

Fluctuation-regularized Front Propagation Dynamics in a Reaction-Diffusion System

David Kessler

Bar-Ilan University

Herbert Levine

UCSD

Elisheva Cohen

Bar-Ilan

Scott Wylie

UCSD

PRL, 94, 158302 (2005)

PRE, 72, 066126 (2005)

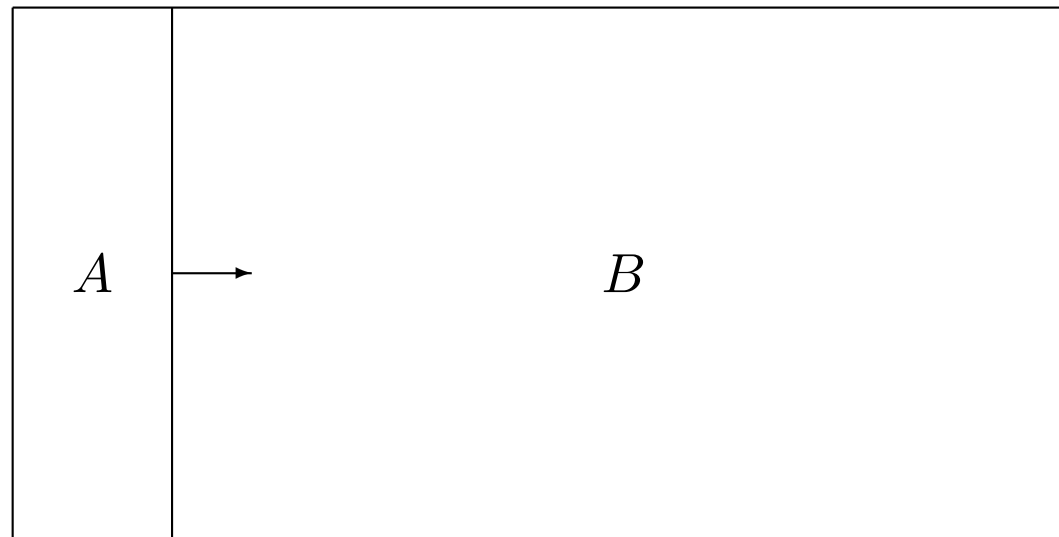
PRE, to appear (cond-mat/0604110)

The Standard Problem: $A + B \rightarrow 2A$

Start with a system full of B 's

Introduce some A 's at left hand edge

Nonlinear "wave" of A 's propagates to right, consuming B 's



Propagation into an Unstable Phase

The Standard Approach: Reaction-Diffusion Equation

If $D_A = D_B$, get Fisher (aka Kolmogorov-Petrovsky-Piscounov) Equation (1937)

$$\dot{A} = D_A \nabla^2 A + rA(N - A)$$

Has Positive Traveling wave Solutions for **all** $v > v_F \equiv 2\sqrt{D_A N r}$

First Sign of Something Funny

All Initial Conditions with Compact Support Lead to Wave with $v = v_F$!
(Aronson-Weinberger, 1978)

$v \rightarrow v_F$ very slowly: $v(t) = v_F \left(1 - \frac{3}{4Nrt}\right)$ (Bramson, 1983)

Why are things funny?

Fisher (1937):

The equation “must omit some essential element of the problem, and it is indeed clear that while a coefficient of diffusion may represent the biological conditions adequately in places where large numbers of individuals of both types are available, it cannot do so at the extreme front and back of the advancing wave, where the numbers ... are small, and where their distribution must be largely sporadic.”

What about Fluctuations?

Can't add Regular Noise! Would Kill Wave Due to Instability!

Noise Amplitude $\propto \sqrt{A}$ -- Kind of Multiplicative Noise

What about Fluctuations?

Can't add Regular Noise! Would Kill Wave Due to Instability!

Noise Amplitude $\propto \sqrt{A}$ -- Kind of Multiplicative Noise

Leads to Compact Interface! (Mueller and Sowers, 1995)

- Difficult Mathematics
- Obvious from Original Particle Model - There is always a "last" A

What about Fluctuations?

Can't add Regular Noise! Would Kill Wave Due to Instability!

Noise Amplitude $\propto \sqrt{A}$ -- Kind of Multiplicative Noise

Leads to Compact Interface! (Mueller and Sowers, 1995)

- Difficult Mathematics
- Obvious from Original Particle Model - There is always a "last" A

What have we gained??!

For recent progress on velocity bounds, see (Conlon and Doering, 2005)

New (Crude) Approach: Cutoff Reaction-Diffusion Eqn.

Since there are no A 's beyond some point, there is no reaction beyond that point.

New (Crude) Approach: Cutoff Reaction-Diffusion Eqn.

Since there are no A 's beyond some point, there is no reaction beyond that point.

Let us kill off the reaction by hand! (Brenner, Levine and Tu (1991), Kepler and Perelson (1993), Kessler, Levine and Tsimring (1996), Brunet and Derrida (1997))

$$r = r_0 \theta(A - A_c)$$

No reaction if number of A 's at a site $< A_c$, an $O(1)$ threshold.

New (Crude) Approach: Cutoff Reaction-Diffusion Eqn.

Since there are no A 's beyond some point, there is no reaction beyond that point.

Let us kill off the reaction by hand! (Brener, Levine and Tu (1991), Kepler and Perelson (1993), Kessler, Levine and Tsimring (1996), Brunet and Derrida (1997))

$$r = r_0 \theta(A - A_c)$$

No reaction if number of A 's at a site $< A_c$, an $O(1)$ threshold.

Amazing Result: (Brunet and Derrida, (1997))

$$v = v_F \left(1 - \frac{\pi^2}{\ln^2(N/A_c)} \right) \quad N \rightarrow \infty$$

Huge Correction to Velocity. In fact, for small N , $v \propto N$, not \sqrt{N} !

New (Crude) Approach: Cutoff Reaction-Diffusion Eqn.

Since there are no A 's beyond some point, there is no reaction beyond that point.

Let us kill off the reaction by hand! (Brener, Levine and Tu (1991), Kepler and Perelson (1993), Kessler, Levine and Tsimring (1996), Brunet and Derrida (1997))

$$r = r_0 \theta(A - A_c)$$

No reaction if number of A 's at a site $< A_c$, an $O(1)$ threshold.

Amazing Result: (Brunet and Derrida, (1997))

$$v = v_F \left(1 - \frac{\pi^2}{\ln^2(N/A_c)} \right) \quad N \rightarrow \infty$$

Huge Correction to Velocity. In fact, for small N , $v \propto N$, not \sqrt{N} !

In Two Dimensions, Cutoff gives rise to instability for small enough D_A . (Kessler and Levine, 2001)

Verified in Particle Simulations.

So much for simple things...

What Happens if Reaction Rate r Not Constant?

Not at all far-fetched

- Imposed Temperature Gradient
- Natural Inhomogeneities - Propagation of Roll State in Convection with Nonparallel Top and Bottom Walls
- Mapping to model of Darwinian Evolution

So much for simple things...

What Happens if Reaction Rate r Not Constant?

Not at all far-fetched

- Imposed Temperature Gradient
- Natural Inhomogeneities - Propagation of Roll State in Convection with Nonparallel Top and Bottom Walls
- Mapping to model of Darwinian Evolution

Naive Answer: Adiabatic Approximation

v is given by local value of r at front position

- Makes sense if r does not change significantly over width of front

So much for simple things...

What Happens if Reaction Rate r Not Constant?

Not at all far-fetched

- Imposed Temperature Gradient
- Natural Inhomogeneities - Propagation of Roll State in Convection with Nonparallel Top and Bottom Walls
- Mapping to model of Darwinian Evolution

Naive Answer: Adiabatic Approximation

v is given by local value of r at front position

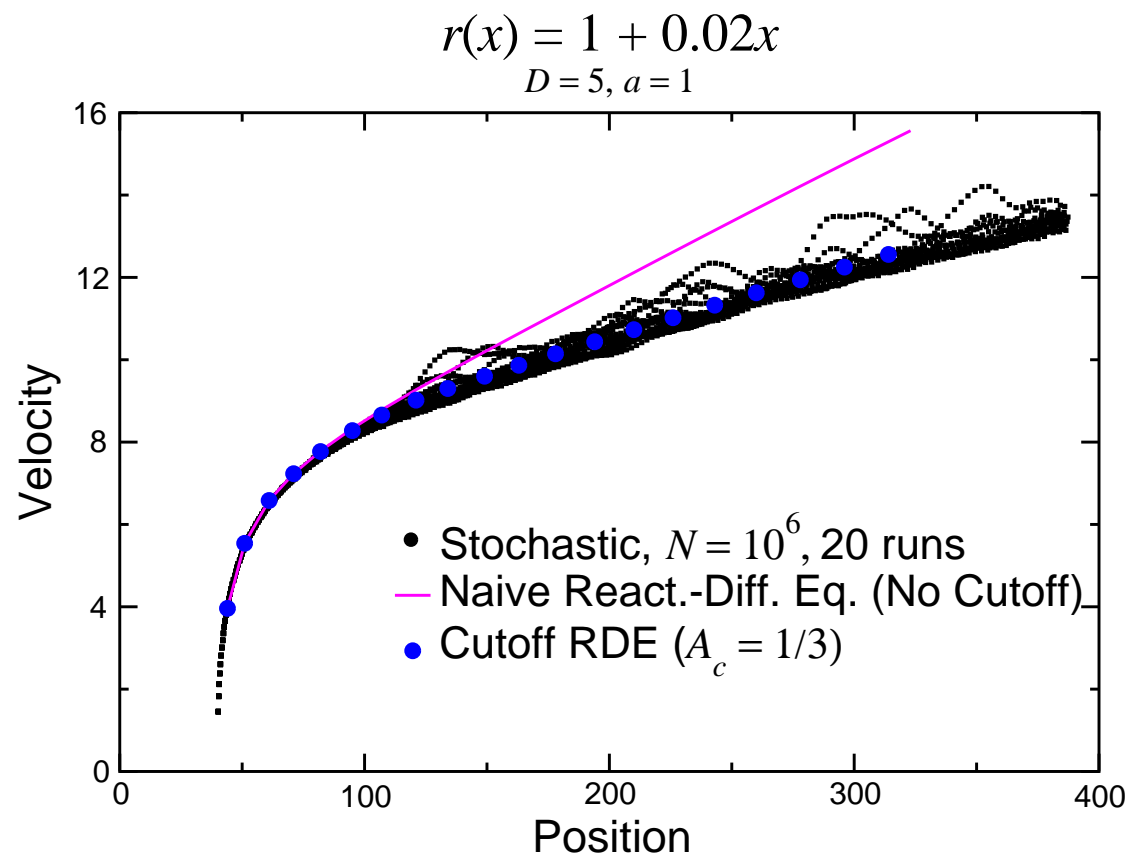
- Makes sense if r does not change significantly over width of front

BUT --- Width of front depends on N , Width $\rightarrow \infty$ as $N \rightarrow \infty$

Conclusion: Does not work for large N

2nd Conclusion: N effects even more interesting than before!

Again: Study N Dependence via Cutoff



Cutoff works quite well!

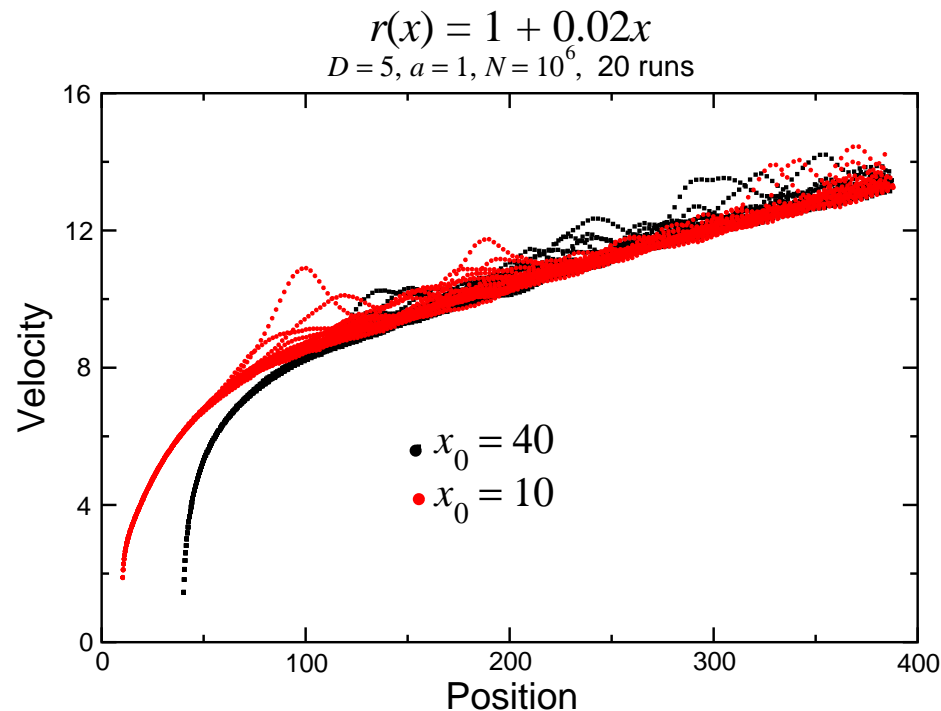
$$\dot{A} = \frac{D}{a^2} (A(x+a) - 2A(x) + A(x-a)) + r(x)\theta(A - A_c)A(N - A)$$
$$r(x) = r_0(1 + \alpha x)$$

The Cutoff and the Attractor

Problem: The Front Accelerates --- What can one say about the velocity?

- Want to make predictions independent of details of the initial conditions
- "Normally", there is an asymptotic steady-state velocity (and front profile) indep. of IC's
- Here, no such solution exists

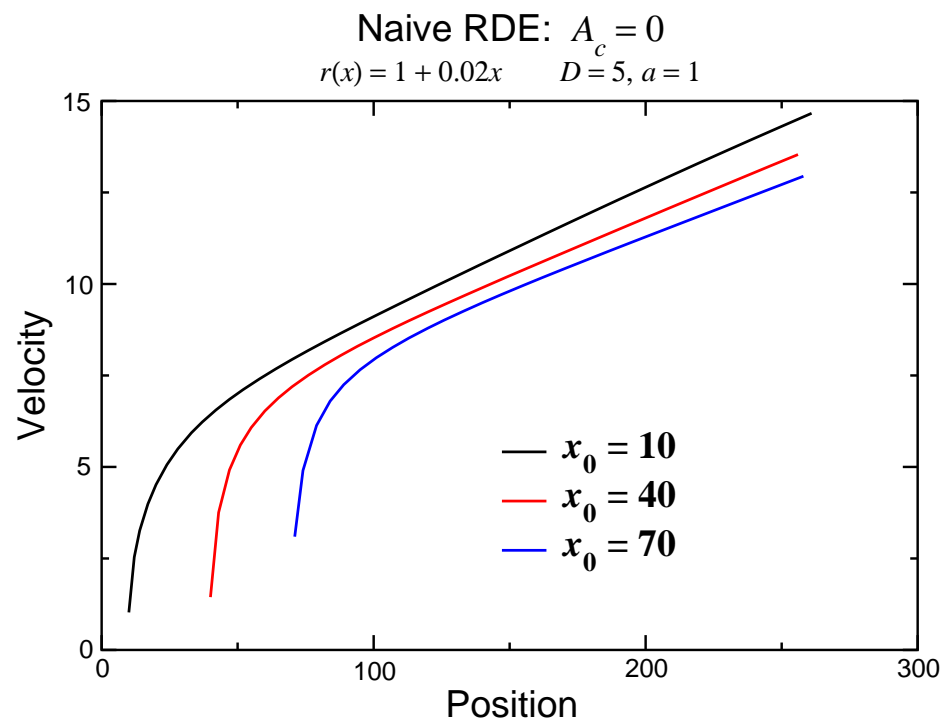
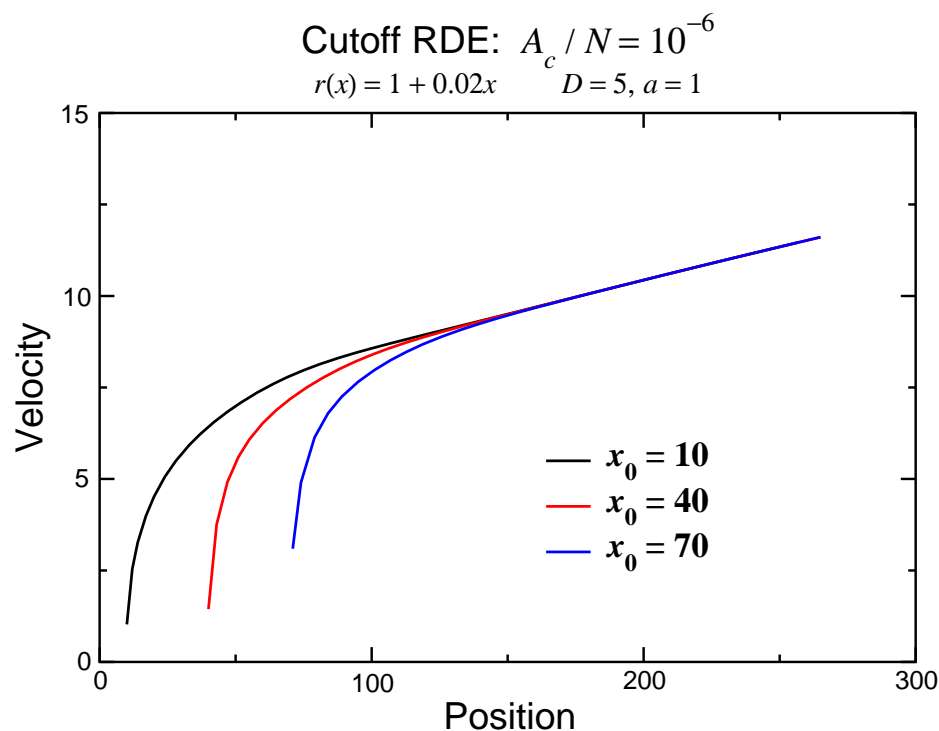
Solution: v asymptotically only depends on front location, not IC's



The Cutoff and the Attractor, cont.

Unsurprisingly, velocity asymptotically only depends on the front location in Cutoff RDE, also

Surprisingly, not true **without** cutoff

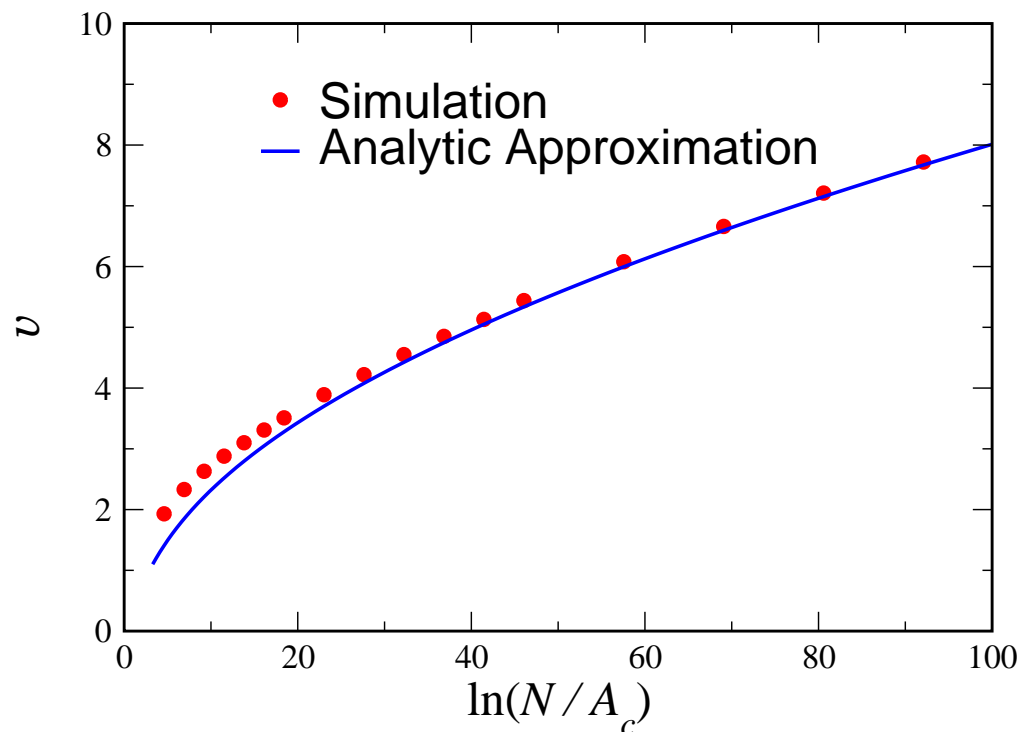


Cutoff regularizes theory, Responsible for attractor
Leading edge becomes more and more unstable \Rightarrow Cutoff Essential

Theory vs. Simulation of Cutoff Quasistatic RDE

Can analytically solve for small cutoff quasistatic case

$$a=1, \alpha=0.1, D=r_0=1$$



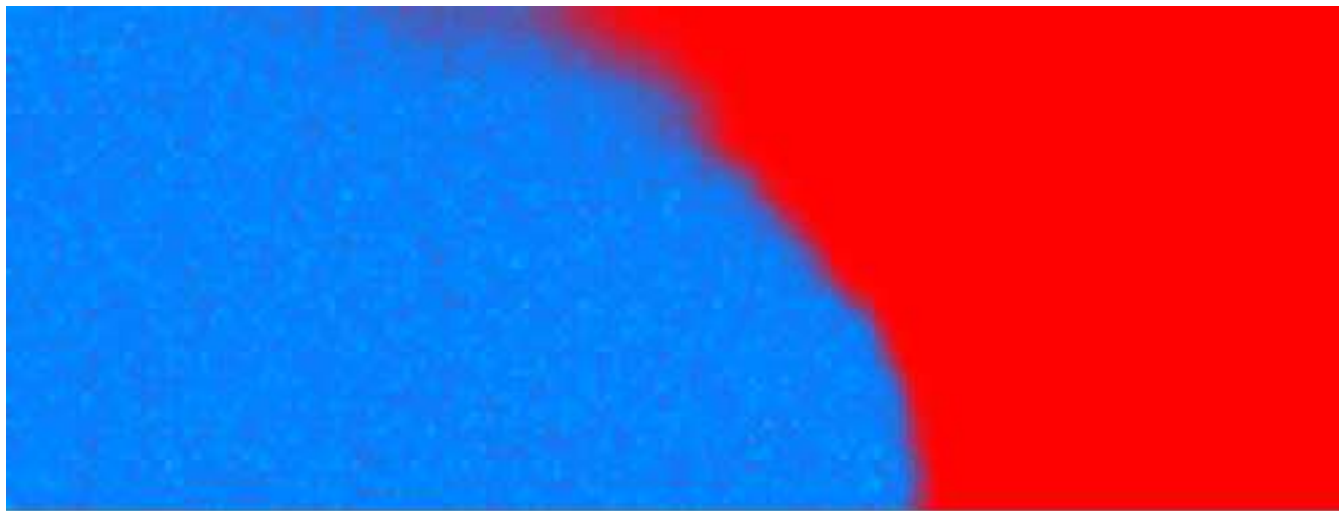
Two Dimensions

Things become even more interesting in 2D

Planar front is unstable

Deterministic Cutoff Model develops into a growing finger

Stochastic Model develops a well-defined finger for large enough N



$$N = 1000, D = 0.25, \alpha = 0.06, L_y = 61, a = 1$$

Take-Home Messages

Discreteness of particles is a singular perturbation --- controls pattern selection

Few “pioneer” particles at leading edge control dynamics

Need better mathematical tools