Longtime behaviors of stochastic reaction-diffusion equations on metric graphs

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Outline

1. Motivation: model comparison
2. Biased voter model and FKPP
3. Stochastic PDE on metric graphs
4. Duality and extinction probability

Partial differential equations

- powerful tools that capture many **space-time organized structures**
- describe the macroscopic behavior of a certain quantity $u(t,x)$ at time t and location x

Eg. **Heat equation**

$$\boxed{\partial_t u(t,x) = \alpha\, \Delta u(t,x)}$$

Suppose initial condition u_0 is "nice at infinity", then the solution on $\mathbb{R}^d$ is

$$u(t,x) = \int_{\mathbb{R}^d} p(t,x,y)\, u_0(y) dy,$$

where $p(t,x,y) = (4\pi\alpha t)^{-d/2} e^{-|x-y|^2/4\alpha t}$.

Eg. **Reaction-Diffusion equation**

$$\boxed{\partial_t u(t,x) = \alpha\, \Delta u(t,x) + F(u(t,x))}$$

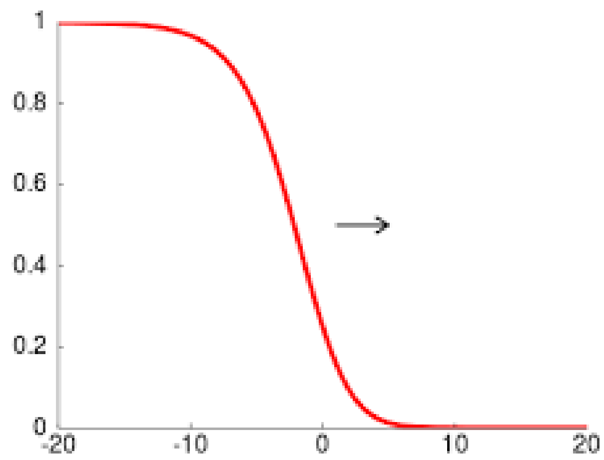
.e.g. $F(u) = \beta u(1-u)$ logistic growth

Partial differential equations

Eg. Fisher-Kolmogorov-Petrovskii-Piscounov (**FKPP**) equation

$$\partial_t u(t,x) = \alpha\, \Delta u(t,x) + \beta\, u(t,x)\big(1 - u(t,x)\big)$$

- models the spatial spread of an advantageous gene type



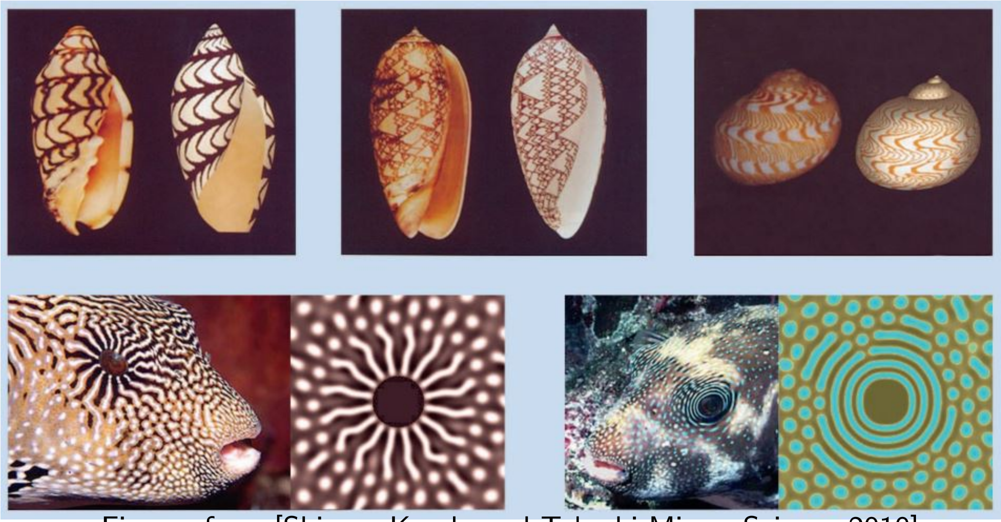
- on $\mathbb{R}$, it has asymptotic speed: $2\sqrt{\alpha\,\beta}$

  [Fisher 1937, KPP 1937, McKean 1975, Bramson 1983, Freidlin 1996, etc]

Partial differential equations

Eg. Turing patterns [Alan Turing 1952] captured by reaction-diffusion systems

$$\begin{cases} \partial_t u &= \alpha_u \Delta u + F(u,v) \\ \partial_t v &= \alpha_v \Delta v + G(u,v) \end{cases}$$



Figures from [Shigeru Kondo and Takashi Miura, Science 2010]

Eg. Transport equation, wave equation, Burgers equation, Navier-Stokes equation, Einstein's equation, Ginzburg-Landau equation, etc.

$u(t, x)$ is usually interpreted as certain continuous quantity

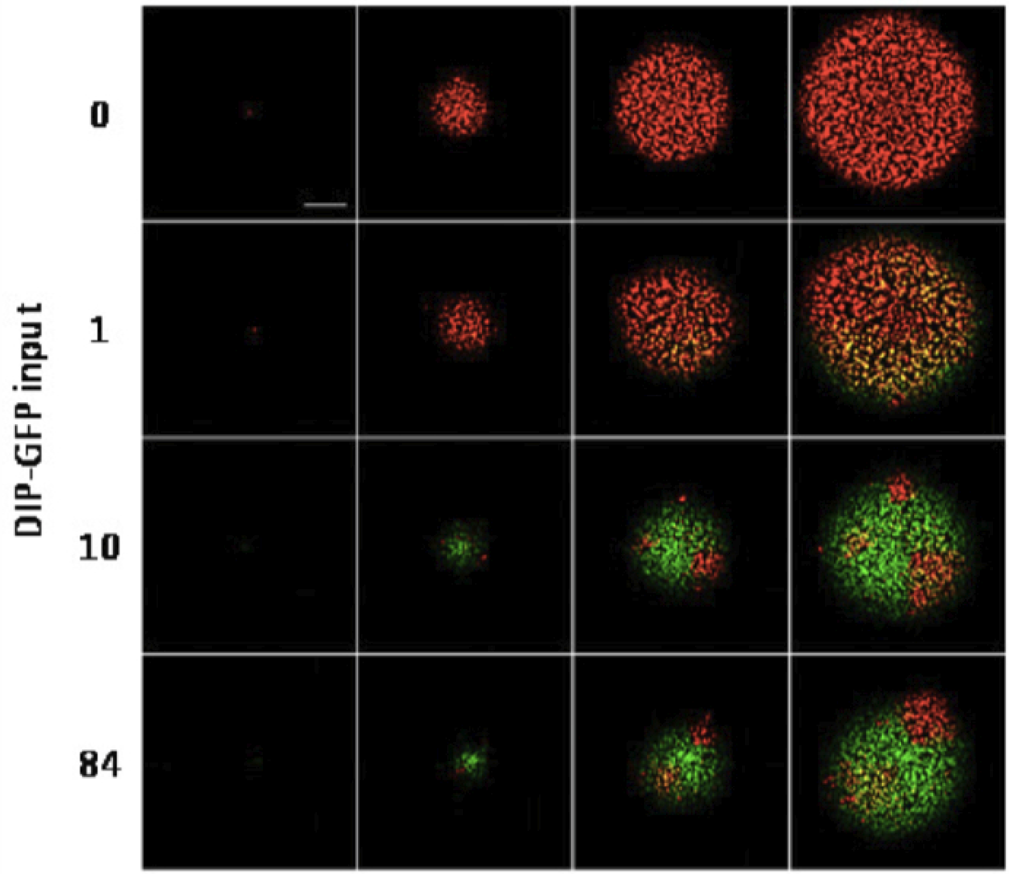
However,

- individuals are **not infinitesimally small**
- observations are often **noisy**

Randomly growing tumor

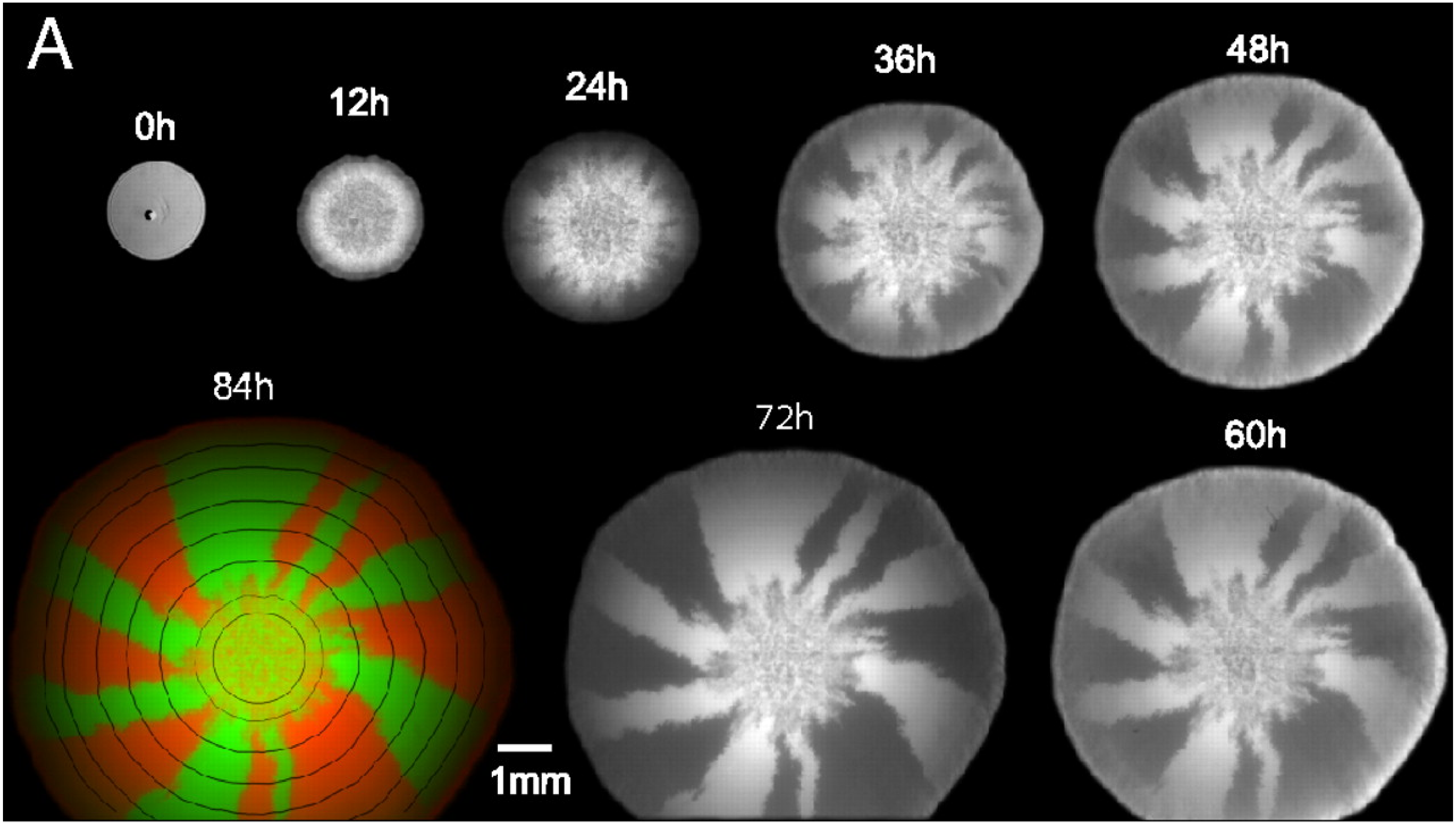
Duke Cancer Institute: http://sites.duke.edu/dukecancerinstitute/

Virus spread



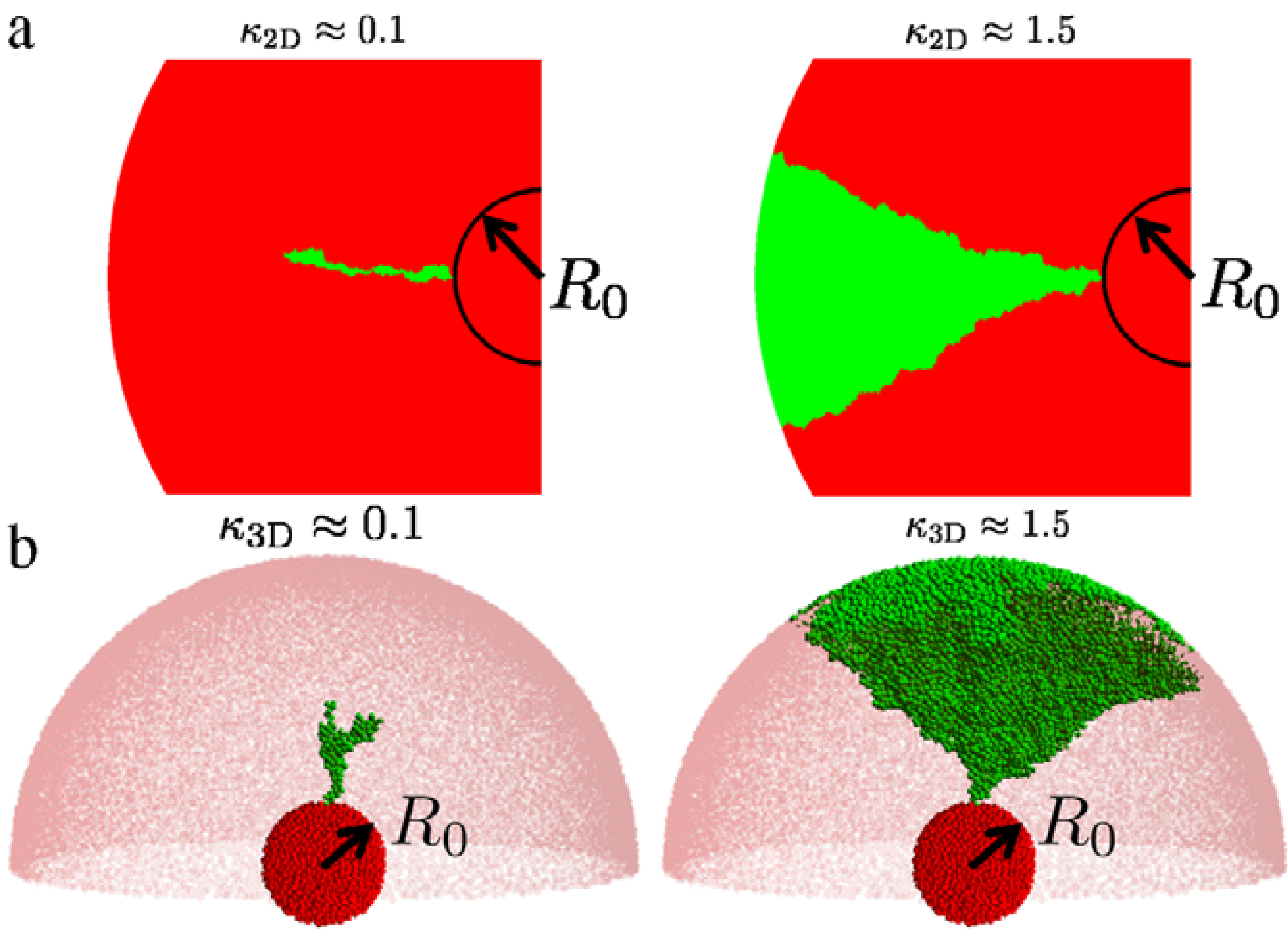
[Baltes, Akpinar, Inankur, and Yin 2017]

Growing bacterial colonies



[Hallatschek, Hersen, Ramanathan and Nelson 2007]

Extinction versus survival

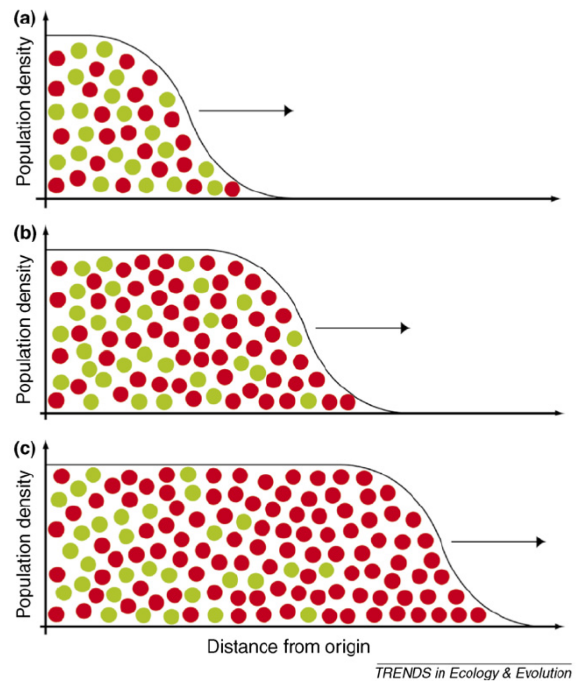


[Lavrentovich and Nelson 2015]

Individual-based model

- cells and particles have positive size
- experimental outcomes are stochastic.

To take **discreteness** and **stochasticity** into account, individual-based models are often used.



However, they are often **computationally and analytically intractable**.

Fundamental challenge in modeling

Which model should we use?

- Individual-based models
- Partial differential equations (PDE)
- Stochastic PDE (SPDE)
- multi-scale models
- hybrid models
- $\cdots$

Key: understand the connections among models.

Why do we care?

Fundamental challenge in modeling

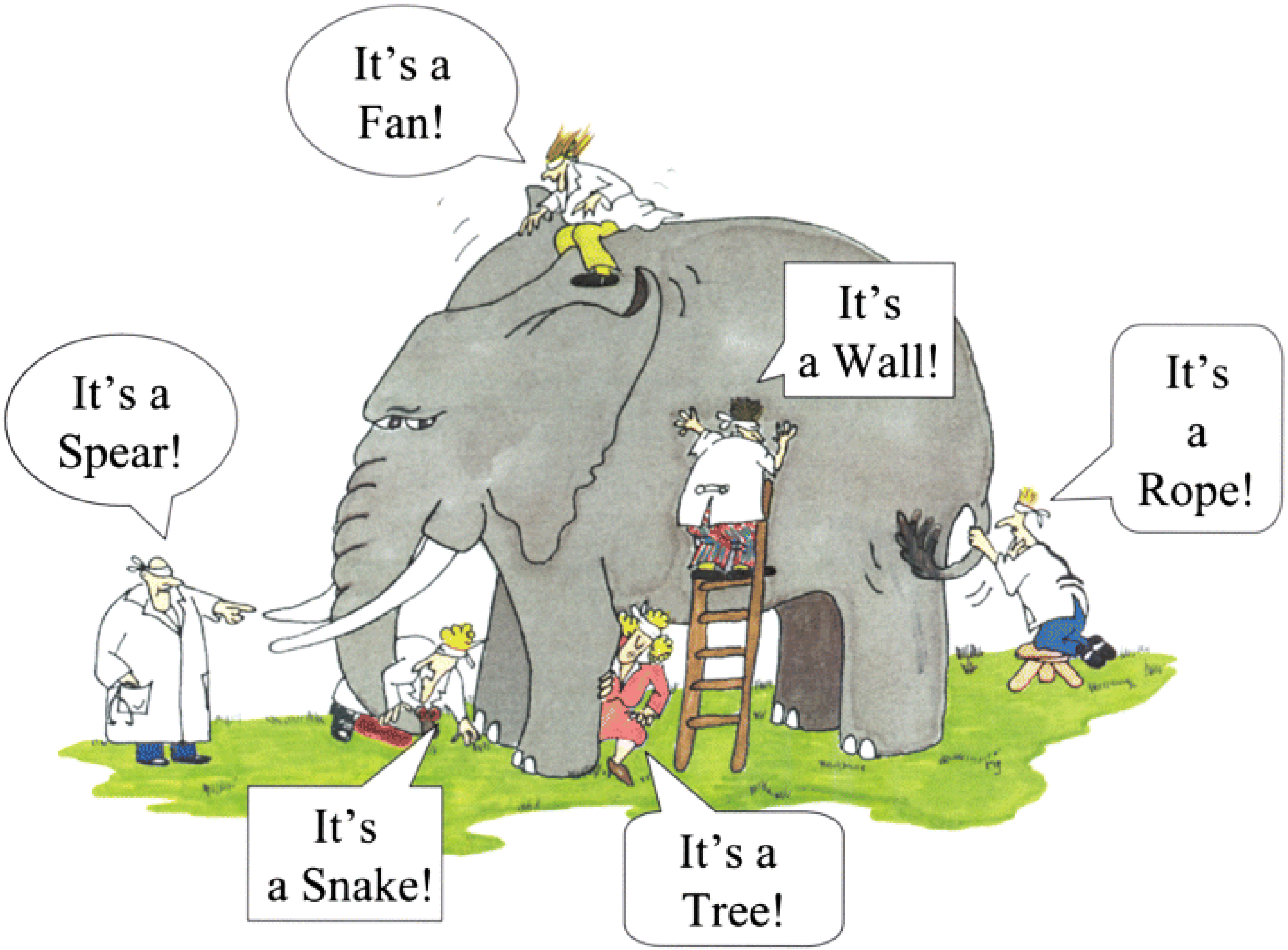
Which model should we use?

- Individual-based models
- Partial differential equations (PDE)
- Stochastic PDE (SPDE)
- multi-scale models
- hybrid models
- ...

Key: understand the connections among models.

Why do we care?

Why do we care about understanding the connections among models ?



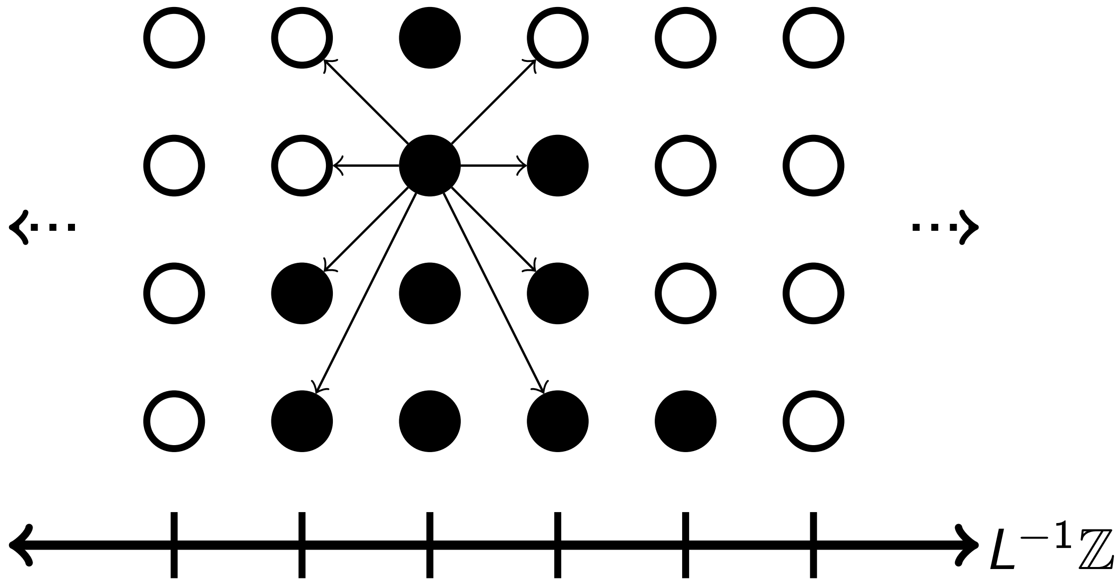
The parable of the blind men and an elephant, figures from cvi teacher - WordPress.com

Outline

Biased Voter Model (BVM)

BVM on

$$(L^{-1}\mathbb{Z}) \times \{1, \dots, M\}.$$

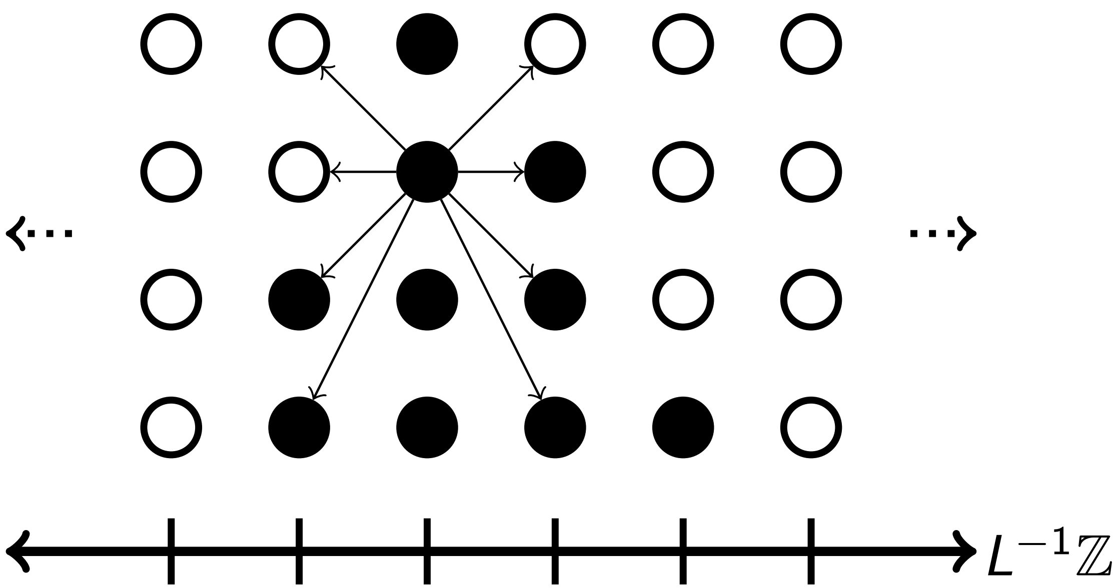


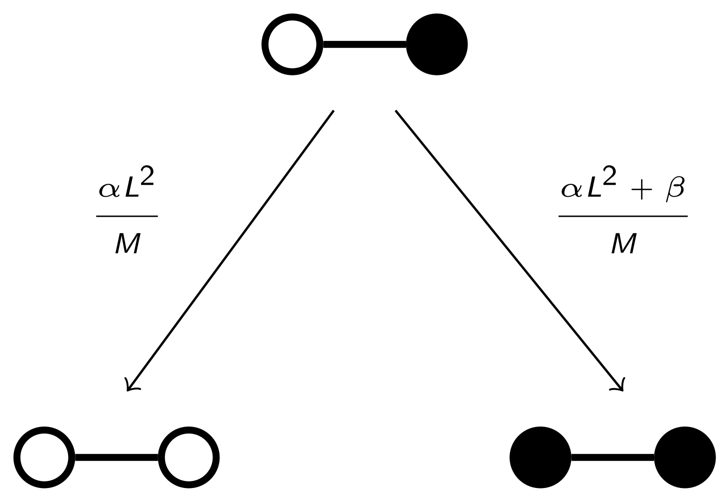
[Hallatschek and Nelson 2007], [Durrett and Fan 2016]

Biased Voter Model (BVM)

$$\begin{cases} \text{Each type-0 reproduces at rate } 2\alpha L^2 \\ \text{Each type-1 reproduces at rate } 2(\alpha L^2 + \beta) \end{cases}$$

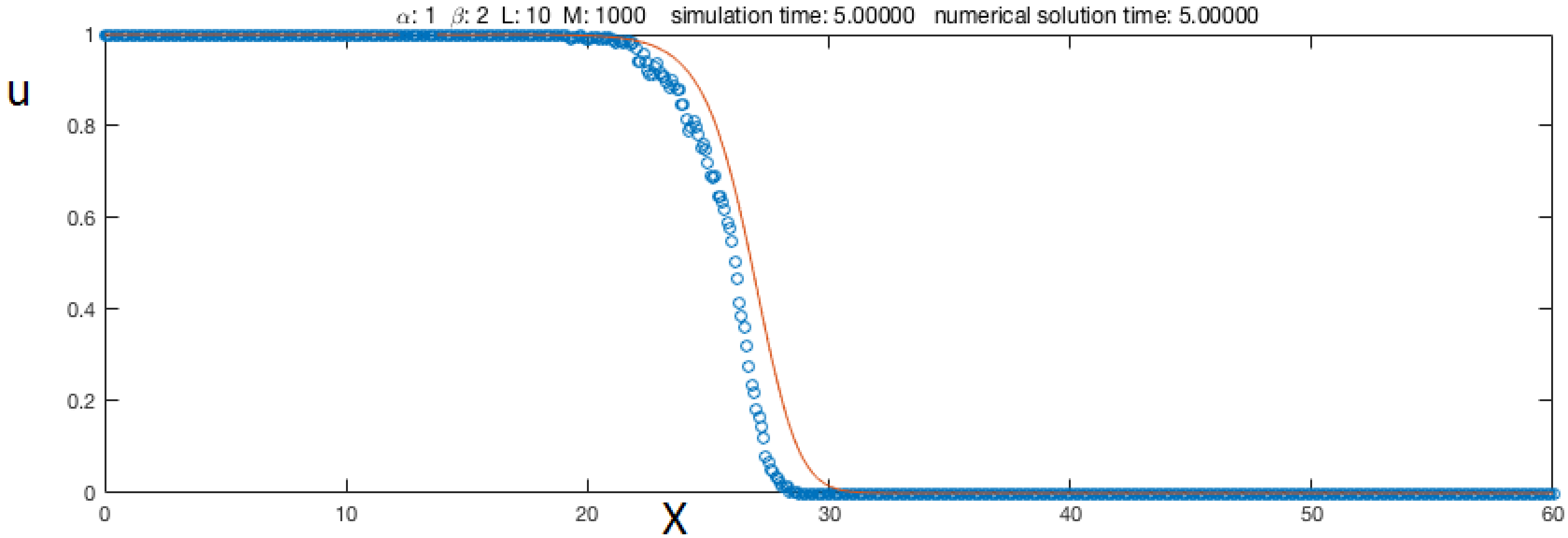
Offspring replaces a randomly chosen neighbor





Simulation for BVM

$$\begin{cases} \text{Each type-0 reproduces at rate 200} \\ \text{Each type-1 reproduces at rate 204,} \end{cases} \qquad L = 10,\ M = 1000.$$



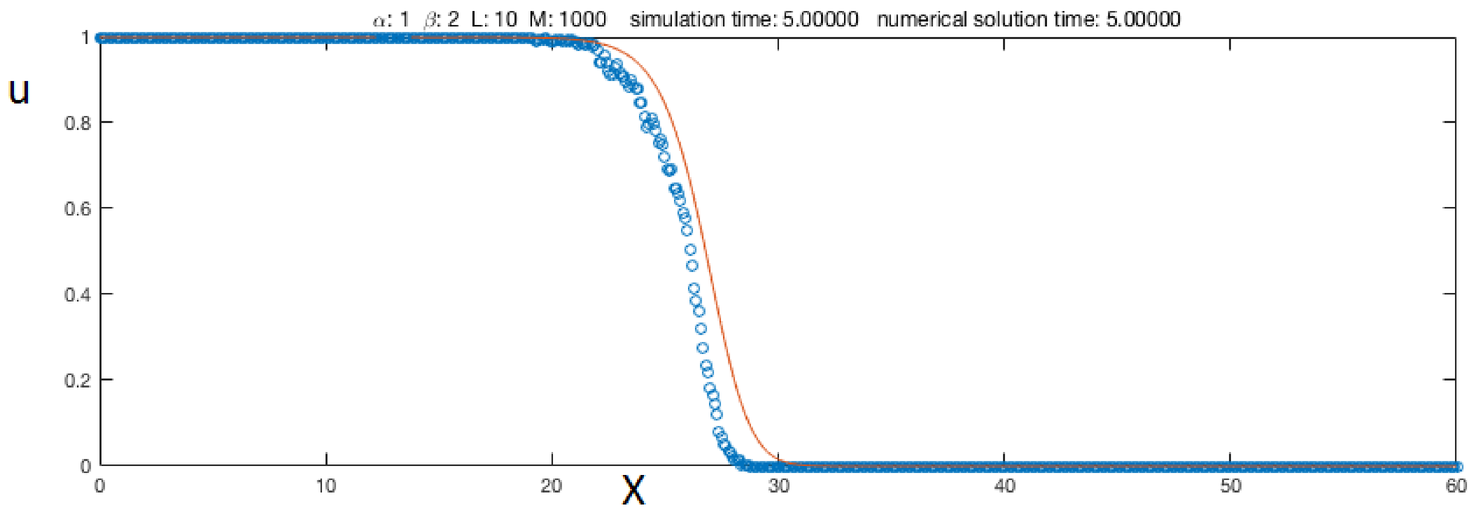
Comparison of the evolution of the **fraction of type 1** with FKPP

$$\partial_t u = \alpha \Delta u + \beta u(1 - u)$$

Biased Voter Model (BVM)

1. Is deterministic FKPP a good approximation?

NOT NECESSARILY. This is annoying.



How to remedy?

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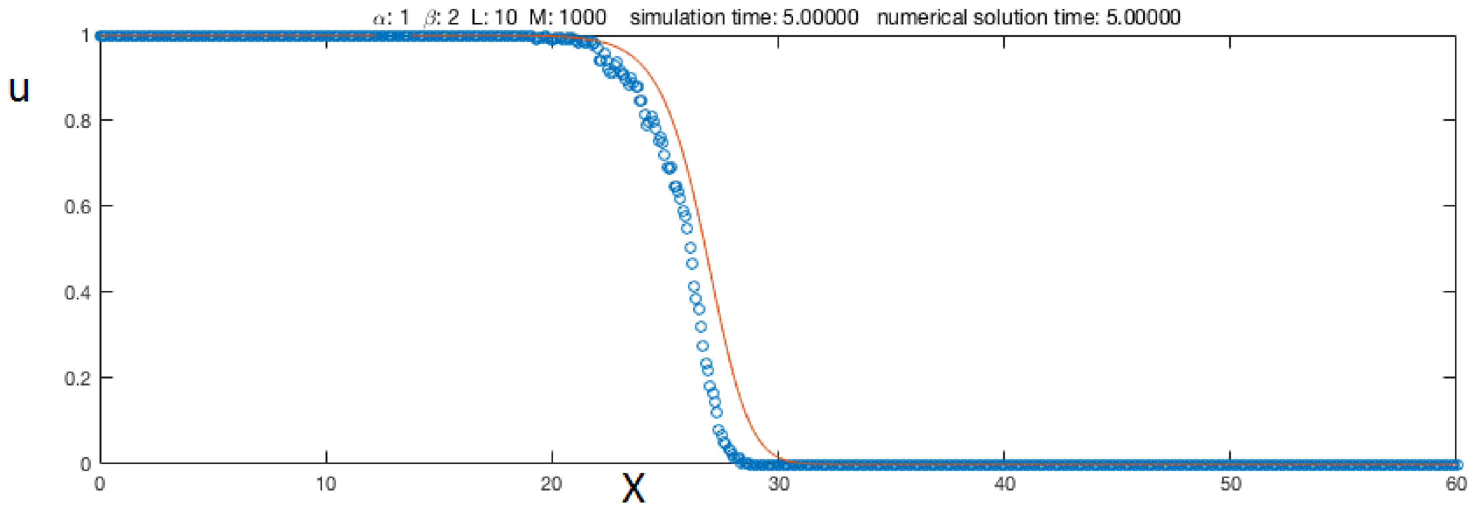

How to remedy?

Stochastic FKPP

$$\partial_t u(t,x) = \alpha\,\Delta u + \beta\, u(1-u) + |\gamma\, u(1-u)|^{1/2}\,\dot{W},$$

where $\dot{W}(t,x)$ is the space-time Gaussian white noise, $x \in \mathbb{R}^d$, $t \in [0,\infty)$.

Roughly speaking, stochastic PDE (SPDE) are

- PDE with random terms
- macroscopic models for systems with randomness

What does it mean by a "solution" ?

Stochastic PDE

How to make sense of parabolic SPDE

$$\boxed{\partial_t u(t,x) = \alpha\,\Delta u(t,x) + b\big(u(t,x)\big) + \sigma\big(u(t,x)\big)\,\dot{W}(t,x)}\ ?$$

- Mild solution

$$u_t(x) = P_t u_0(x) + \int_0^t P_{t-s}\big(b(u_s)\big)(x)\,ds + \int_{[0,t]\times\mathbb{R}^d} p(t-s,x,y)\sigma(u_s(y))\,dW(s,y),$$

where $p(t,x,y) = (4\pi\alpha t)^{-d/2}e^{-|x-y|^2/4\alpha t}$.

[Gihman and Skorohod 1979, Métivier and Pellaumeil 1980, Walsh 1986]

Stochastic PDE

How to make sense of parabolic SPDE

$$\boxed{\partial_t u(t,x) = \alpha\, \Delta u(t,x) + b\big(u(t,x)\big) + \sigma\big(u(t,x)\big)\, \dot{W}(t,x)}\ ?$$

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[Gihman and Skorohod 1979, Métivier and Pellaumeil 1980, Walsh 1986]

Stochastic FKPP on $\mathbb{R}$

$$\partial_t u = \alpha\, \Delta u + \beta\, u(1-u) + |\gamma\, u(1-u)|^{1/2}\, \dot{W}$$

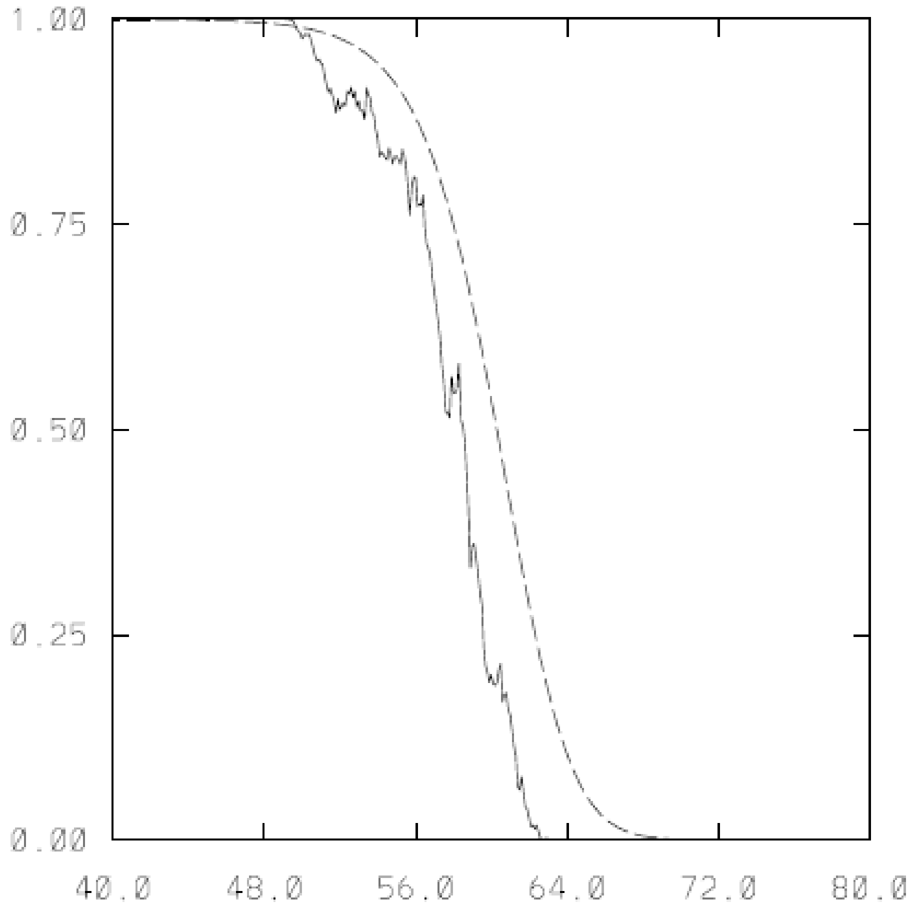


Figure from [Doering, Mueller and Smereka 2003]

Stochastic FKPP on $\mathbb{R}$

$$\partial_t u = \alpha\,\Delta u + \beta\, u(1-u) + |\gamma\, u(1-u)|^{1/2}\,\dot{W} \qquad (t,x) \in \mathbb{R}_+ \times \mathbb{R}$$

- Arise as scaling limits of various discrete models [Muller and Tribe 1995, Durrett and Fan 2016, Fan 2021]
- Backward-in-time lineage dynamics [Hallatschek and Nelson 1997, Durrett and Fan 2016]
- Wavefront is formed, compact containment holds [Mueller and Sowers 1995]
- Conditioned on non-extinction, asymptotic speed is

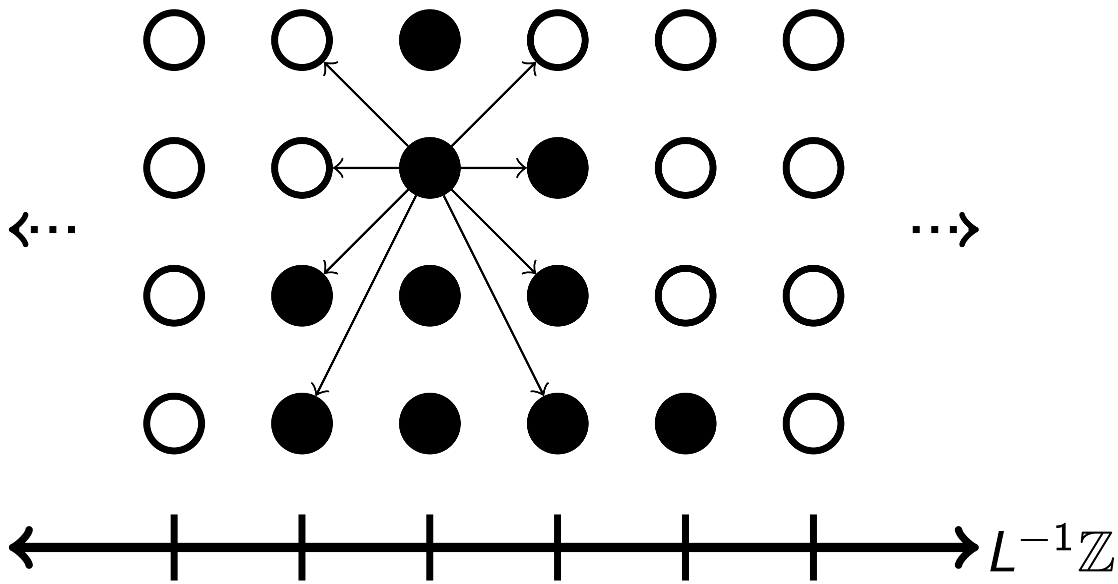
$$2\sqrt{\alpha\,\beta} - O(|\log^{-2}\gamma|)$$

  for small $\gamma > 0$. [Brunet and Derrida 1997, Mueller, Mytnik and Quastel 2011]
- Probability of extinction is

$$\exp\left\{\frac{-2\beta}{\gamma}\int_{\mathbb{R}} u_0(x)dx\right\}$$

  [Doering, Mueller and Smereka 2003]

FKPP or Stochastic FKPP ?

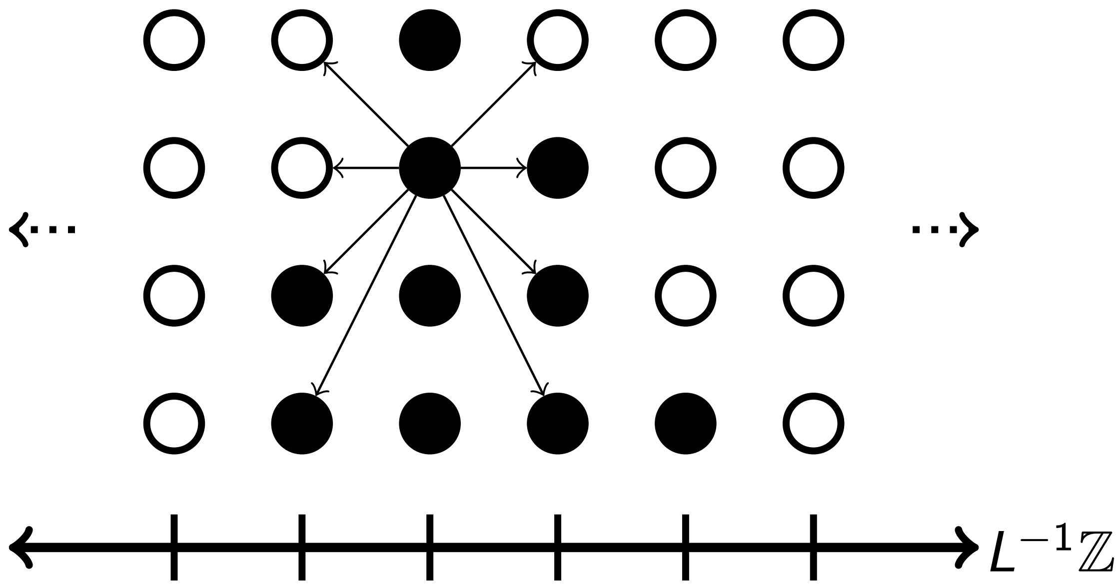


Define the **approximate density of type 1**

$$u^{(M,L)}(t,x) = \frac{\text{number of type 1 at } x}{M}$$

Want: $u^{(M,L)}(t,\cdot) \to u(t,\cdot) \in \mathcal{C}_{[0,1]}(\mathbb{R})$.

FKPP or Stochastic FKPP ?



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Want: $u^{(M,L)}(t,\cdot) \to u(t,\cdot) \in \mathcal{C}_{[0,1]}(\mathbb{R})$.

BVM on $(L^{-1}\mathbb{Z}) \times \{1, \ldots, M\}$.

$$\begin{cases} \text{Each type-0 reproduces at rate } 2\alpha L^2 \\ \text{Each type-1 reproduces at rate } 2(\alpha L^2 + \beta) \end{cases}$$

Theorem (Durrett and Fan, 2016)

Suppose $L/M \to \gamma/(4\alpha) \in [0, \infty)$ *and the initial approximate density converges. Then* $u^{(M,L)}(t, \cdot) \to u(t, \cdot) \in \mathcal{C}_{[0,1]}(\mathbb{R})$ *where*

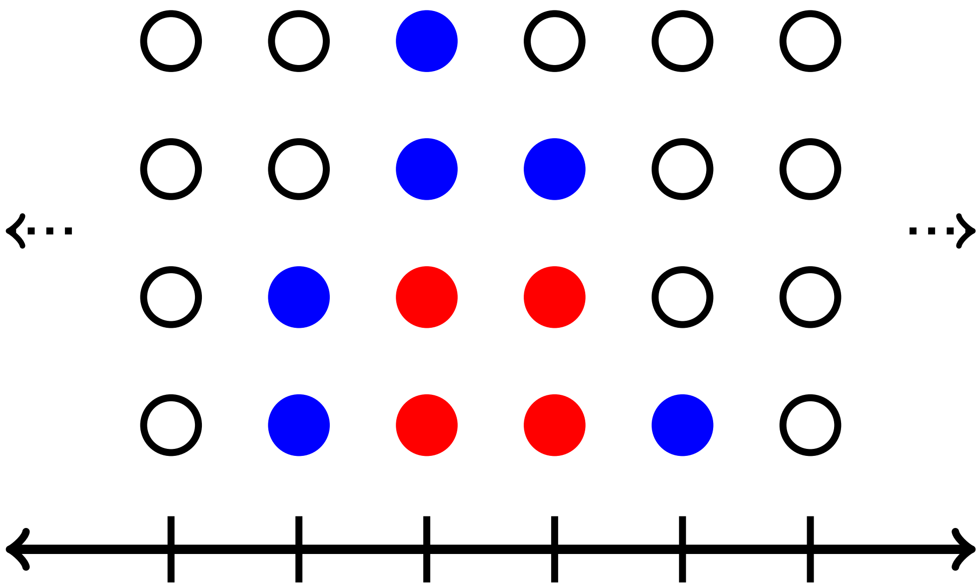
$$\partial_t u = \alpha\, \Delta u + 2\beta\, u(1-u) + |\gamma\, u(1-u)|^{1/2}\, \dot{W}$$

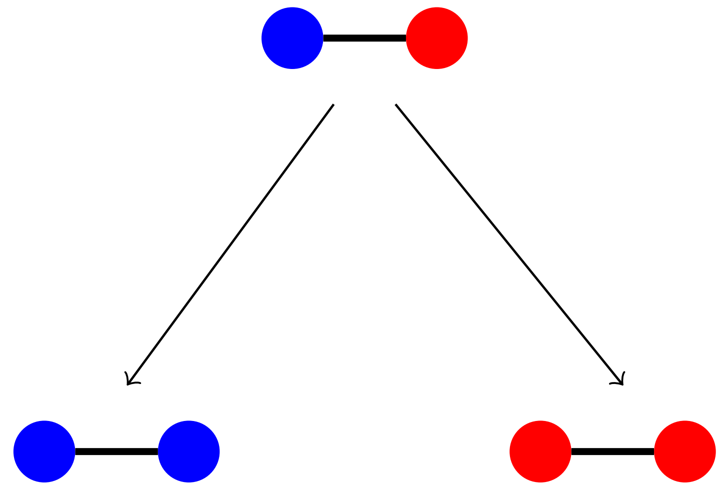
where $\alpha > 0$, $\beta \geq 0$ *and* $\gamma \geq 0$.

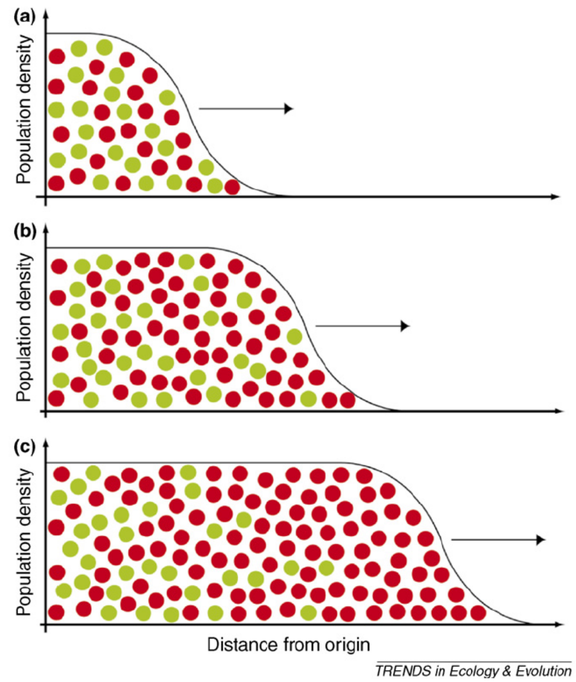
$\gamma = 0$ (deterministic FKPP) $L = n^{1/b}$, $M = \alpha n^{2/b - 1/a}$, $2a > b > a > 0$

$\gamma > 0$ (stochastic FKPP) $M = n^a$, $L = \gamma M/(4\alpha)$

BVM with neutral labels







Theorem (Durrett and Fan, 2016)

Suppose $L/M \to \gamma/(4\alpha)$ and initial densities converge. The **pair** *of densities of type 1 and labeled type 1 converges weakly to the coupled SPDE*

$$\partial_t u = \alpha \Delta u + 2\beta u(1-u) + |\gamma \ell (1-u)|^{1/2}\, \dot{W}^0 + |\gamma (u-\ell)(1-u)|^{1/2}\, \dot{W}^1$$

$$\partial_t \ell = \alpha \Delta \ell + 2\beta \ell\,(1-u) + |\gamma \ell (1-u)|^{1/2}\, \dot{W}^0 + |\gamma \ell\,(u-\ell)|^{1/2}\, \dot{W}^2$$

Applications: lineage dynamics, extinction probability, probability of gene surfing

Outline

Stochastic FKPP on $\mathbb{R}$

Wellposedness for

$$\partial_t u = \alpha\,\Delta u + \beta\, u(1-u) + \left|\gamma\, u(1-u)\right|^{1/2} \dot{W} \qquad (t,x) \in \mathbb{R}_+ \times \mathbb{R}$$

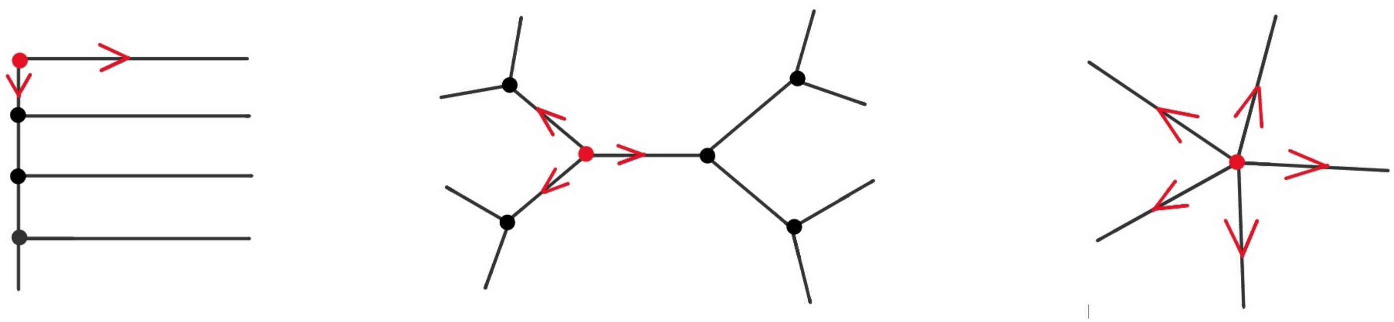
- Stochastic FKPP has a unique weak solution for $d = 1$.
- Solution theory for $d \geq 2$ not available (!!).

Usual approach: Discretize space
New approach: Model space as a metric graph

SPDE on metric graphs

$$\boxed{\partial_t u(t,x) = \underbrace{\mathcal{L}u}_{\text{spatial motion}} + \underbrace{b(u)}_{\text{reactions}} + \underbrace{\sigma(u)\,\dot{\mathbb{W}}}_{\text{noise}}, \qquad \underbrace{x \in \mathbb{X}}_{\text{metric graph}}}$$

with suitable boundary conditions on the vertices.



- Wellposed in the weak sense if $\mathbb{X}$ is "nice"
- Gaussian heat kernels and Holder continuity holds for the underlying diffusion [Fan 2021]

SPDE on metric graphs

$$\begin{cases} \partial_t u = \mathcal{L}u(t,x) + b\big(x,\, u(t,x)\big) + \sigma\big(x,\, u(t,x)\big)\,\dot{W} & \text{for } x \in \mathring{G} \\ \nabla_{out} u \cdot \vec{\alpha} = -\hat{\beta}(v,\, u(t,v)) & \text{for } v \in V \end{cases}$$

is the shorthand of

$$\begin{aligned} u_t(x) = P_t u_0(x) &+ \int_0^t P_{t-s}\big(b(\cdot, u_s)\big)(x)\, ds \\ &+ \int_{[0,t]\times G} p(t-s,x,y)\sigma(y, u_s(y))\, dW(s,y) \\ &+ \int_0^t \sum_{v\in V} p(t-s,x,v)\, \hat{\beta}(v, u_s(v))\, ds, \end{aligned}$$

where $p(t,x,y)$ the transition density for the $\mathcal{L}$-diffusion on G. [Cerrai and Freidlin 2019, Fan 2021]

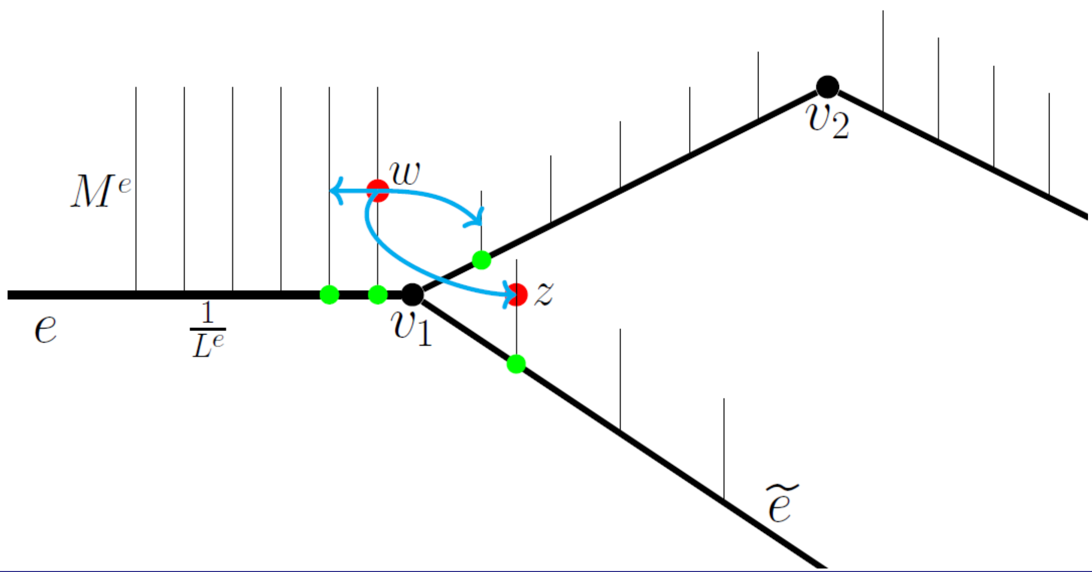
SPDE on metric graphs

(I) Our SPDE are more general (well-posedness not known apriori)

$$\begin{cases} \partial_t u = \mathcal{L}u + b(u) + \sigma(u)\,\dot{W} & \text{on } \mathring{G} \\ \nabla_{out} u = -\hat{\beta}(u) & \text{on } V. \end{cases}$$

- More general metric graphs G and operators $\mathcal{L}$
- Nontrivial boundary conditions

(III) We obtain the first scaling limit results which connect individual based models to both deterministic and SPDE on metric graphs.



Theorem (Fan 2021)

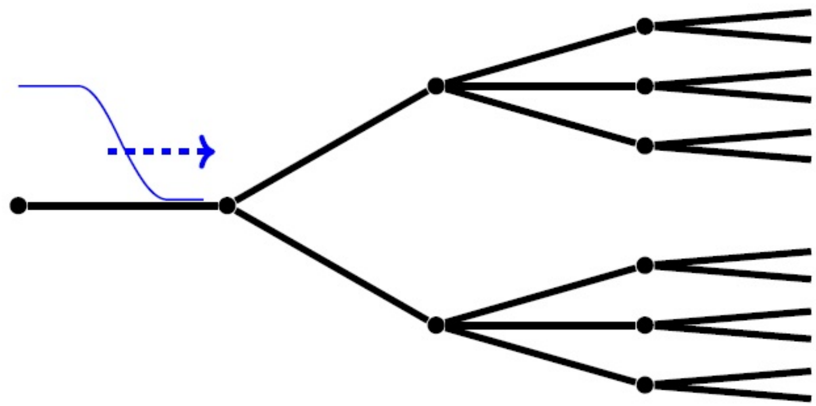
Let G be a metric graph admitting suitable regularity conditions (such as volume-doubling property and Poincaré inequality). Suppose the initial approximate densities converge, then under suitable scaling, the approximate density processes converge in $\mathcal{D}([0,\infty), \mathcal{C}_{[0,1]}(G))$ to the solution of

$$\begin{cases} \partial_t u = \alpha_e \, \Delta u + \beta_e \, u(1-u) + \sqrt{\gamma_e \, u(1-u)}\,\dot{W} & \text{on } \mathring{e} \\ \nabla_{out} u \cdot \vec{\alpha} = -\hat{\beta}\, u(1-u) & \text{on } V. \end{cases}$$

- We also have a numerical scheme via **interacting Itô SDEs**
- Same method expected to work for several other parabolic SPDE

Example: FKPP on trees

We consider the FKPP equation on an infinite regular tree $\mathbb{T}_{\vec{d},\vec{\ell}}$



What is the wavespeed on a tree? Is it faster or slower than that on $\mathbb{R}$?

FKPP on $\mathbb{T}_{\vec{d},\vec{\ell}}$

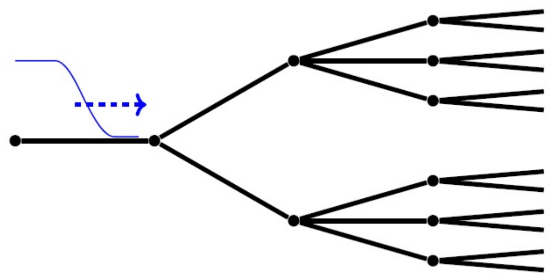
- FKPP equation on an infinite regular tree $\mathbb{T}_{\vec{d},\vec{\ell}}$:

$$\begin{cases} \dfrac{\partial u}{\partial t}(t,x) = \dfrac{1}{2}\dfrac{\partial^2 u}{\partial x^2} + \beta u(1-u) & , \quad (t,x) \in (0,\infty) \times \mathring{\mathbb{T}}_{\vec{d},\vec{\ell}} \ , \\ \nabla u(t,v) = 0 & , \quad (t,v) \in (0,\infty) \times V \ , \\ u(0,x) = u_0(x) & , \quad x \in \mathring{\mathbb{T}}_{\vec{d},\vec{\ell}} \ , \end{cases}$$

- The condition $\nabla u(t,v) = \sum_i \partial_i u(t,v) = 0$ in which ∂_i is the outward derivative along the i-th edge attached to the vertex v, specifies that the *flow-in equals flow-out* of mass at each vertex.
- The initial condition $u_0(x) = 1_{(-\delta,\delta)}(x)$ for some small $\delta > 0$.

Wavespeed for FKPP on trees

- Consider the FKPP equation on $\mathbb{T}_{\vec{d},\vec{\ell}}$
- i.i.d. branching degrees $\vec{d} = (d_i)_{i \in \mathbb{Z}_+}$
- i.i.d. branch lengths $\vec{\ell} = (\ell_i)_{i \in \mathbb{Z}_+}$



Theorem (Fan, Hu and Terlov 2021)

There is a **critical growth rate** $\beta_c > 0$ *such that if* $\beta \in (\beta_c, \infty)$, *a wavefront is formed. The wavefront travels with a positive asymptotic speed* $c_* \leq \sqrt{2\beta}$, *with equality holds if and only if the tree* $\mathbb{T}_{\vec{d},\vec{\ell}}$ *is the real line* $\mathbb{R}$.

- We obtained a variational representation for c_*.

Corollary: d-ary tree

Theorem (Fan, Hu and Terlov 2021)

Consider the d-ary tree with branch length ℓ. There is a critical growth rate $\beta_c := \frac{d-2}{\ell\, d}\ln(d-1)$ above which the asymptotic speed is

$$\inf_{\lambda\geq 0} \frac{\lambda+\beta}{\sqrt{2\lambda}+\frac{1}{\ell}\ln\left(\frac{4p}{1+\gamma^2-\sqrt{(\gamma^2-1)^2+4(2p-1)^2\gamma^2}}\right)} \in (0,\sqrt{2\beta}\,]\,,$$

where $p=(d-1)/d$ and $\gamma := e^{\ell\sqrt{2\lambda}}$.

Idoof

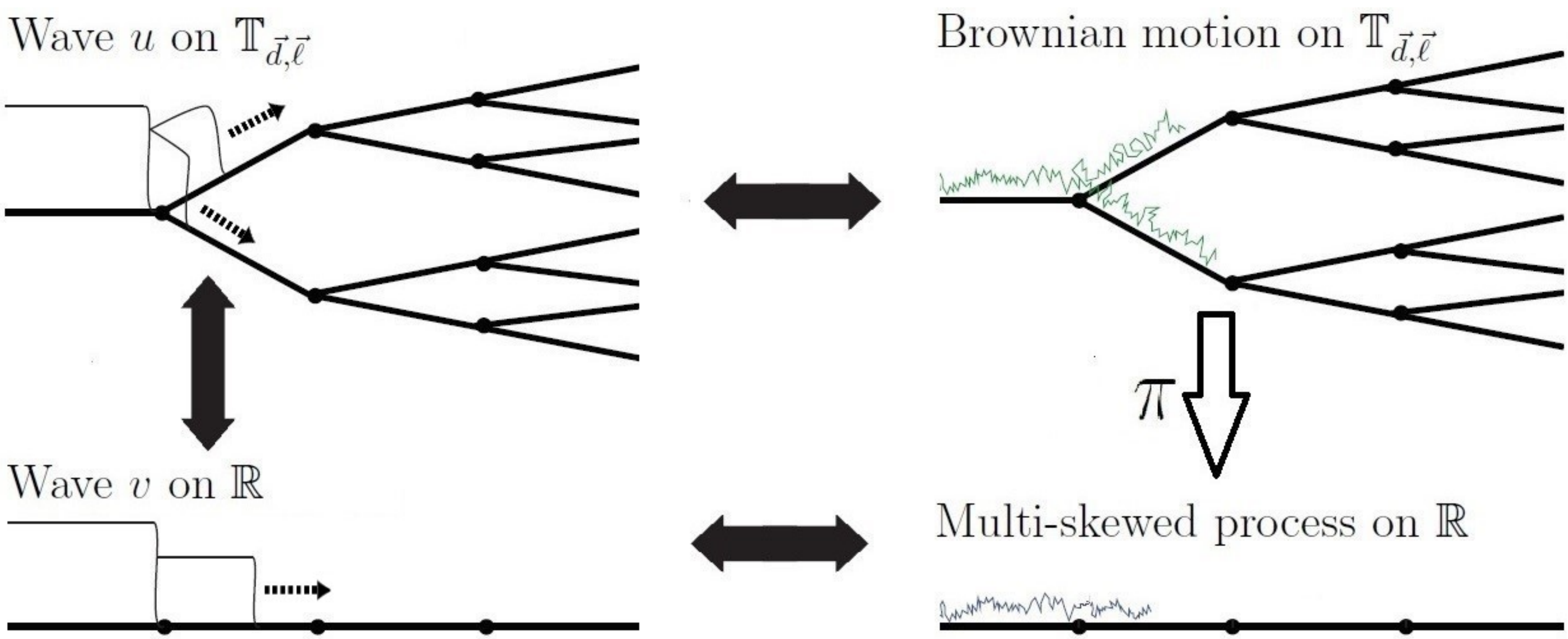


Figure: Connection with multi-skewed Brownian motion via projection π.

Idoof

- If $y = \pi(x)$ then $u(t,x) = v(t,y)$, where

$$v(t,y) = E_y^{(\vec{d},\vec{\ell})}\left[1_{(-\delta,\delta)}(Y_t)\exp\left\{\beta\int_0^t \Big(1 - v(t-s, Y_s)\Big)\,ds\right\}\right].$$

Our problem is reduced to large deviations principle (LDP) and the analysis of wavefront propagation associated with the multi-skewed Brownian motion Y_t.

Outline

Proof outline for convergence theorems

The approximate density is

$$u_t^{(n)}(x) = \frac{\text{number of type 1 at } x}{M^e}.$$

View $u_t^{(n)} \in \mathcal{C}_{[0,1]}(G)$ for each $t \in [0,\infty)$. We want to show

$$u^{(n)} \to u \in D([0,\infty), \mathcal{C}_{[0,1]}(G)).$$

(I) Show that $\{u^{(n)}\}$ is relatively compact.

(II) Show that all limit points u^{∞} satisfy the limiting martingale problem: $F(u_t) - F(u_0) - \int_0^t \mathcal{L}F(u_s)\,ds$ are martingales.

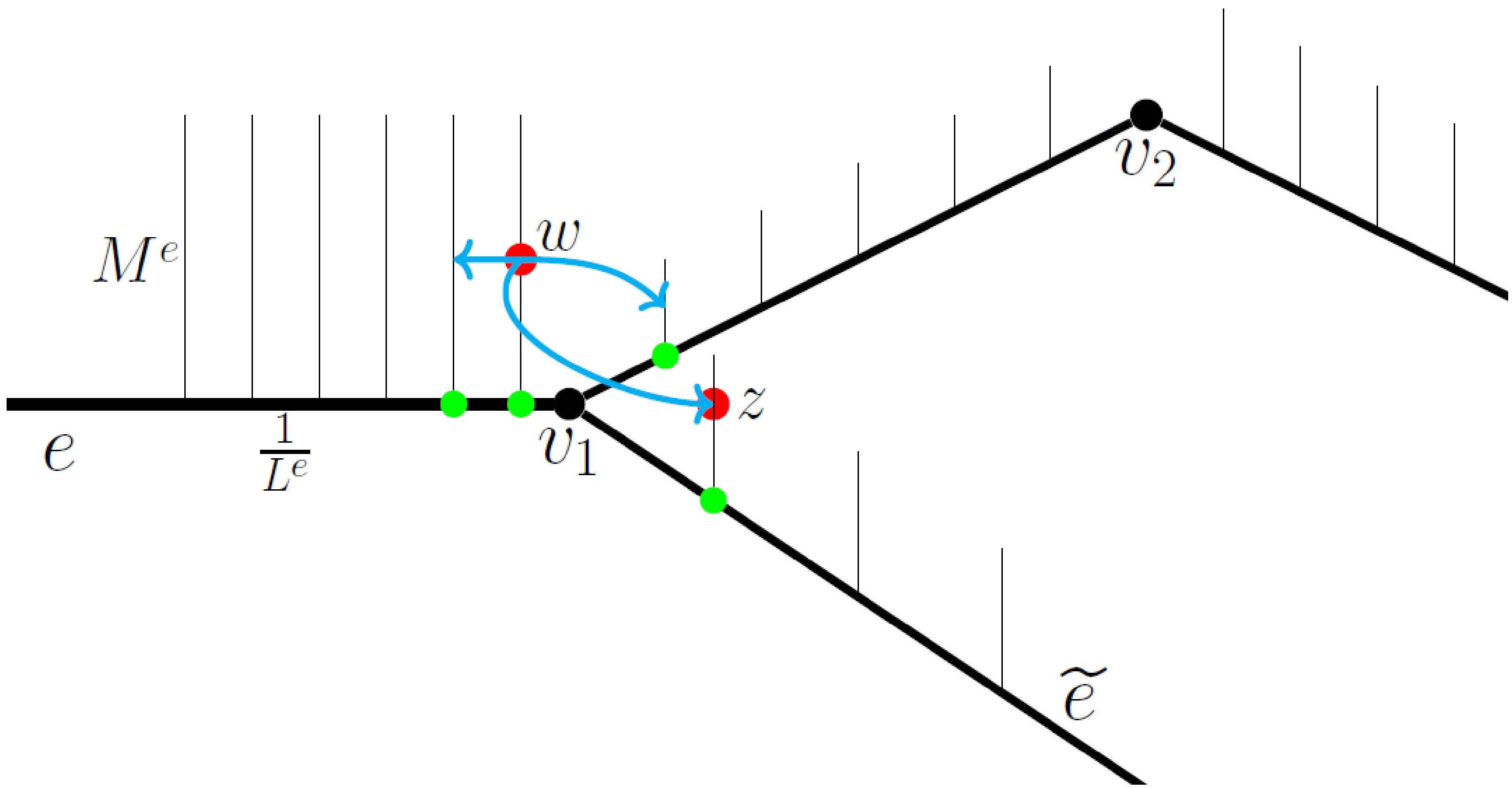
(III) Uniqueness of solution of the limiting martingale problem.

Proof has to address **new challenges:**

(A) Interactions near vertex singularities in relation to $\{M_n^e\}$ and $\{L_n^e\}$.

(B) Weak uniqueness via a new duality

(C) Uniform heat kernel estimates on G_n.



Non-uniqueness of SPDE

Theorem (Mueller, Mytnik and Perkins 2014)

If $0 < \gamma < 3/4$, then uniqueness in law and pathwise uniqueness **fail** *for*

$$\partial_t u(t,x) = \frac{1}{2}\Delta u(t,x) + |u(t,x)|^{\gamma}\, \dot{W}(t,x), \qquad u(0,x) = 0$$

on the space of $\mathcal{C}(\mathbb{R})$-valued adapted processes.

Open problems:

- strong uniqueness for case $\gamma = 3/4$.
- strong uniqueness for stochastic FKPP on $\mathcal{C}_+(\mathbb{R})$-valued processes

Duality and weak uniqueness

The stochastic FKPP

$$\partial_t u = \alpha \Delta u + \beta u(1-u) + \sqrt{\gamma u(1-u)}\dot{W}.$$

is dual to the Branching Coalescing Brownian motions

$$X_t := (x_1(t), x_2(t), \cdots, x_{n(t)}(t)).$$

Precisely, the following **duality** exists between u and X

$$\mathbb{E}\prod_{i=1}^{n(0)}\Big(1-u(t,x_i(0))\Big) = \mathbb{E}\prod_{i=1}^{n(t)}\Big(1-u(0,x_i(t))\Big).$$

[Shiga and Uchiyama 1986, Athreya and Tribe 2000]

This duality implies **weak uniqueness** of stochastic FKPP on $C_{[0,1]}(\mathbb{R})$, and is useful in obtaining the **probability of extinction**.

Duality and extinction probability

Recall the duality

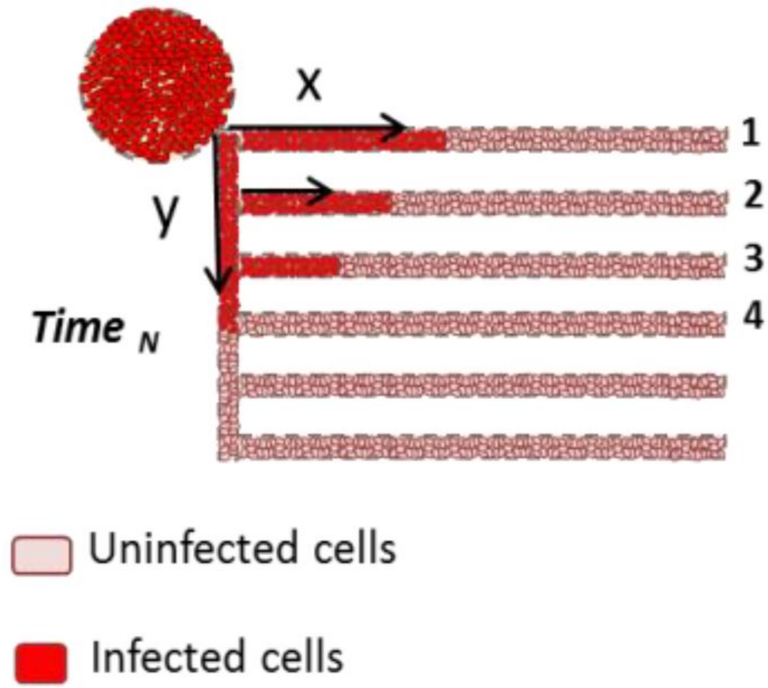
$$\mathbb{E}\prod_{i=1}^{n(0)}\Big(1-u(t,x_i(0))\Big)=\mathbb{E}\prod_{i=1}^{n(t)}\Big(1-u(0,x_i(t))\Big). \tag{4.1}$$

Suppose $\int u_0(x)dx<\infty$. The LHS of (4.1) tends to the **extinction probability** $\mathbb{P}(u_\infty=0)$ as $t\to\infty$. The RHS of (4.1) tends to

$$\exp\left\{\frac{-2\beta}{\gamma}\int u_0(x)\,dx\right\}$$

since the BCBM converges to a Poisson point process with intensity $\frac{2\beta}{\gamma}$ as $t\to\infty$.
[Doering, Mueller and Smereka 2003], [Fan and Yang 2022+]

Ongoing/Future work

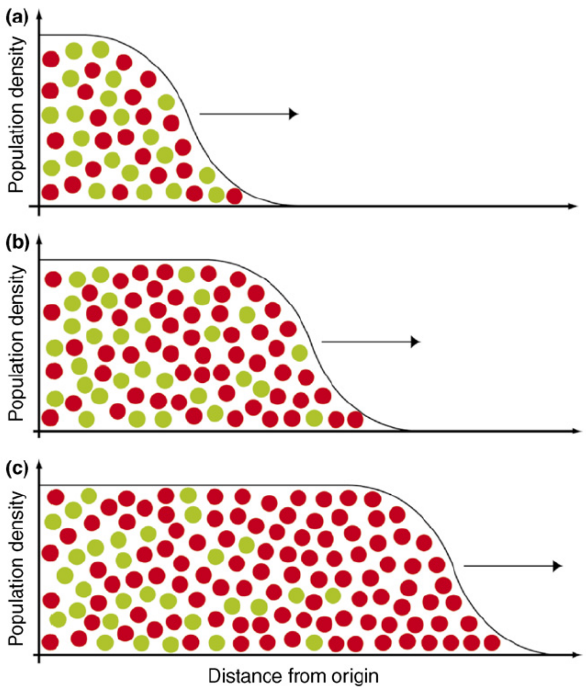


[Inankur and Yin 2017, Fan and Yin 2022+]

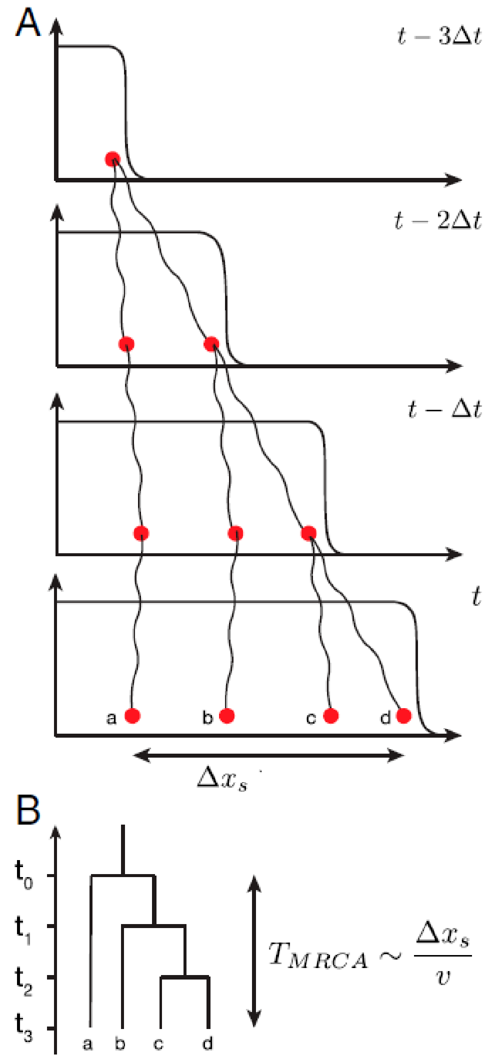
How do spatial structures affect the dynamics, competition outcome and genealogies of interacting populations?

Ongoing/Future work

Understand the general principles governing the dynamics and the genealogies of expanding populations



TRENDS in Ecology & Evolution



Ongoing/Future work

1. Develop duality and field-theoretic techniques in the analysis of co-existence, fixation probabilities, quasi-stationary and quasi-ergodic behaviors
2. More general reaction terms (e.g. pushed waves) and metric graphs

$$\partial_t u = \underbrace{\mathcal{L}u}_{\text{spatial motion}} + \underbrace{F(u)}_{\text{reactions}} + \underbrace{\sigma(u)\,\dot{\mathbb{W}}}_{\text{noise}}, \qquad \underbrace{x \in \mathbb{X}}_{\text{metric graph}}$$

3. Coupled SPDE on graphs, fractals, and other metric spaces
   - Coexistence, competition outcome
   - Propagating speeds and spatial patterns of stochastic waves
   - Lineage dynamics and genealogies

Thank you for your attention!

- *Reversibility and convergence of Branching-coalescing Brownian motions.* With Yifan (Johnny) Yang.
- *Quasi-stationary behavior for the stochastic FKPP on compact spaces.* With Oliver Tough.
- *Stochastic PDEs on graphs as scaling limits of discrete interacting systems.* Bernoulli. 27(3), 2021.
- *Wave propagation for reaction-diffusion equations on infinite trees.* With W. Hu and G. Terlov. Communications in Mathematical Physics. 384, 2021.
- *Genealogies in expanding populations.* With R. Durrett. Annals of Applied Probability. 26(6), 2016.

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