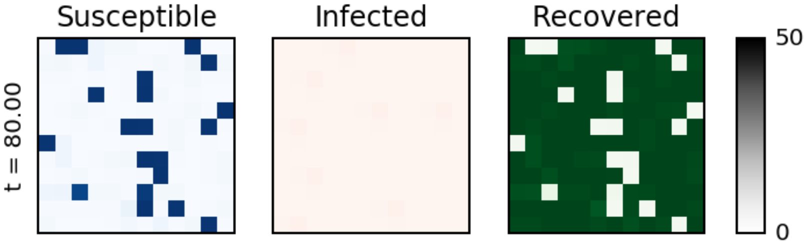

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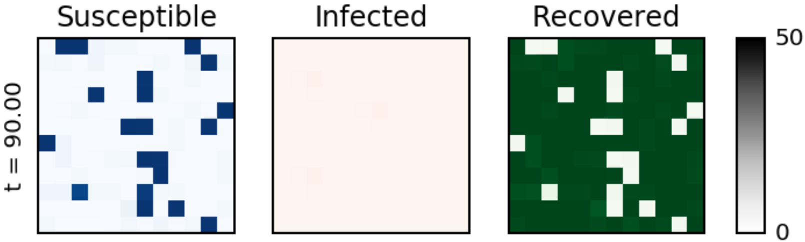

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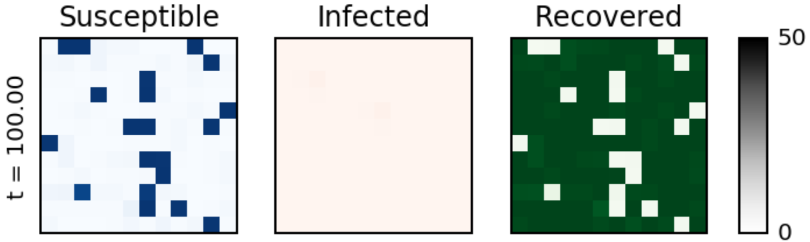

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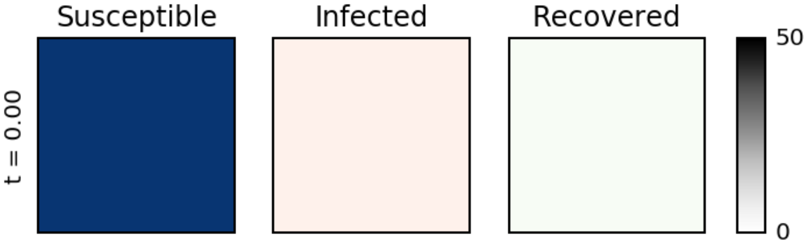

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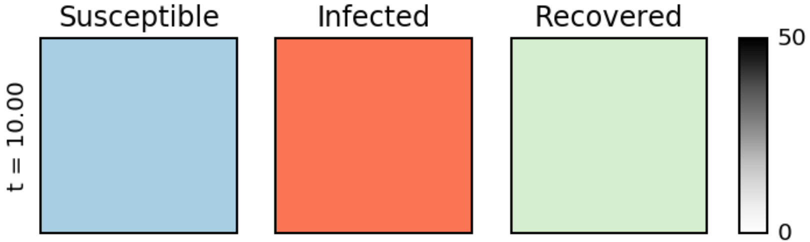

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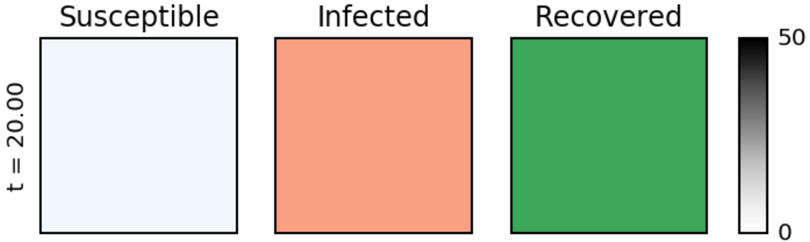

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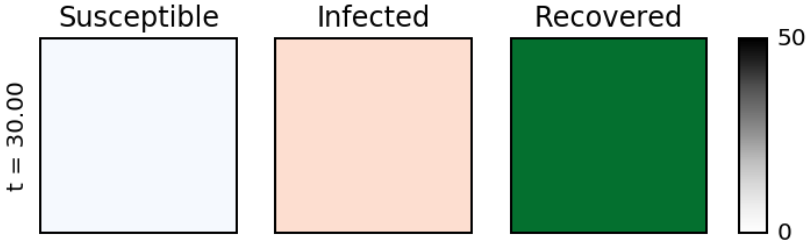

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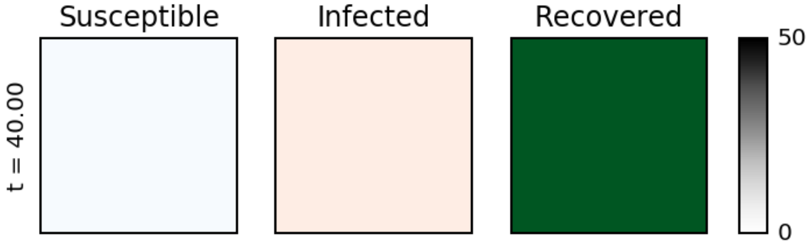

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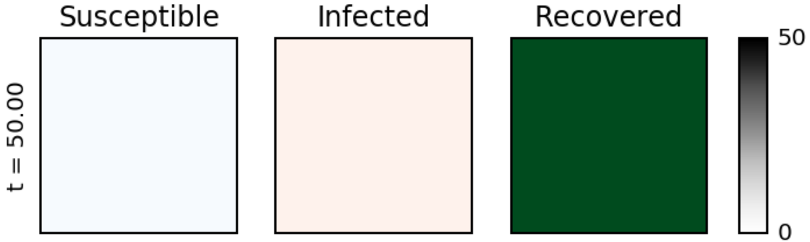

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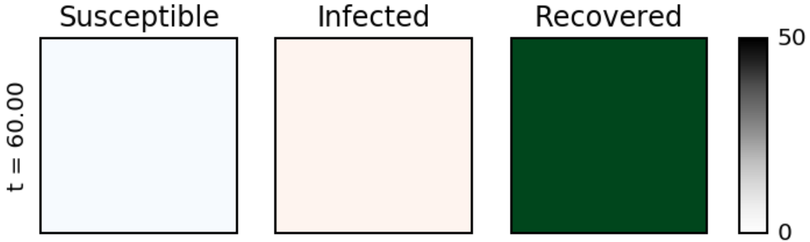

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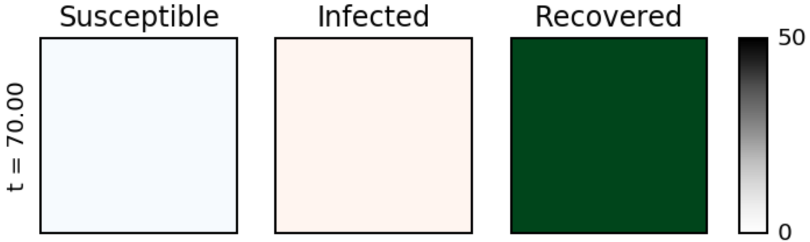

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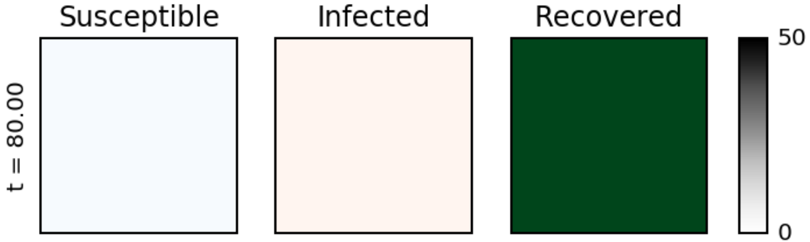

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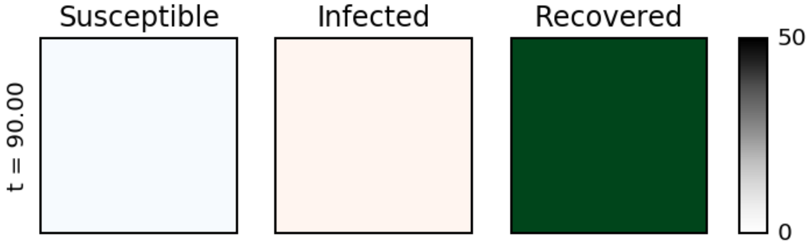
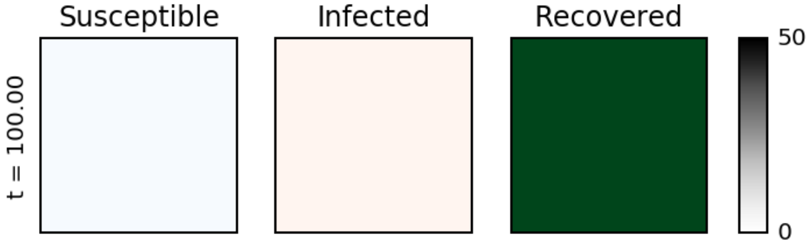
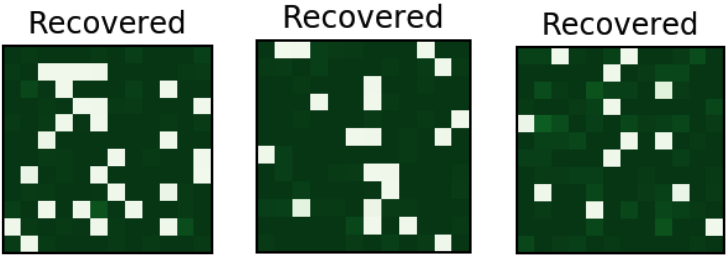


Initial values: $S^{(i)}(0) = 49, I^{(i)}(0) = 1, R^{(i)}(0) = 0$
Parameters: $k = 0.011,\ r = 0.1,\ m_s = m_i = 0.00001$



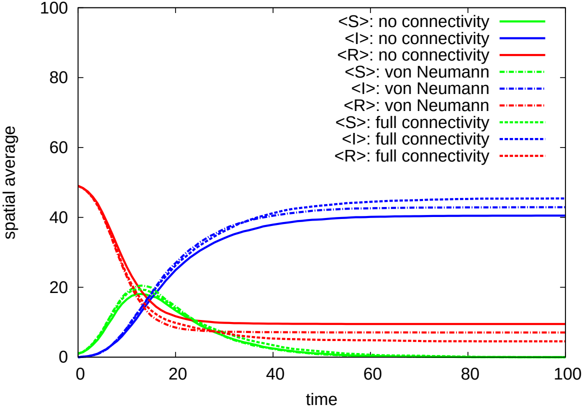
Initial values: $S^{(i)}(0) = 49, I^{(i)}(0) = 1, R^{(i)}(0) = 0$

Parameters: $k = 0.011,\ r = 0.1,\ m_s = m_i = 0.00001$



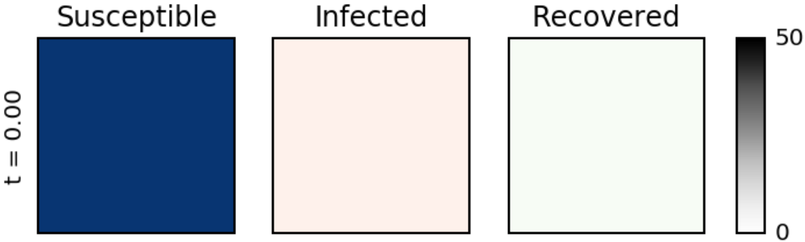
No connectivity | Von Neumann neighbourhood | full connectivity

Initial values: $S^{(i)}(0) = 49, I^{(i)}(0) = 1, R^{(i)}(0) = 0$
Parameters: $k = 0.011,\ r = 0.1,\ m_s = m_i = 0.00001$

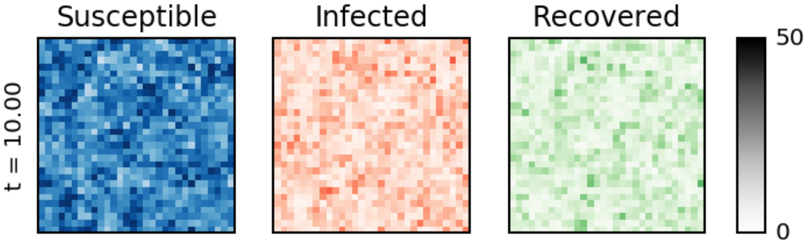


Initial values: $S^{(i)}(0) = 30, I^{(i)}(0) = 10, R^{(i)}(0) = 0$

Parameters: $k = 0.01,\ r = 0.2,\ m_s = m_i = 0.05$

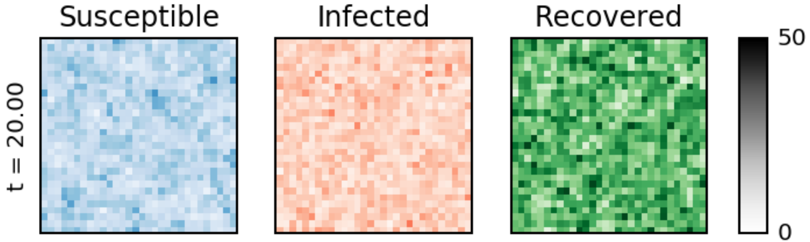


Initial values: $S^{(i)}(0) = 30, I^{(i)}(0) = 10, R^{(i)}(0) = 0$
Parameters: $k = 0.01,\ r = 0.2,\ m_s = m_i = 0.05$



Initial values: $S^{(i)}(0) = 30, I^{(i)}(0) = 10, R^{(i)}(0) = 0$

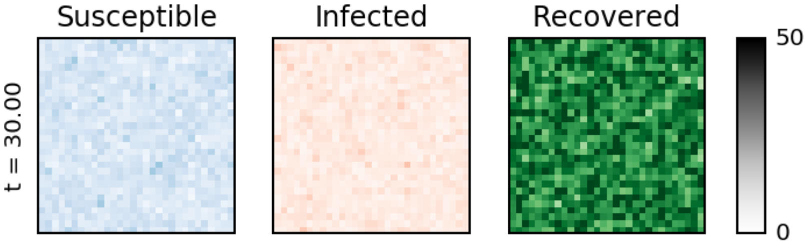
Parameters: $k = 0.01,\ r = 0.2,\ m_s = m_i = 0.05$



SIR model on 30x30 grid

Stochastic: von Neumann neighbourhood

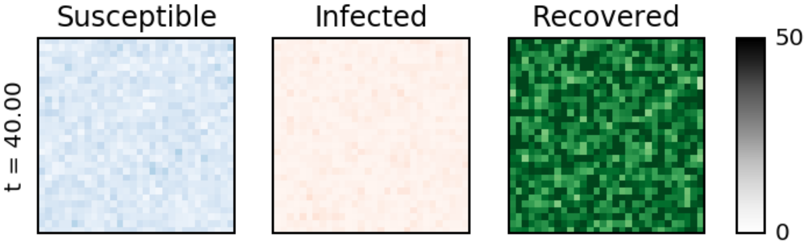
Initial values: $S^{(i)}(0) = 30, I^{(i)}(0) = 10, R^{(i)}(0) = 0$
Parameters: $k = 0.01,\ r = 0.2,\ m_s = m_i = 0.05$



SIR model on 30x30 grid

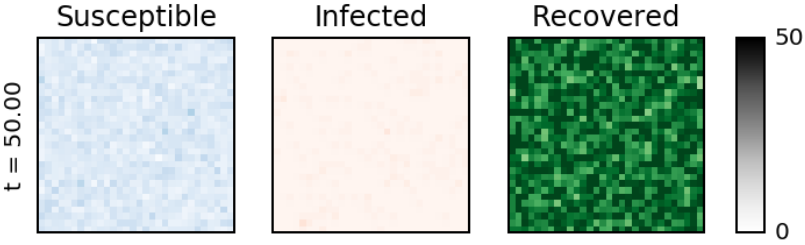
Stochastic: von Neumann neighbourhood

Initial values: $S^{(i)}(0) = 30, I^{(i)}(0) = 10, R^{(i)}(0) = 0$
Parameters: $k = 0.01,\ r = 0.2,\ m_s = m_i = 0.05$

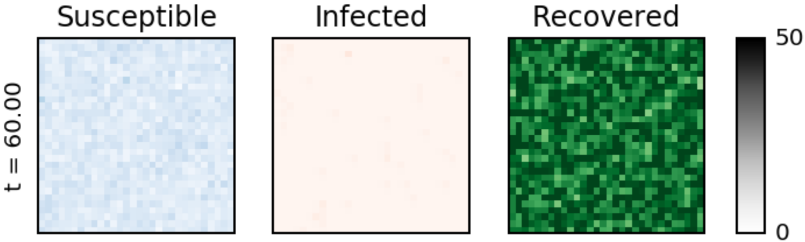


Initial values: $S^{(i)}(0) = 30, I^{(i)}(0) = 10, R^{(i)}(0) = 0$

Parameters: $k = 0.01,\ r = 0.2,\ m_s = m_i = 0.05$



Initial values: $S^{(i)}(0) = 30, I^{(i)}(0) = 10, R^{(i)}(0) = 0$
Parameters: $k = 0.01$, $r = 0.2$, $m_s = m_i = 0.05$



SIR model on 30x30 grid
Stochastic: von Neumann neighbourhood

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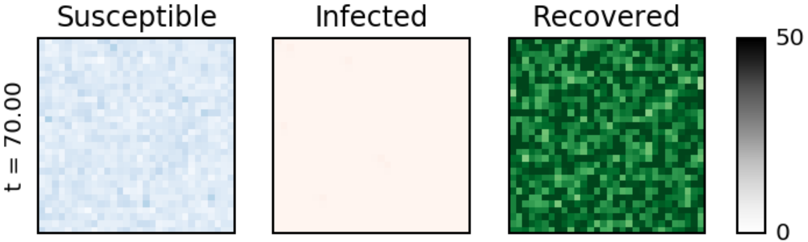
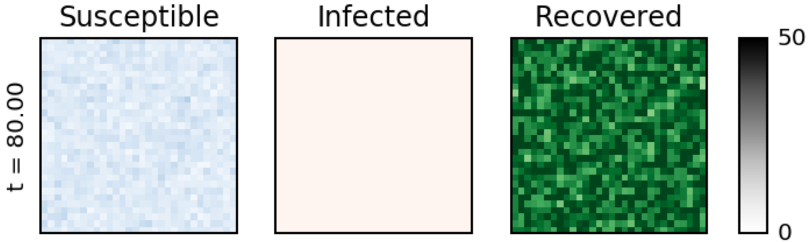
Initial values: $S^{(i)}(0) = 30, I^{(i)}(0) = 10, R^{(i)}(0) = 0$
Parameters: $k = 0.01,\ r = 0.2,\ m_s = m_i = 0.05$



SIR model on 30x30 grid
Stochastic: von Neumann neighbourhood

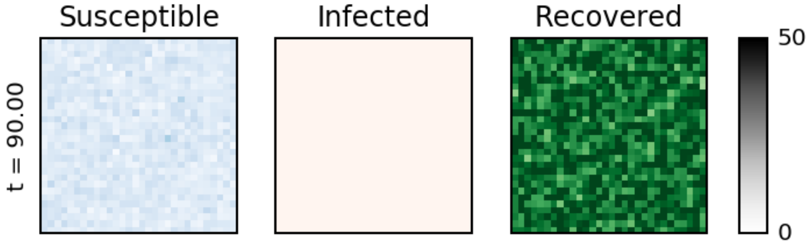
Initial values: $S^{(i)}(0) = 30, I^{(i)}(0) = 10, R^{(i)}(0) = 0$
Parameters: $k = 0.01,\ r = 0.2,\ m_s = m_i = 0.05$



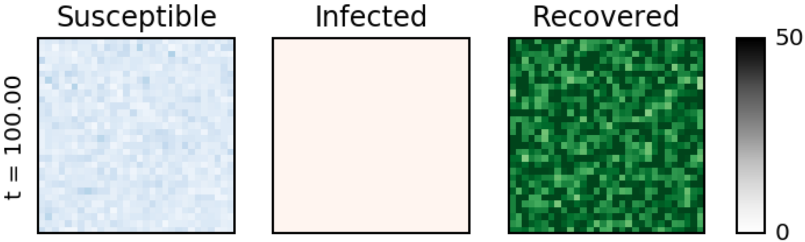
SIR model on 30x30 grid

Stochastic: von Neumann neighbourhood

Initial values: $S^{(i)}(0) = 30, I^{(i)}(0) = 10, R^{(i)}(0) = 0$
Parameters: $k = 0.01,\ r = 0.2,\ m_s = m_i = 0.05$



Initial values: $S^{(i)}(0) = 30, I^{(i)}(0) = 10, R^{(i)}(0) = 0$
Parameters: $k = 0.01$, $r = 0.2$, $m_s = m_i = 0.05$

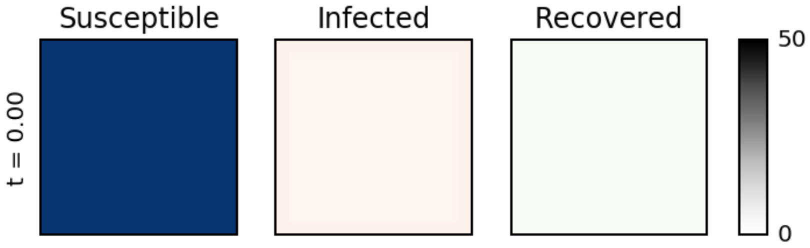


SIR model on 30x30 grid

Stochastic: von Neumann neighbourhood

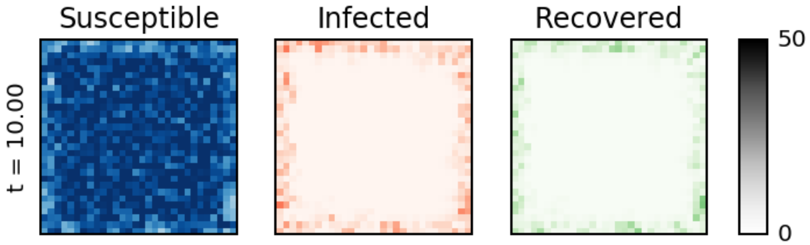
Initial values: $S^{(i)}(0) = 30, I^{(i)}(0) = 0, R^{(i)}(0) = 0$
except border, $I^{(i)}(0) = 10$

Parameters: $k = 0.01,\ r = 0.2,\ m_s = m_i = 0.05$



Initial values: $S^{(i)}(0) = 30, I^{(i)}(0) = 0, R^{(i)}(0) = 0$
except border, $I^{(i)}(0) = 10$

Parameters: $k = 0.01,\ r = 0.2,\ m_s = m_i = 0.05$

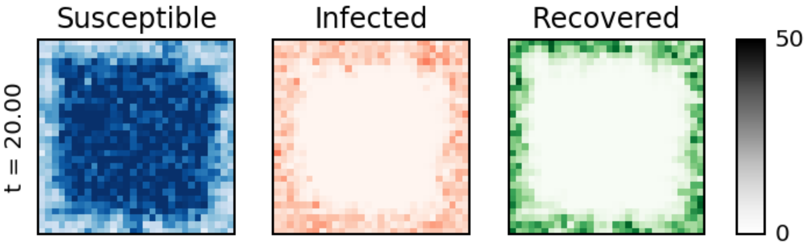


SIR model on 30x30 grid

Stochastic: von Neumann neighbourhood

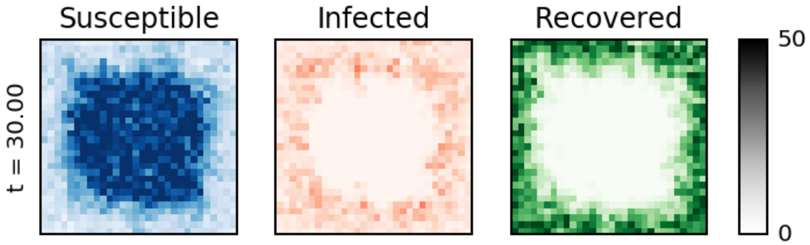
Initial values: $S^{(i)}(0) = 30, I^{(i)}(0) = 0, R^{(i)}(0) = 0$
except border, $I^{(i)}(0) = 10$

Parameters: $k = 0.01$, $r = 0.2$, $m_s = m_i = 0.05$



Initial values: $S^{(i)}(0) = 30, I^{(i)}(0) = 0, R^{(i)}(0) = 0$
except border, $I^{(i)}(0) = 10$

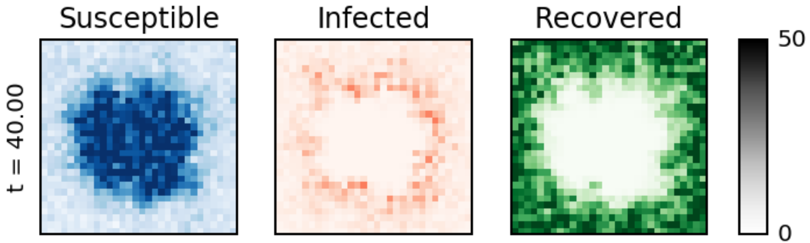
Parameters: $k = 0.01$, $r = 0.2$, $m_s = m_i = 0.05$



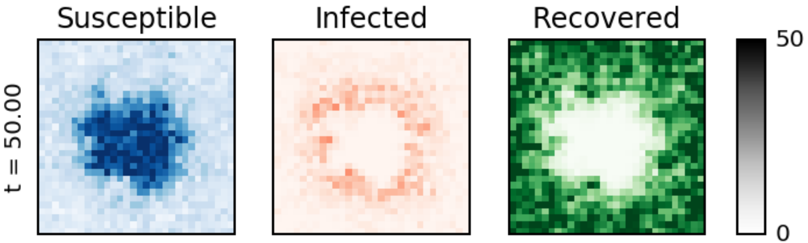
SIR model on 30x30 grid
Stochastic: von Neumann neighbourhood

Initial values: $S^{(i)}(0) = 30, I^{(i)}(0) = 0, R^{(i)}(0) = 0$
except border, $I^{(i)}(0) = 10$

Parameters: $k = 0.01$, $r = 0.2$, $m_s = m_i = 0.05$

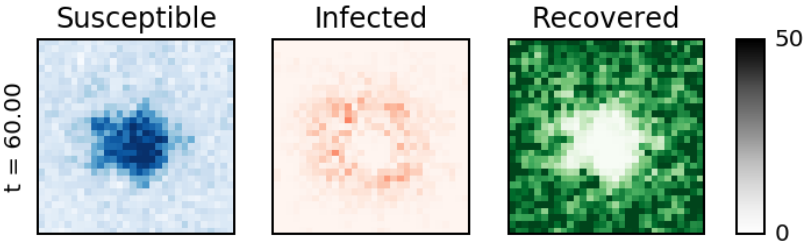


Initial values: $S^{(i)}(0) = 30, I^{(i)}(0) = 0, R^{(i)}(0) = 0$
except border, $I^{(i)}(0) = 10$
Parameters: $k = 0.01,\ r = 0.2,\ m_s = m_i = 0.05$



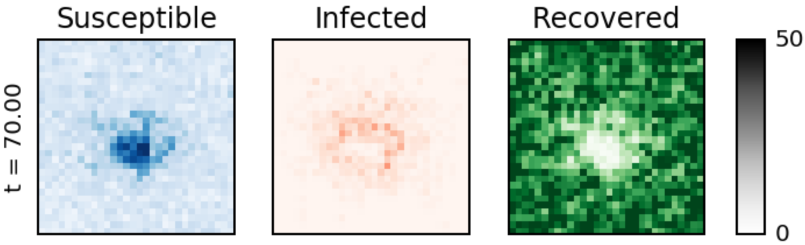
Initial values: $S^{(i)}(0) = 30, I^{(i)}(0) = 0, R^{(i)}(0) = 0$
except border, $I^{(i)}(0) = 10$

Parameters: $k = 0.01$, $r = 0.2$, $m_s = m_i = 0.05$



Initial values: $S^{(i)}(0) = 30, I^{(i)}(0) = 0, R^{(i)}(0) = 0$
except border, $I^{(i)}(0) = 10$

Parameters: $k = 0.01,\ r = 0.2,\ m_s = m_i = 0.05$

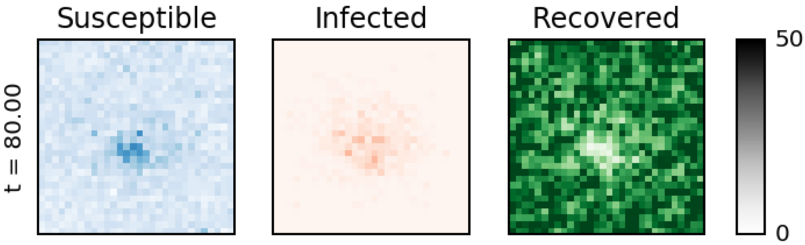


SIR model on 30x30 grid

Stochastic: von Neumann neighbourhood

Initial values: $S^{(i)}(0) = 30, I^{(i)}(0) = 0, R^{(i)}(0) = 0$
except border, $I^{(i)}(0) = 10$

Parameters: $k = 0.01,\ r = 0.2,\ m_s = m_i = 0.05$



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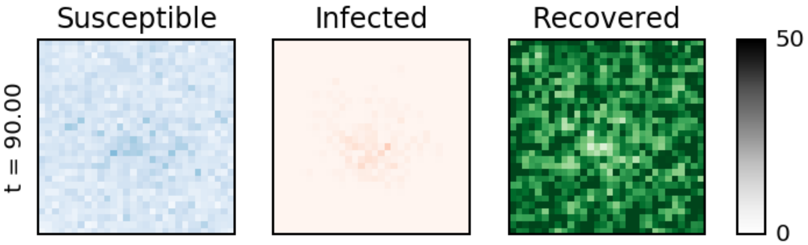
except border, $I^{(i)}(0) = 10$

Parameters: $k = 0.01,\ r = 0.2,\ m_s = m_i = 0.05$



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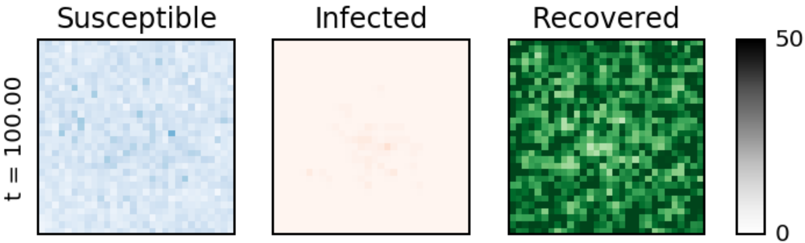
except border, $I^{(i)}(0) = 10$
Parameters: $k = 0.01$, $r = 0.2$, $m_s = m_i = 0.05$



SIR model on 30x30 grid

Stochastic: von Neumann neighbourhood

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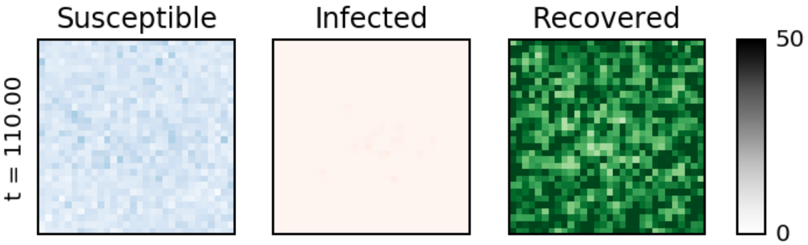
except border, $I^{(i)}(0) = 10$

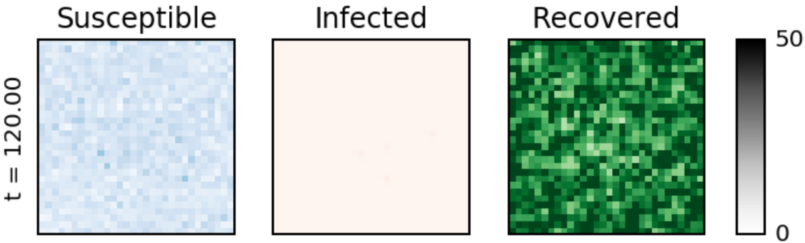
Parameters: $k = 0.01,\ r = 0.2,\ m_s = m_i = 0.05$



SIR model on 30x30 grid
Stochastic: von Neumann neighbourhood

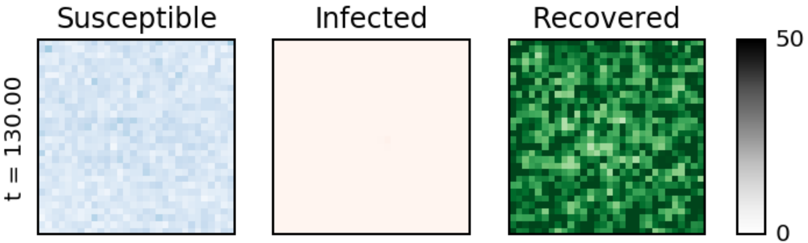
Initial values: $S^{(i)}(0) = 30, I^{(i)}(0) = 0, R^{(i)}(0) = 0$
except border, $I^{(i)}(0) = 10$

Parameters: $k = 0.01,\ r = 0.2,\ m_s = m_i = 0.05$



Initial values: $S^{(i)}(0) = 30, I^{(i)}(0) = 0, R^{(i)}(0) = 0$
except border, $I^{(i)}(0) = 10$

Parameters: $k = 0.01,\ r = 0.2,\ m_s = m_i = 0.05$



SIR model on 30x30 grid

Stochastic: von Neumann neighbourhood

Initial values: $S^{(i)}(0) = 30, I^{(i)}(0) = 0, R^{(i)}(0) = 0$
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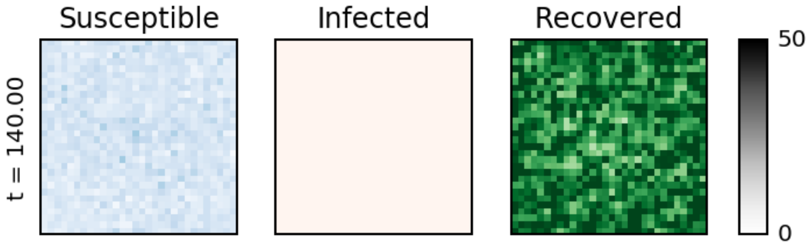
Parameters: $k = 0.01$, $r = 0.2$, $m_s = m_i = 0.05$



SIR model on 30x30 grid

Stochastic: von Neumann neighbourhood

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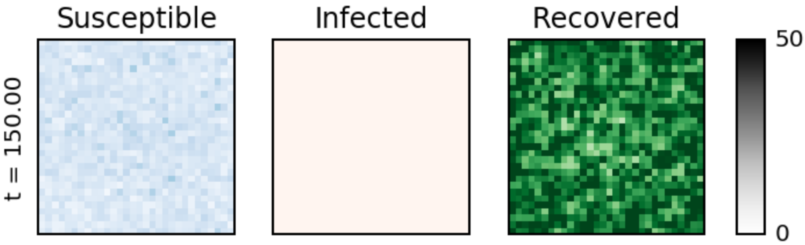
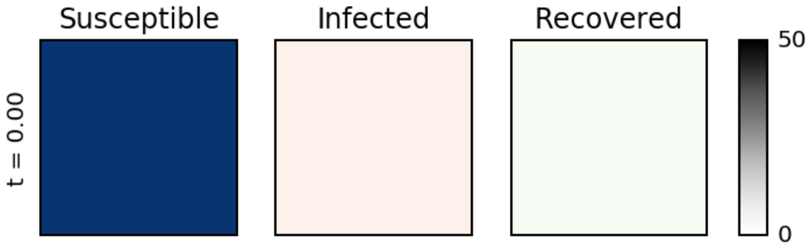
Initial values: $S^{(i)}(0) = 30, I^{(i)}(0) = 0, R^{(i)}(0) = 0$
except border, $I^{(i)}(0) = 10$

Parameters: $k = 0.01,\ r = 0.2,\ m_s = m_i = 0.05$



Initial values: $S^{(i)}(0) = 30, I^{(i)}(0) = 10, R^{(i)}(0) = 0$
Parameters: $k = 0.01,\ r = 0.2,\ m_s = m_i = 0.05$
except bottom third $k = 0.05$



Initial values: $S^{(i)}(0) = 30, I^{(i)}(0) = 10, R^{(i)}(0) = 0$
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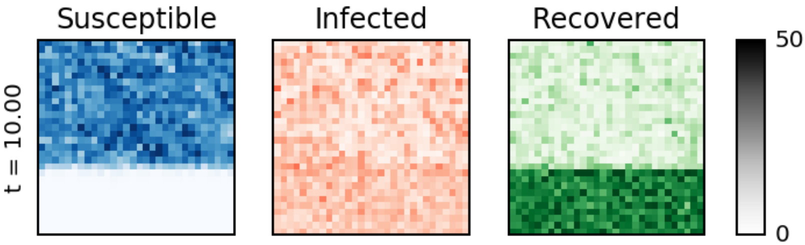

SIR model on 30x30 grid

Stochastic: von Neumann neighbourhood

Initial values: $S^{(i)}(0) = 30, I^{(i)}(0) = 10, R^{(i)}(0) = 0$
Parameters: $k = 0.01,\ r = 0.2,\ m_s = m_i = 0.05$
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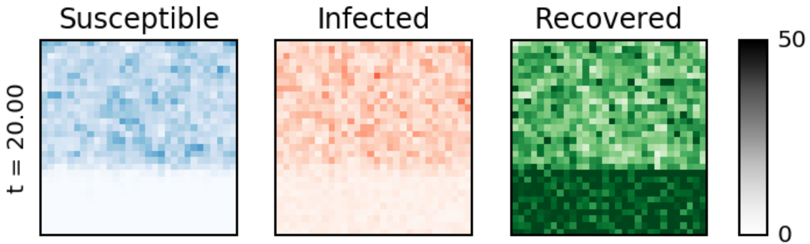

SIR model on 30x30 grid
Stochastic: von Neumann neighbourhood

Initial values: $S^{(i)}(0) = 30, I^{(i)}(0) = 10, R^{(i)}(0) = 0$
Parameters: $k = 0.01,\ r = 0.2,\ m_s = m_i = 0.05$
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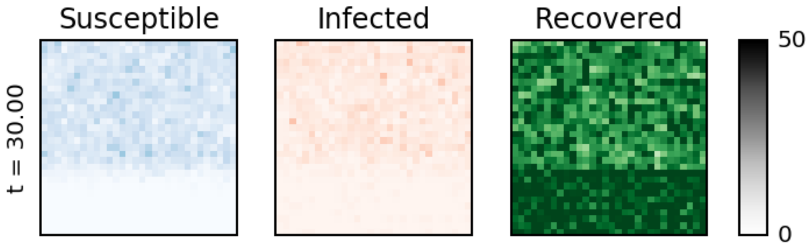

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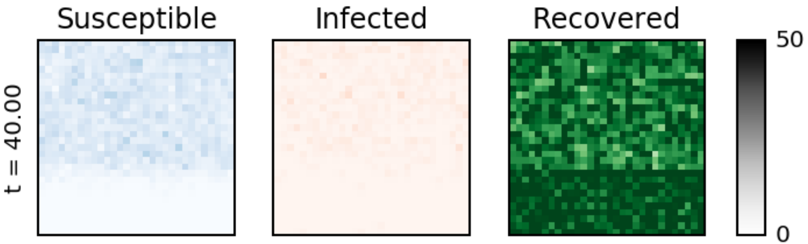
Parameters: $k = 0.01,\ r = 0.2,\ m_s = m_i = 0.05$

except bottom third $k = 0.05$



SIR model on 30x30 grid
Stochastic: von Neumann neighbourhood

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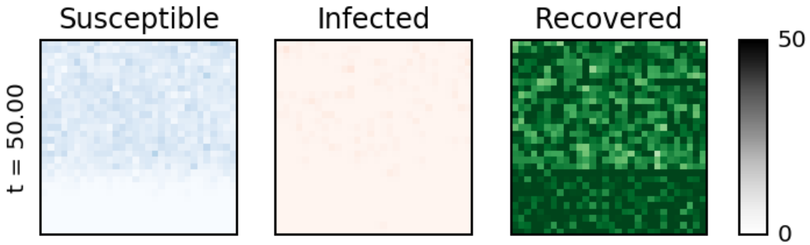
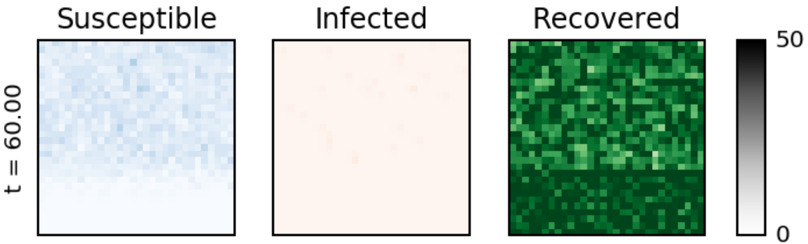


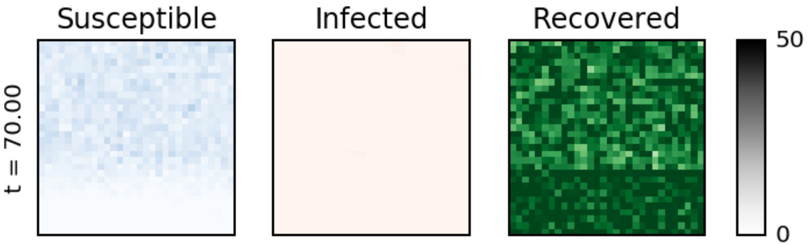
Initial values: $S^{(i)}(0) = 30, I^{(i)}(0) = 10, R^{(i)}(0) = 0$

Parameters: $k = 0.01,\ r = 0.2,\ m_s = m_i = 0.05$

except bottom third $k = 0.05$



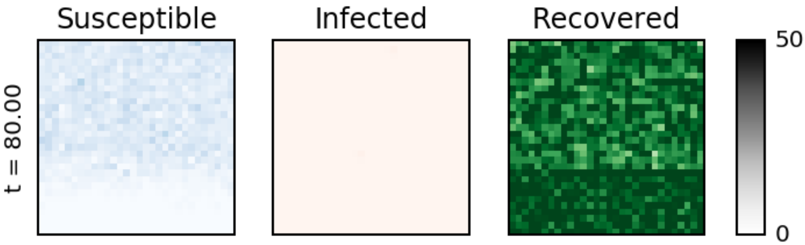
Initial values: $S^{(i)}(0) = 30, I^{(i)}(0) = 10, R^{(i)}(0) = 0$
Parameters: $k = 0.01$, $r = 0.2$, $m_s = m_i = 0.05$
except bottom third $k = 0.05$



SIR model on 30x30 grid

Stochastic: von Neumann neighbourhood

Initial values: $S^{(i)}(0) = 30, I^{(i)}(0) = 10, R^{(i)}(0) = 0$
Parameters: $k = 0.01,\ r = 0.2,\ m_s = m_i = 0.05$
except bottom third $k = 0.05$



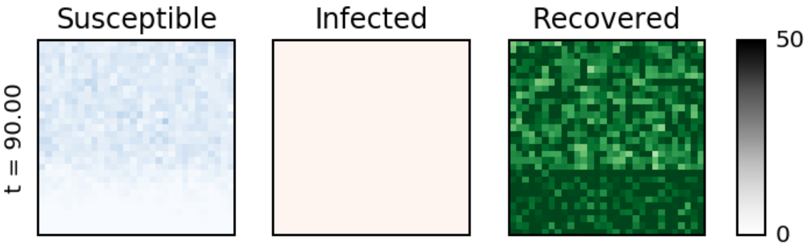
SIR model on 30x30 grid

Stochastic: von Neumann neighbourhood

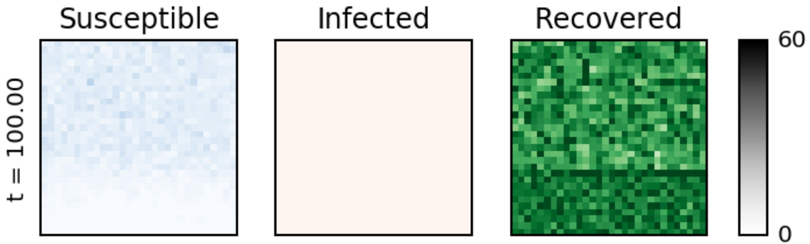
Initial values: $S^{(i)}(0) = 30, I^{(i)}(0) = 10, R^{(i)}(0) = 0$

Parameters: $k = 0.01,\ r = 0.2,\ m_s = m_i = 0.05$

except bottom third $k = 0.05$



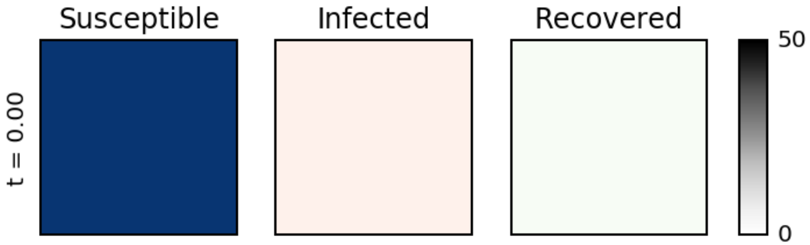
Initial values: $S^{(i)}(0) = 30, I^{(i)}(0) = 10, R^{(i)}(0) = 0$
Parameters: $k = 0.01,\ r = 0.2,\ m_s = m_i = 0.05$
except bottom third $k = 0.05$



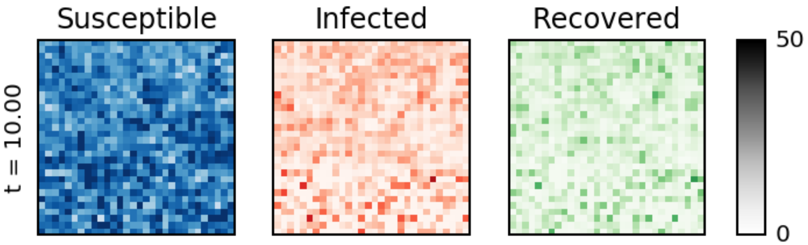
Initial values: $S^{(i)}(0) = 30, I^{(i)}(0) = 10, R^{(i)}(0) = 0$

Parameters: $k = 0.01,\ r = 0.2,\ m_s = m_i = 0.05$

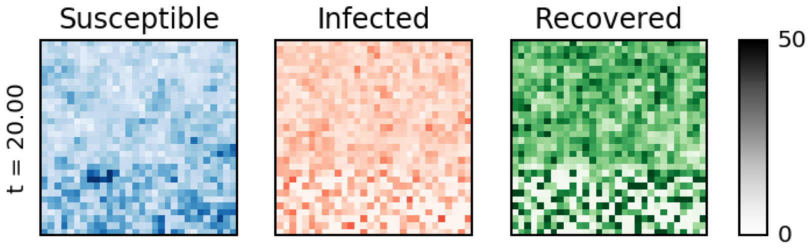
except bottom third $m_i = 0.001$



Initial values: $S^{(i)}(0) = 30, I^{(i)}(0) = 10, R^{(i)}(0) = 0$
Parameters: $k = 0.01,\ r = 0.2,\ m_s = m_i = 0.05$
except bottom third $m_i = 0.001$



Initial values: $S^{(i)}(0) = 30, I^{(i)}(0) = 10, R^{(i)}(0) = 0$
Parameters: $k = 0.01,\ r = 0.2,\ m_s = m_i = 0.05$
except bottom third $m_i = 0.001$



SIR model on 30x30 grid

Stochastic: von Neumann neighbourhood

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Initial values: $S^{(i)}(0) = 30, I^{(i)}(0) = 10, R^{(i)}(0) = 0$

Parameters: $k = 0.01,\ r = 0.2,\ m_s = m_i = 0.05$

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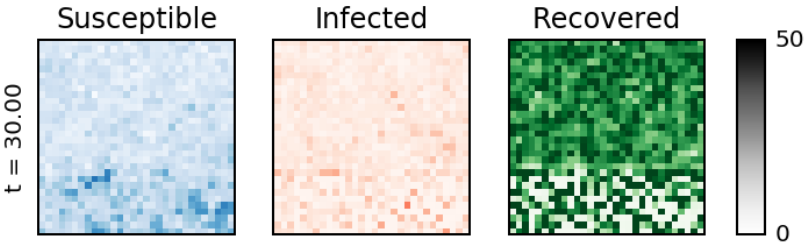

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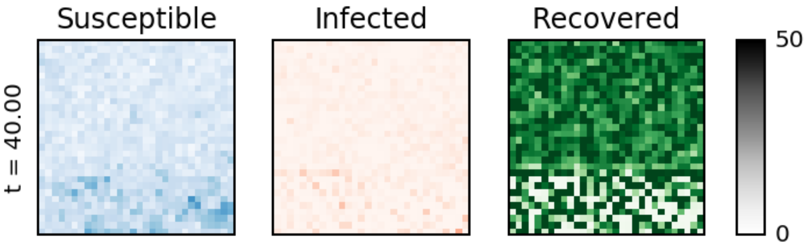

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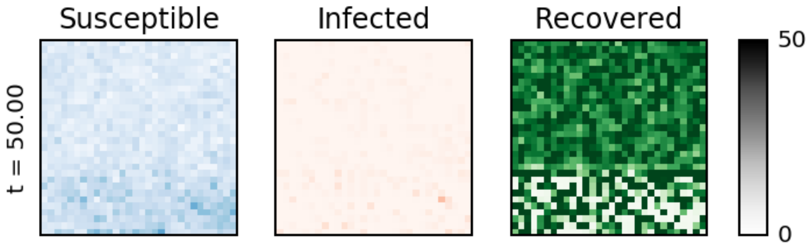

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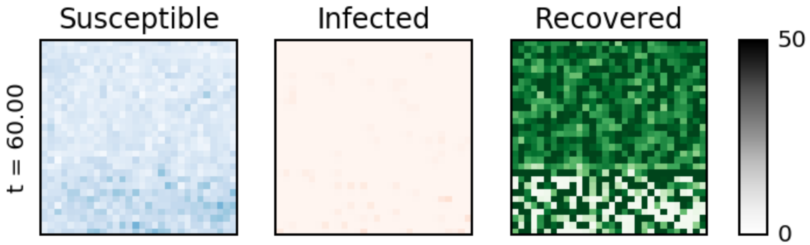

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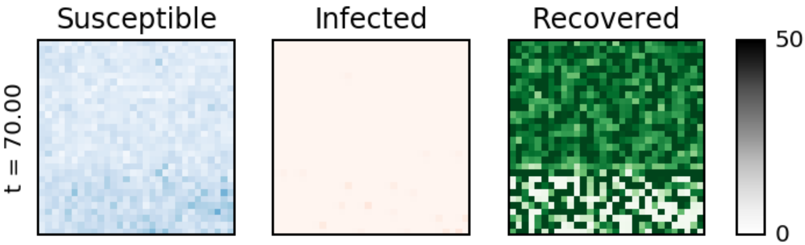

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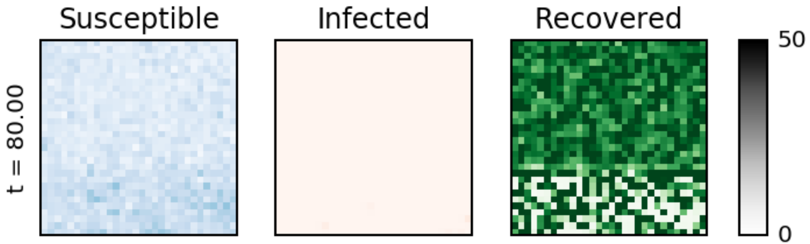

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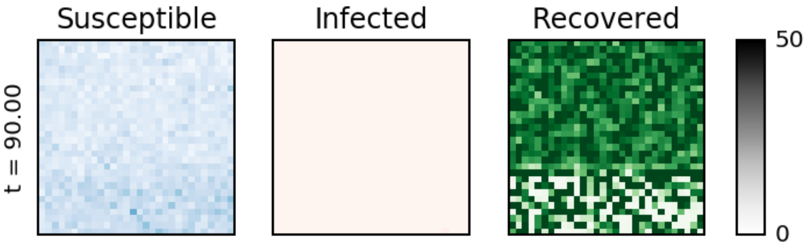

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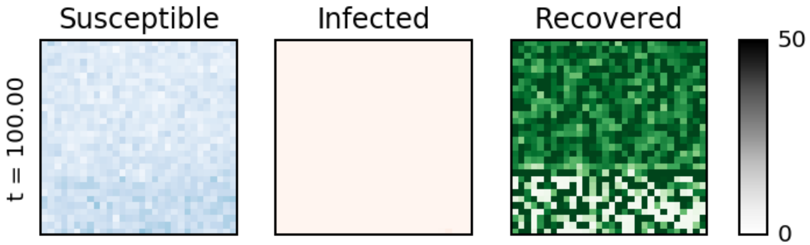

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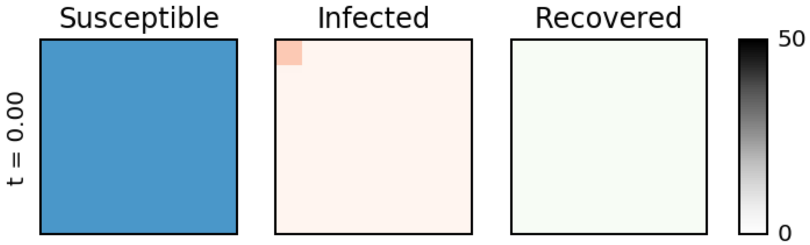

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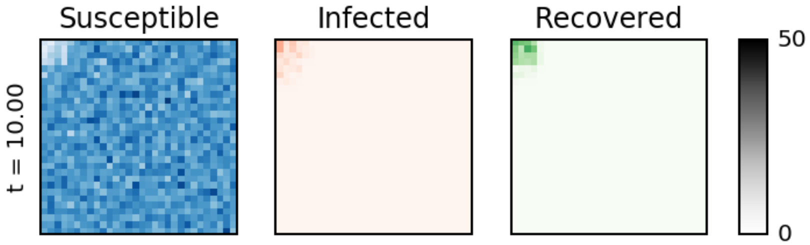

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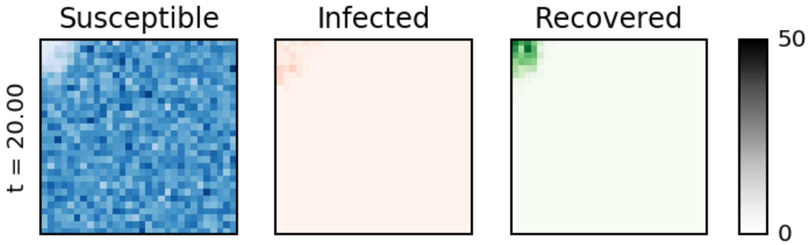

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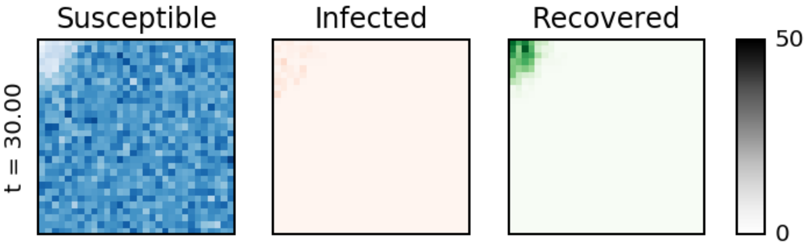

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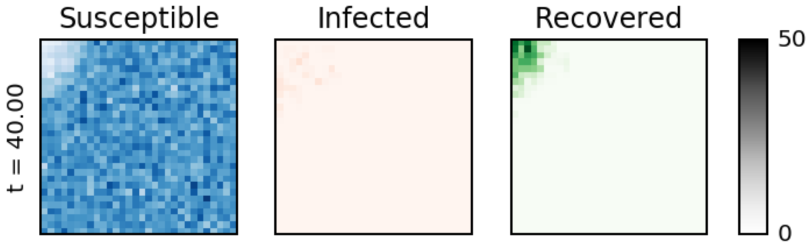

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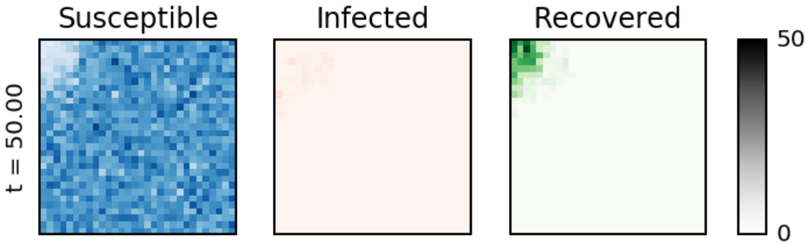

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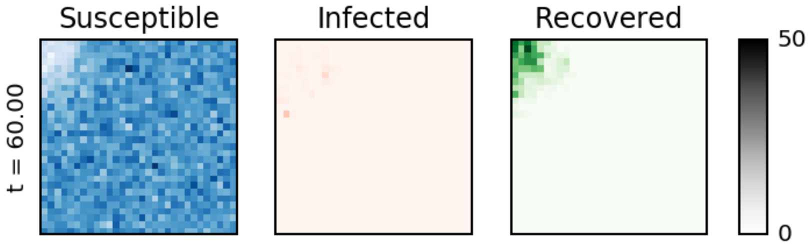

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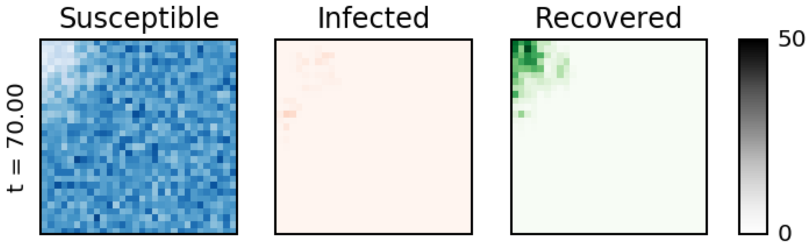

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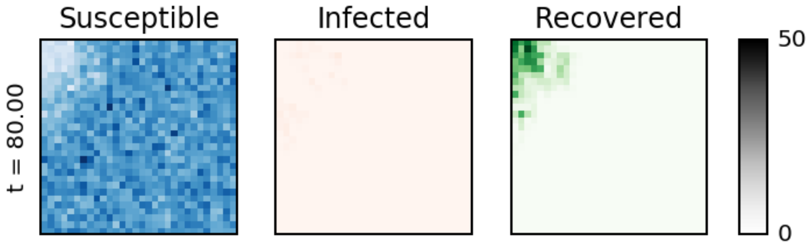

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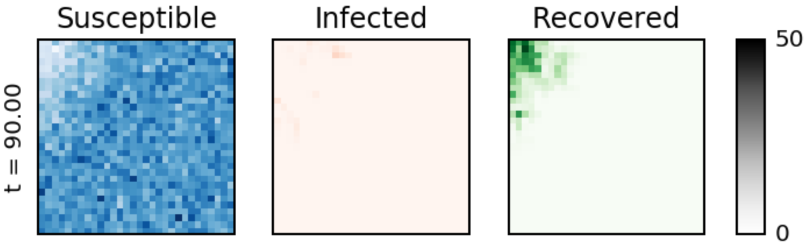

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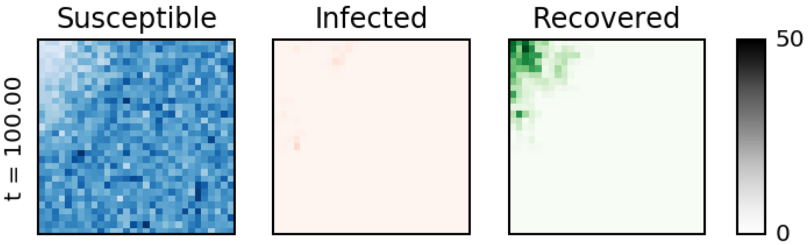

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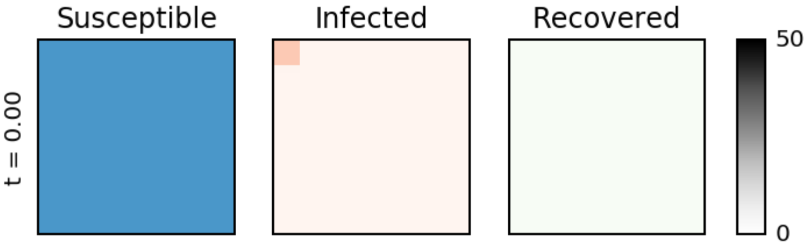

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Spatial moment closure

- technique that abstracts from space
- provides spatial averages for each subpopulation
- closure of ODEs for averages give approximations
- useful for large discrete space models
- no general theory yet; model specific
- potential use
  - large model with a few interesting locations
  - hybrid treatment of locations
  - approximate most locations with spatial moment ODEs
  - use other techniques for interesting locations

Moment ODEs

- Moments are the expected values of products of variables considered at a single time point
- $\mathbf{E}[X]$ is the first moment of X and the average value of X
- $\mathbf{E}[XY]$ is a second joint moment and the average value of XY
- $\mathrm{Var}[X] = \mathbf{E}[X^2] - \mathbf{E}[X]^2$ is a second central moment and the variance of X
- $\mathrm{Cov}(X, Y) = \mathbf{E}[XY] - \mathbf{E}[X]\mathbf{E}[Y]$ is a second central joint moment and the covariance of X and Y
- In general, $\mathbf{E}[X_1^{n_1} X_2^{n_2} \ldots X_k^{n_k}]$ is the nth joint moment when $n = \sum_{j=1}^{k} n_j$

Moment ODEs

- For a population CTMC, the behavior of each moment is defined by an ODE (Engblom, 2006)

$$\frac{d\mathbf{E}[M(\mathbf{Y})]}{dt} = \sum_{\tau=(\mathbf{v},r)} \mathbf{E}[r(\mathbf{Y}) \cdot (M(\mathbf{Y}+\mathbf{v}) - M(\mathbf{Y}))]$$

- Typically, each moment ODE involves higher moments
- Infinite system of ODEs which can't be simulated
- Use moment closure to truncate system

Types of moment closure

- Stochastic linearisation
  - approximate $\mathbf{E}[XY]$ by $\mathbf{E}[X]\mathbf{E}[Y]$ (or similar products)
  - equivalent to the assumption that $\mathrm{Cov}(X, Y) = 0$
- Distribution assumption
  - approximate higher moments with moments from chosen distribution
  - log-normal is good for populations since it has non-negative support
- Assume higher-order moments are negligible
  - approximate them with zero

Spatial moment ODEs

- Spatial moments are the expected value of products of variables average over all locations, at a single time point
- Typically, leads to infinite system of ODEs
- Apply moment closure techniques [Marion *et al*, 2002, 2005]
- No general expression for ODEs (yet)
- Consider for SIR model with homogeneous parameters and full connectivity

SIR: spatial moment ODEs

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$$
\begin{aligned}
d\mathbf{E}[\langle S \rangle]/dt &= -k\mathbf{E}[\langle SI \rangle] \\
d\mathbf{E}[\langle I \rangle]/dt &= k\mathbf{E}[\langle SI \rangle] - r\mathbf{E}[\langle I \rangle] \\
d\mathbf{E}[\langle R \rangle]/dt &= r\mathbf{E}[\langle I \rangle]
\end{aligned}
$$

$$
\begin{aligned}
d\mathbf{E}[\langle SI \rangle]/dt &= k(\mathbf{E}[\langle S^2 I \rangle] - \mathbf{E}[\langle SI^2 \rangle]) - r\mathbf{E}[\langle SI \rangle] \\
&\quad -m_s p(\mathbf{E}[\langle SI \rangle] - \mathbf{E}[\langle S \rangle\langle I \rangle]) \\
&\quad -m_i p(\mathbf{E}[\langle SI \rangle] - \mathbf{E}[\langle S \rangle\langle I \rangle]) \\
d\mathbf{E}[\langle S^2 \rangle]/dt &= -2k(\mathbf{E}[\langle S^2 I \rangle] \\
&\quad +m_s p(\mathbf{E}[\langle S^2 \rangle] - \mathbf{E}[\langle S \rangle\langle S \rangle])) \\
d\mathbf{E}[\langle I^2 \rangle]/dt &= 2(k\mathbf{E}[\langle SI^2 \rangle] - r\mathbf{E}[\langle I^2 \rangle] \\
&\quad -m_i p(\mathbf{E}[\langle I^2 \rangle] - \mathbf{E}[\langle I \rangle\langle I \rangle])
\end{aligned}
$$

SIR: spatial moment ODEs

$$\begin{aligned}
d\mathbf{E}[\langle S^2 I\rangle]/dt &= k(\mathbf{E}[\langle S^3 I\rangle] - 2\mathbf{E}[\langle S^2 I^2\rangle]) - r\mathbf{E}[\langle S^2 I\rangle] \\
&\quad - m_s p(\mathbf{E}[\langle S^2 I\rangle] - \mathbf{E}[\langle S^2\rangle\langle I\rangle]) \\
&\quad - m_i p(\mathbf{E}[\langle S^2 I\rangle] - \mathbf{E}[\langle S^2\rangle\langle I\rangle])
\end{aligned}$$

$$\begin{aligned}
d\mathbf{E}[\langle S I^2\rangle]/dt &= -k\mathbf{E}[\langle S I^3\rangle] + 2k\mathbf{E}[\langle S^2 I^2\rangle] - r\mathbf{E}[\langle S^2 I\rangle] \\
&\quad - m_s p(\mathbf{E}[\langle S I^2\rangle] - \mathbf{E}[\langle S I\rangle\langle I\rangle]) \\
&\quad - m_i p(\mathbf{E}[\langle S I^2\rangle] - \mathbf{E}[\langle S I\rangle\langle I\rangle])
\end{aligned}$$

Derivations

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Rate	$S^{(i)}$	$S^{(j)}$	$I^{(i)}$	$E^{(j)}$	$R^{(i)}$
$kS^{(i)}I^{(i)}$	-1	0	+1	0	0
$rI^{(i)}$	0	0	-1	0	+1
$m_s S^{(i)}$	-1	+1	0	0	0
$m_i I^{(i)}$	0	0	-1	+1	0

$$
\begin{aligned}
S^{(i)}(t+\delta t) - S^{(i)}(t) &= \delta S^{(i)} \\
&= [-kS^{(i)}(t)I^{(i)}(t) \\
&\quad -m_s \sum_{j=1}^{p} S^{(i)}(t) + m_s \sum_{j=1}^{p} S^{(j)}(t)]\delta t
\end{aligned}
$$

Derivations

Rate	$S^{(i)}$	$S^{(j)}$	$I^{(i)}$	$E^{(j)}$	$R^{(i)}$
$kS^{(i)}I^{(i)}$	-1	0	$+1$	0	0
$rI^{(i)}$	0	0	-1	0	$+1$
$m_s S^{(i)}$	-1	$+1$	0	0	0
$m_i I^{(i)}$	0	0	-1	$+1$	0

$$
\begin{aligned}
I^{(i)}(t+\delta t) - I^{(i)}(t) &= \delta I^{(i)} \\
&= [kS^{(i)}(t)I^{(i)}(t) - rI^{(i)}(t) \\
&\quad -m_i \sum_{j=1}^{p} I^{(i)}(t) + m_i \sum_{j=1}^{p} I^{(j)}(t)]\delta t
\end{aligned}
$$

Derivations

Rate	$S^{(i)}$	$S^{(j)}$	$I^{(i)}$	$E^{(j)}$	$R^{(i)}$
$kS^{(i)}I^{(i)}$	-1	0	$+1$	0	0
$rI^{(i)}$	0	0	-1	0	$+1$
$m_sS^{(i)}$	-1	$+1$	0	0	0
$m_iI^{(i)}$	0	0	-1	$+1$	0

$$\begin{aligned} R^{(i)}(t+\delta t) - R^{(i)}(t) &= \delta R^{(i)} \\ &= [rI^{(i)}(t)]\delta t \end{aligned}$$

Derivation of first moment

$$
\begin{aligned}
S^{(i)}(t+\delta t) - S^{(i)}(t) &= [-kS^{(i)}(t)I^{(i)}(t) \\
&\quad -m_s \sum_{j=1}^{p} S^{(i)}(t) + m_s \sum_{j=1}^{p} S^{(j)}(t)]\delta t
\end{aligned}
$$

Take spatial averages

$$
\begin{aligned}
1/p \sum_{i=1}^{p} (S^{(i)}(t+\delta t) + S^{(i)}(t)) &= [-1/p \sum_{i=1}^{p} (kS^{(i)}(t)I^{(i)}(t) \\
&\quad -m_s \sum_{j=1}^{p} S^{(i)}(t) + m_s \sum_{j=1}^{p} S^{(j)}(t))]\delta t
\end{aligned}
$$

Derivation of first moment

Rewrite with spatial average notation

$$
\begin{aligned}
\langle S\rangle(t+\delta t)+\langle S\rangle(t) &= [-k\langle SI\rangle(t) \\
&\quad -m_s\sum_{j=1}^{p}\langle S\rangle(t)+m_s\sum_{j=1}^{p}\langle S\rangle(t)]\delta t \\
&= -k\langle SI\rangle(t)\delta t
\end{aligned}
$$

Take expectations

$$\mathbf{E}[\langle S\rangle](t+\delta t)+\mathbf{E}[\langle S\rangle](t) = -k\langle SI\rangle(t)\delta t$$

Divide by δt and take the limit as $\delta t \to 0$

$$d\mathbf{E}[\langle S\rangle](t) = -k\langle SI\rangle$$

Derivation of second moment

Expand

$$
\begin{aligned}
S^{(i)}I^{(i)}(t+\delta t) &= S^{(i)}(t+\delta t)I^{(i)}(t+\delta t) \\
&= (S^{(i)}(t)+\delta S^{(i)})(I^{(i)}(t)+\delta I^{(i)}) \\
&= S^{(i)}I^{(i)}(t) + S^{(i)}\delta I^{(i)} + I^{(i)}\delta S^{(i)} + \delta S^{(i)}\delta I^{(i)}
\end{aligned}
$$

Hence

$$
\begin{aligned}
& S^{(i)}I^{(i)}(t+\delta t) - S^{(i)}I^{(i)}(t) \\
= \;& S^{(i)}\delta I^{(i)} + I^{(i)}\delta S^{(i)} + K \\
= \;& S^{(i)}[kS^{(i)}I^{(i)} - rI^{(i)} - m_s\sum_{j=1}^{p} S^{(i)} + m_s\sum_{j=1}^{p} S^{(j)}]\delta + \\
+ \;& I^{(i)}[-kS^{(i)}I^{(i)} - m_i\sum_{j=1}^{p} I^{(i)} + m_i\sum_{j=1}^{p} I^{(j)}]\delta + K
\end{aligned}
$$

Derivation of second moment

Taking spatial averages

$$
\begin{aligned}
& \langle SI\rangle(t+\delta t) - \langle SI\rangle(t) \\
= \;& [k(\langle S^2 I\rangle - \langle S^2 I\rangle) - r\langle SI\rangle - \\
& m_s \sum_{j=1}^{p} \langle SI\rangle + m_s\langle S\rangle \sum_{j=1}^{p} S^{(j)} - m_i \sum_{j=1}^{p} \langle SI\rangle + m_i\langle S\rangle \sum_{j=1}^{p} I^{(j)}]\delta + K \\
= \;& [k(\langle S^2 I\rangle - \langle S^2 I\rangle) - r\langle SI\rangle - \\
& m_s p(\langle SI\rangle - \langle S\rangle\langle I\rangle) - m_i p(\langle SI\rangle - \langle S\rangle\langle I\rangle)]\delta + K
\end{aligned}
$$

Following the same procedure as before

$$
\begin{aligned}
d\mathbf{E}[\langle SI\rangle](t+\delta t)/dt \;=\;& k(\mathbf{E}[\langle S^2 I\rangle] - \mathbf{E}[\langle S^2 I\rangle]) - r\mathbf{E}[\langle SI\rangle] \\
& - m_s p(\mathbf{E}[\langle SI\rangle] - \mathbf{E}[\langle S\rangle\langle I\rangle]) \\
& - m_i p(\mathbf{E}[\langle SI\rangle] - \mathbf{E}[\langle S\rangle\langle I\rangle])
\end{aligned}
$$

Derivation of second moment

Taking spatial averages

$$
\begin{aligned}
& \langle SI\rangle(t+\delta t) - \langle SI\rangle(t) \\
= \;& [k(\langle S^2 I\rangle - \langle S^2 I\rangle) - r\langle SI\rangle - \\
& m_s \sum_{j=1}^{p} \langle SI\rangle + m_s\langle S\rangle \sum_{j=1}^{p} S^{(j)} - m_i \sum_{j=1}^{p} \langle SI\rangle + m_i\langle S\rangle \sum_{j=1}^{p} I^{(j)}]\delta + K \\
= \;& [k(\langle S^2 I\rangle - \langle S^2 I\rangle) - r\langle SI\rangle - \\
& m_s p(\langle SI\rangle - \langle S\rangle\langle I\rangle) - m_i p(\langle SI\rangle - \langle S\rangle\langle I\rangle)]\delta + K
\end{aligned}
$$

Following the same procedure as before

$$
\begin{aligned}
d\mathbf{E}[\langle SI\rangle](t+\delta t)/dt \;=\;& k(\mathbf{E}[\langle S^2 I\rangle] - \mathbf{E}[\langle S^2 I\rangle]) - r\mathbf{E}[\langle SI\rangle] \\
& - m_s p(\mathbf{E}[\langle SI\rangle] - \mathbf{E}[\langle S\rangle]\mathbf{E}[\langle I\rangle]) \\
& - m_i p(\mathbf{E}[\langle SI\rangle] - \mathbf{E}[\langle S\rangle]\mathbf{E}[\langle I\rangle])
\end{aligned}
$$

SIR: spatial moment ODEs

$$\begin{aligned}
d\mathbf{E}[\langle S\rangle]/dt &= -k\mathbf{E}[\langle SI\rangle] \\
d\mathbf{E}[\langle I\rangle]/dt &= \ \ k\mathbf{E}[\langle SI\rangle] - r\mathbf{E}[\langle I\rangle] \\
d\mathbf{E}[\langle R\rangle]/dt &= \ \ r\mathbf{E}[\langle I\rangle]
\end{aligned}$$

$$\begin{aligned}
d\mathbf{E}[\langle SI\rangle]/dt &= \ \ k(\mathbf{E}[\langle S^2 I\rangle] - \mathbf{E}[\langle SI^2\rangle]) - r\mathbf{E}[\langle SI\rangle] \\
&\quad -m_s p(\mathbf{E}[\langle SI\rangle] - \mathbf{E}[\langle S\rangle\langle I\rangle]) \\
&\quad -m_i p(\mathbf{E}[\langle SI\rangle] - \mathbf{E}[\langle S\rangle\langle I\rangle]) \\
d\mathbf{E}[\langle S^2\rangle]/dt &= -2k(\mathbf{E}[\langle S^2 I\rangle] \\
&\quad +m_s p(\mathbf{E}[\langle S^2\rangle] - \mathbf{E}[\langle S\rangle\langle S\rangle])) \\
d\mathbf{E}[\langle I^2\rangle]/dt &= \ \ 2(k\mathbf{E}[\langle SI^2\rangle] - r\mathbf{E}[\langle I^2\rangle] \\
&\quad -m_i p(\mathbf{E}[\langle I^2\rangle] - \mathbf{E}[\langle I\rangle\langle I\rangle])
\end{aligned}$$

SIR: spatial moment ODEs

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$$
\begin{aligned}
d\mathbf{E}[\langle S\rangle]/dt &= -k\mathbf{E}[\langle SI\rangle] \\
d\mathbf{E}[\langle I\rangle]/dt &= \quad k\mathbf{E}[\langle SI\rangle] - r\mathbf{E}[\langle I\rangle] \\
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\end{aligned}
$$

$$
\begin{aligned}
d\mathbf{E}[\langle SI\rangle]/dt &= \quad k(\mathbf{E}[\langle S^2 I\rangle] - \mathbf{E}[\langle SI^2\rangle]) - r\mathbf{E}[\langle SI\rangle] \\
&\quad -m_s p(\mathbf{E}[\langle SI\rangle] - \mathbf{E}[\langle S\rangle\langle I\rangle]) \\
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d\mathbf{E}[\langle I^2\rangle]/dt &= \quad 2(k\mathbf{E}[\langle SI^2\rangle] - r\mathbf{E}[\langle I^2\rangle] \\
&\quad -m_i p(\mathbf{E}[\langle I^2\rangle] - \mathbf{E}[\langle I\rangle\langle I\rangle])
\end{aligned}
$$

SIR: spatial moment ODEs

quanticol
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$$
\begin{aligned}
d\mathbf{E}[\langle S^2 I\rangle]/dt &= k(\mathbf{E}[\langle S^3 I\rangle] - 2\mathbf{E}[\langle S^2 I^2\rangle]) - r\mathbf{E}[\langle S^2 I\rangle] \\
&\quad - m_s p(\mathbf{E}[\langle S^2 I\rangle] - \mathbf{E}[\langle S^2\rangle\langle I\rangle]) \\
&\quad - m_i p(\mathbf{E}[\langle S^2 I\rangle] - \mathbf{E}[\langle S^2\rangle\langle I\rangle])
\end{aligned}
$$

$$
\begin{aligned}
d\mathbf{E}[\langle S I^2\rangle]/dt &= -k\mathbf{E}[\langle S I^3\rangle] + 2k\mathbf{E}[\langle S^2 I^2\rangle] - r\mathbf{E}[\langle S^2 I\rangle] \\
&\quad - m_s p(\mathbf{E}[\langle S I^2\rangle] - \mathbf{E}[\langle S I\rangle\langle I\rangle]) \\
&\quad - m_i p(\mathbf{E}[\langle S I^2\rangle] - \mathbf{E}[\langle S I\rangle\langle I\rangle])
\end{aligned}
$$

SIR: spatial moment ODEs

$$
\begin{aligned}
d\mathbf{E}[\langle S^2 I\rangle]/dt &= k(\mathbf{E}[\langle S^3 I\rangle] - 2\mathbf{E}[\langle S^2 I^2\rangle]) - r\mathbf{E}[\langle S^2 I\rangle] \\
&\quad -m_s p(\mathbf{E}[\langle S^2 I\rangle] - \mathbf{E}[\langle S^2\rangle\langle I\rangle]) \\
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$$

$$
\begin{aligned}
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&\quad -m_i p(\mathbf{E}[\langle S I^2\rangle] - \mathbf{E}[\langle S I\rangle\langle I\rangle])
\end{aligned}
$$

SIR: spatial moment ODEs

- stochastic linearisation for third order moments
  - approximate $\mathbf{E}[\langle S^2 I\rangle]$ with $\mathbf{E}[\langle S\rangle]\mathbf{E}[\langle SI\rangle]$ or $\mathbf{E}[\langle S^2\rangle]\mathbf{E}[\langle I\rangle]$
  - approximate $\mathbf{E}[\langle SI^2\rangle]$ with $\mathbf{E}[\langle S\rangle]\mathbf{E}[\langle I^2\rangle]$ or $\mathbf{E}[\langle SI\rangle]\mathbf{E}[\langle I\rangle]$
- stochastic linearisation for fourth order moments
  - approximate $\mathbf{E}[\langle S^3 I\rangle]$, $\mathbf{E}[\langle SI^3\rangle]$ and $\mathbf{E}[\langle S^2 I^2\rangle]$
- log-normal distribution to approximate third order moments

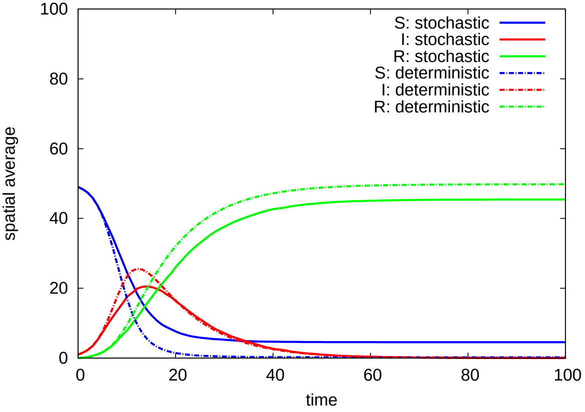
$$\mathbf{E}[\langle S^2 I\rangle] = \frac{\mathbf{E}[\langle S^2\rangle]\mathbf{E}[\langle SI\rangle]^2}{\mathbf{E}[\langle S\rangle]^2\mathbf{E}[\langle I\rangle]}$$

$$\mathbf{E}[\langle SI^2\rangle] = \frac{\mathbf{E}[\langle I^2\rangle]\mathbf{E}[\langle SI\rangle]^2}{\mathbf{E}[\langle I\rangle]^2\mathbf{E}[\langle S\rangle]}$$

SIR model on 12x12 grid

Initial values: $S^{(i)}(0) = 49, I^{(i)}(0) = 1, R^{(i)}(0) = 0$
Parameters: $k = 0.011,\ r = 0.1,\ m_s = m_i = 0.00001$

Stochastic versus deterministic



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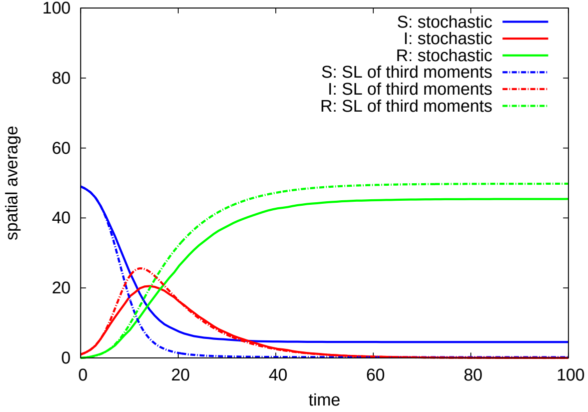
Stochastic versus stochastic linearisation of third moments



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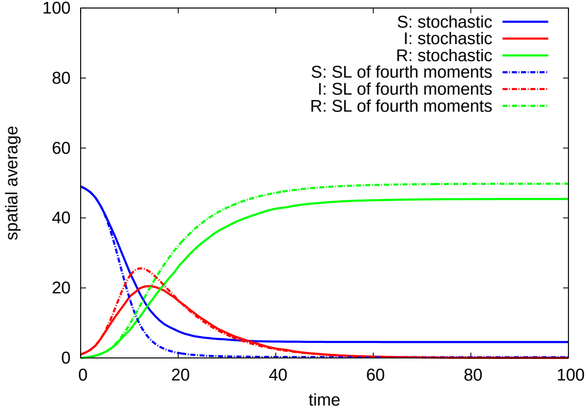
Stochastic versus stochastic linearisation of fourth moments



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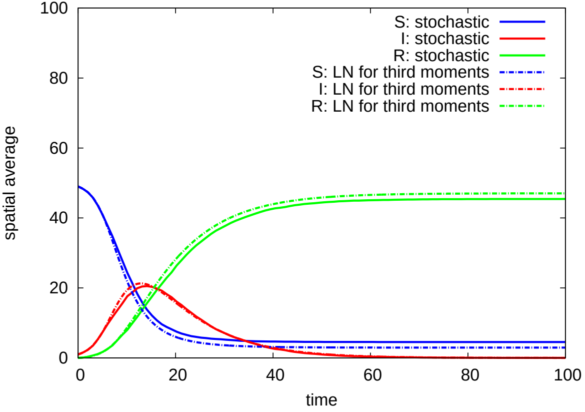
Parameters: $k = 0.011$, $r = 0.1$, $m_s = m_i = 0.00001$

Stochastic versus log normal third moments



Spatial moment closure

- techniques for approximating average behaviour *over space*
- generality: when does it work?
  - different parameter ranges for SIR
  - other models – SEIS
  - general definition of ODEs
- applications
  - for global behaviour
  - to abstract "uninteresting" parts of a model
- ongoing research

Going to the (spatial) limit

Current approach for scalable modelling

Current approach for scalable modelling

State-space explosion $\xrightarrow{\text{fluid approximation}}$ ODEs

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State-space explosion $\xrightarrow{\text{fluid approximation}}$ ODEs

Does this work with discrete space?

Current approach for scalable modelling

State-space explosion $\xrightarrow{\text{fluid approximation}}$ ODEs

Does this work with discrete space?

Add space

Current approach for scalable modelling

State-space explosion $\xrightarrow{\text{fluid approximation}}$ ODEs

Does this work with discrete space?

Bigger state-space explosion $\xrightarrow{\text{fluid approximation}}$ PDEs

Current approach for scalable modelling

State-space explosion $\xrightarrow{\text{fluid approximation}}$ ODEs

Does this work with discrete space?

Bigger state-space explosion $\xrightarrow{\text{fluid approximation}}$ PDEs

Yes, here is how it can be done

Using PDES for discrete space

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population discrete-space model on grid

$\Downarrow$ fluidisation of space

partial differential equation model

PDE solver uses $\Downarrow$ discretisation of space

results for population discrete-space model

[Tschaikowski and Tribastone, 2014]

Mobile agents on a grid

- Consider agents which are moving on a lattice in the unit square.

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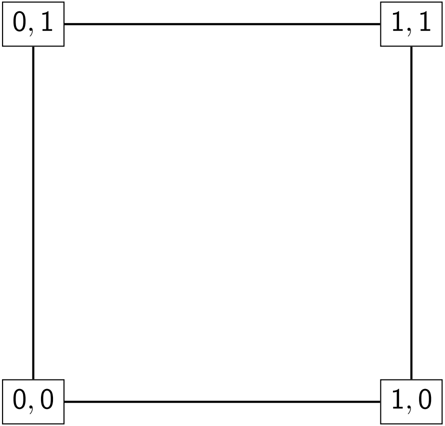
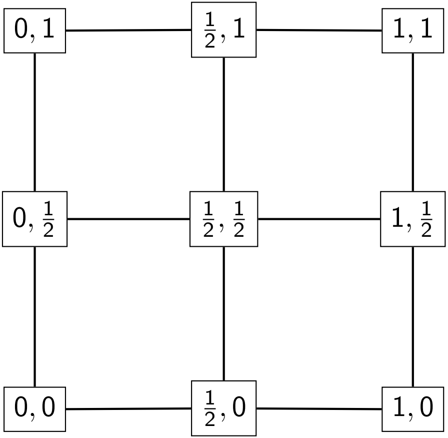
$K = 1$



Mobile agents on a grid

- Consider agents which are moving on a lattice in the unit square.
- The lattice consists of $(K+1)^2$ regions.

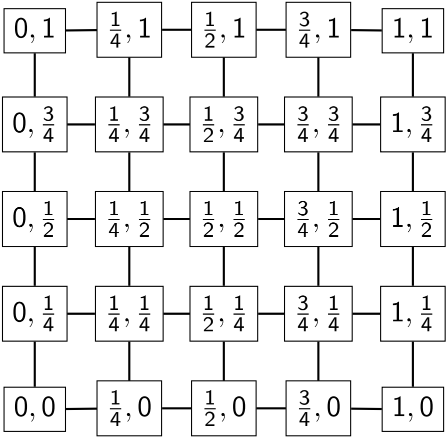
$K = 2$



Mobile agents on a grid

- Consider agents which are moving on a lattice in the unit square.
- The lattice consists of $(K+1)^2$ regions.

$$K = 4$$



Mobile agents on a grid

- agents moving on a grid using von Neumann neighbourhood and with random, unbiased walk
- with many agents, we know how to approximate behaviour with ODEs
- the number of ODEs is proportional to number of grid points
- the finer the granularity of the space, the larger the ODE system
- we can approximate the ODE system by a system of partial differential equations that does not depend on the number of grid points
- technique supported by Spatial Fluid Extended Process Algebra (SFEPA) [Tschaikowski and Tribastone, 2014]

Predator-prey example

- The fluid approximation applied to agents give the ODEs for the nonspatial model

$$dS/dt = qrSR - sS \qquad\qquad dR/dt = zR - rRS$$

Predator-prey example

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- Considering this fluid approximation over a grid gives the ODEs

$$dS^{(x,y)}/dt = qrS^{(x,y)}R^{(x,y)} - sS^{(x,y)} + \mu_S \triangle^d S^{(x,y)}$$
$$dR^{(x,y)}/dt = zR^{(x,y)} - rS^{(x,y)}R^{(x,y)} + \mu_R \triangle^d R^{(x,y)}$$

Predator-prey example

- The fluid approximation applied to agents give the ODEs for the nonspatial model

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- Considering this fluid approximation over a grid gives the ODEs

$$dS^{(x,y)}/dt = qrS^{(x,y)}R^{(x,y)} - sS^{(x,y)} + \mu_S \triangle^d S^{(x,y)}$$
$$dR^{(x,y)}/dt = zR^{(x,y)} - rS^{(x,y)}R^{(x,y)} + \mu_R \triangle^d R^{(x,y)}$$

- These can be approximated by the following PDE system [Okuba and Levin, 2001]

$$\partial_t S = qrSR - sS + \mu_S \triangle S$$
$$\partial_t R = zR - rSR + \mu_R \triangle R$$

Predator-prey example

- generalise model to d predators
- results

K	$d=1$ Error	$d=1$ ODE Time	$d=3$ Error	$d=3$ ODE Time	$d=5$ Error	$d=5$ ODE Time
4	0.082	0 s	0.086	0 s	0.090	0 s
8	0.026	0 s	0.030	3 s	0.034	11 s
16	0.014	5 s	0.018	68 s	0.021	241 s
20	0.013	13 s	0.017	195 s	0.020	764 s
PDE Time		0 s		1 s		2 s

- The ODEs and PDEs were solved using *ode15s* and *parabolic*, respectively

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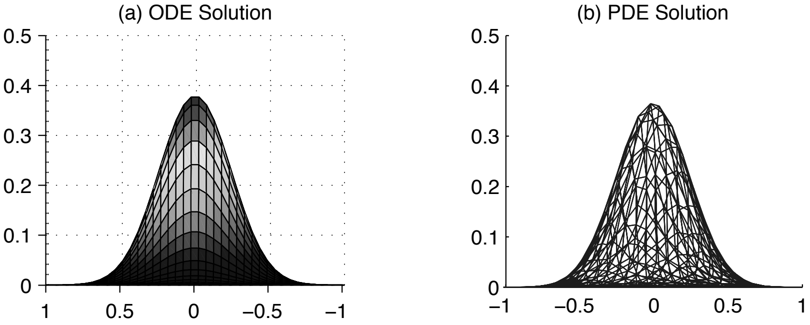
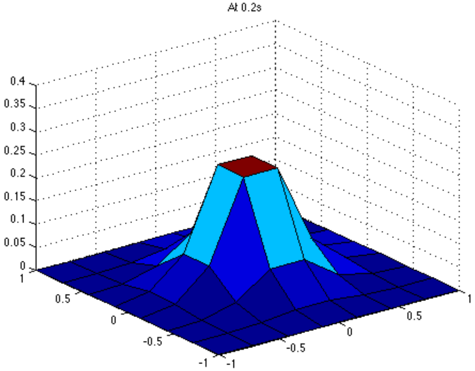
PDE Time		0 s		1 s		2 s

- The ODEs and PDEs were solved using *ode15s* and *parabolic*, respectively
- PDEs solver is faster because the underlying spatial discretization is governed by the PDEs and not by K

Predetor-prey example

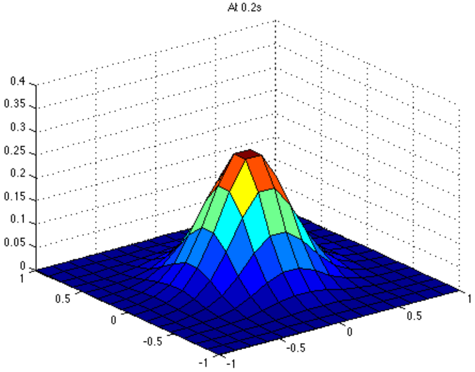


Example: Spatial Lotka Volterra



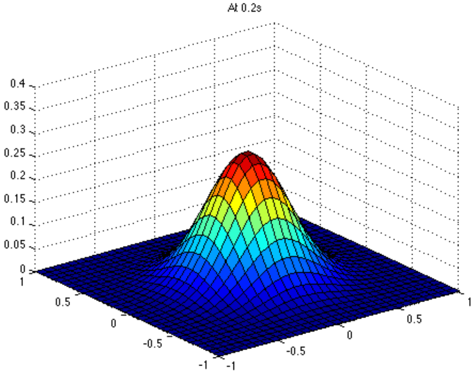
ODE with 8x8 points

Example: Spatial Lotka Volterra



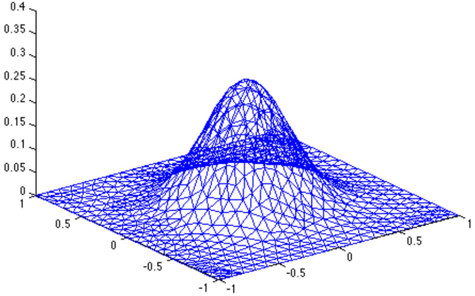
ODE with 16x16 points

Example: Spatial Lotka Volterra



ODE with 32x32 points

Example: Spatial Lotka Volterra



PDE

Conclusion

- spatial representations
  - discrete versus continuous
  - others: hybrid, topological
- spatial analysis techniques
  - dependent on representation
  - general overview
  - two in some detail
- choice for modelling CAS
  - discrete space with population aggregation
  - questions to be answered by modelling

References

- A.T. Bittig and A.M. Uhrmacher, Spatial modeling in cell biology at multiple levels, *Proceedings of Winter Simulation Conference (WSC 2010)*, 608619, 2010
- T. Camp, J. Boleng, and V. Davies. A survey of mobility models for ad hoc network research, *Wireless Communications and Mobile Computing*, 2:483502, 2002
- D. Cerotti, M. Gribaudo, A. Bobbio, C.T. Calafate and P. Manzoni, A Markovian agent model for fire propagation in outdoor environments, *Proceedings of the Seventh European Performance Engineering Workshop (EPEW 2010)*, LNCS 6342, 131146, 2010
- A. Chaintreau, J.-Y. Le Boudec and N. Ristanovic, The age of gossip: spatial mean field regime, *Proceedings of SIGMETRICS/Performance 2009*, 109120, 2009
- E.A Codling, M.J Plank and S. Benhamou, Random walk models in biology, *Journal of the Royal Society Interface*, 5:813834, 2008
- E.E. Holmes, M.A. Lewis, J.E. Banks and R.R. Veit, Partial differential equations in ecology: spatial interactions and population dynamics, *Ecology*, 75:1729, 1994
- H. Hu, S. Myers, V. Colizza and A. Vespignani, WiFi networks and malware epidemiology, *Proceedings of the National Academy of Sciences*, 106:13181323, 2009

References

- P. Juang, H. Oki, Y. Wang, M. Martonosi, L.S. Peh and D. Rubenstein, Energy-efficient computing for wildlife tracking: Design tradeoffs and early experiences with ZebraNet, *SIGPLAN Notices*, 37:96107, 2002
- G. Marion, X. Mao, E. Renshaw and J. Liu, Spatial heterogeneity and the stability of reaction states in autocatalysis, *Physical Review E*, 66:051915, 2002.
- G. Marion, D.L. Swain and M.R. Hutchings, Understanding foraging behaviour in spatially heterogeneous environments, *Journal of Theoretical Biology*, 232:127142, 2005
- M. Musolesi and C. Mascolo, Mobility models for systems evaluation. *Middleware for Network Eccentric and Mobile Applications*, 4362, 2009
- A. Okubo and S.A. Levin, *Diffusion and Ecological Problems: Modern Perspectives*, 2001
- S. Riley, Large-scale spatial-transmission models of infectious disease, *Science*, 316:12981301, 2007
- M. Tschaikowski and M. Tribastone, A Partial-differential Approximation for Spatial Stochastic Process Algebra, *Proceedings of VALUETOOLS 2014*