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2 CATALYTIC AND MUTUALLY CATALYTIC BRANCHING

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2.1 OUTLINE

• Catalytic reactions - lattice models
• Measure-valued processes as a tool in studying spatial phenomea
• Case study: singular catalysts
Catalytic Reactions

Example: Glycolysis

- Chain of reactions taking place inside a cell
  - described by a system of reaction-diffusion equations
- Each reaction initiated by a enzyme catalyst
- Within the cell there is a network of “filamentous actin”
  - enzyme molecules bind to filaments leading to highly concentrated catalytic regions

Problems

- Development of mezoscopic models of these reaction-diffusions
- Determination of effective reaction rates

Mathematical Problems

1. Brownian motion in random field of obstacles
2. Reaction-diffusion equations with random singular coefficients
3. Microscopic models of the reaction diffusion processes.

2.2 MODELS

- Multitype branching random walk on $Z^d$
  - $R_1 \rightarrow R_2 \rightarrow R_3 \rightarrow \ldots \rightarrow R_n$
  - Supercritical branching with removal of final product
- Catalytic multitype branching random walk
  - Both catalytic and reactant particle perform random walks
- Mutually catalytic branching random walk
- Closed catalytic chains
2.3 Key Phenomenological Questions

- These mechanisms lead to highly heterogeneous distribution of reactants - spatial clumping. How do we describe and quantify this?
- The heterogeneous distribution of catalysts and reactants has a profound effect on the rate of product formation - how do we determine this?

Particle Level Description:

* Catalytic Reaction: Reaction rate proportional to amount of catalyst locally present

* Catalytic branching
  
  Catalyst: Red - does Branching RW  
  Green: Reactant - RW + catalytic branching

\[
\begin{align*}
\text{Red+Green} & \rightarrow \text{Green dies: prob. } \frac{1}{2} \\
\text{Red+Green} & \rightarrow \text{Green offspring: prob. } \frac{1}{2}
\end{align*}
\]
Mutually Catalytic Branching
Orange catalyses Blue
Blue catalyses Orange

Orange+Blue $\rightarrow$ Blue offspring: prob. $\frac{1}{4}$
Orange+Blue $\rightarrow$ Orange offspring: prob. $\frac{1}{4}$
Orange+Blue $\rightarrow$ Blue death: prob. $\frac{1}{4}$
Orange+Blue $\rightarrow$ Orange death: prob. $\frac{1}{4}$
Continuous state Lattice Models
[Continuous state BRW in a Uniform Medium]
Medium:

\[ V_t \equiv \gamma \]

\[ U_t(k\varepsilon) = \text{amount of reactant at site } k\varepsilon \text{ at time } t. \]

System of SDE: \( \{q_{jk}\} \) jump rates for a symmetric random walk on \( \varepsilon \mathbb{Z}^d \),

\( 1 > \varepsilon > 0 \).

For \( k \in \mathbb{Z}^d \):

\[
U_t(k\varepsilon) = U_0(k\varepsilon) + \int_0^t \sum_j U_s(j\varepsilon)q_{jk}^s ds \\
+ \int_0^t \sqrt{\gamma U_s(k\varepsilon)} dB_k(s)
\]

\( \{B_k(\cdot) : k \in \mathbb{Z}^d\} \) are a system of independent Brownian motions.

[Reactant: Continuous State Catalytic Branching]

\[
\varepsilon^{-d} V_t(k\varepsilon) \\
= \text{density of catalyst at site } k\varepsilon \text{ at time } t.
\]

\( U_t(k\varepsilon) = \text{amount of reactant at site } k\varepsilon \text{ at time } t. \)

\[
U_t(k\varepsilon) = U_0(k\varepsilon) + \int_0^t \sum_j U_s(j\varepsilon)q_{jk}^s ds \\
+ \int_0^t \sqrt{\varepsilon^{-d} U_s(k\varepsilon)} e^{-dV_s(k\varepsilon)} \varepsilon^{d/2} dB_k(s)
\]
\[ U_t(k\varepsilon) = U_0(k\varepsilon) + \int_0^t \sum_j U_s(j\varepsilon) q_{jk} ds \]

\[ + \int_0^t \sqrt{\varepsilon - dU_s(k)} dV_s(k) \varepsilon^{d/2} dB_s^1 \]

\[ V_t(k\varepsilon) = V_0(k\varepsilon) + \int_0^t \sum_j V_s(j\varepsilon) q_{jk} ds \]

\[ + \int_0^t \sqrt{\varepsilon - dU_s(k)} dV_s(k) \varepsilon^{d/2} dB_s^2 \]
2.4 Questions:

- Existence and mathematical characterization of these processes?
- Spatial Structure: Does there exist a continuum limit?
  - Rescale RW rates on $\varepsilon Z^d$ so that RW converge to Brownian motion on $R^d$ as $\varepsilon \to 0$.
  - Describe the spatial heterogeneity and clumping of the catalyst and reactant and their relation between these.

2.5 Some Basic Tools

- Measure-valued diffusions
  - Martingale problem reformulation of SDE's
- Clumping structure is obtained in the continuum limit - geometry of random measures
2.6 Existence and structure of Continuum Limits: $\varepsilon \to 0$.

2.6.1 The Microscopic Particle Perspective

Branching Clock for “Tagged reactant particle”.

*Collision time between reactant particle and continuum catalyst* (Barlow-Evans-Perkins):

$$\Gamma^V_t(w) := \int_0^t \int V_s(dy)\delta_s(w_x)ds$$

in the sense that

$$\sup_{s \leq t} \left[ \sup_{x \leq r} \left| \int_0^s (p_n \ast V)(r, w_r)\psi(r, w_r)dr - \int_s^t \Gamma^V(dr, w)\psi(r, w_r)^2 \right| \right] \to 0 \text{ as } \eta \downarrow 0$$

2.6.2
Measure-valued Diffusion Continuum Models

2.6.3 Martingale Problem Formulation of Catalytic Branching

We characterize $U_t$ as a continuous $M(R^d)$-valued process which is the unique solution to the MP

$$U_t(\phi) = U_0(\phi) + \int_0^t U_s(\Delta \phi) ds + M_t(\phi)$$

$$ < M(\phi) >_t = \int_0^t \int \phi^2(x) K_\gamma^V(dx, ds)$$

where $K_\gamma^V$ is a “strong lifting” of the additive functional $\Gamma^V$.

2.7 SBM: Branching in a Uniform Medium

$$V_t \equiv \gamma$$

$$\Gamma^V_t (w) \equiv \gamma t$$

$$E \left( e^{-\int \varphi(x) U_t(dx)} | U_0 \right) = e^{-\int u(t,x) U_0(dx)}$$

$$\frac{\partial u}{\partial t} = \frac{1}{2} (\Delta u - \gamma u^2)$$

$U = \text{Super-Brownian Motion}$

2.7.1 Spatial Structure

- $U_t(dx) \perp dx$ and $\dim(\text{supp}(U_t)) = 2$ if $d > 1$
- Two independent SBM meet iff $d < 6$
- A Brownian particle meets the support of a SMB iff $d < 4$. 

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2.8 Catalytic SBM

Quenched Singular Catalyst in $R^d$

\[
E \left( e^{- \int \varphi(x) U_t (dx)} \bigg| U_0 \right) = e^{- \int \varphi(t,z) U_0 (dx)}
\]

\[
\frac{\partial u}{\partial t} = \frac{1}{2} (\Delta u - V_0 u^2) \text{ LLE} \tag{1}
\]

Existence:
The condition (Delmas (1996))

\[
\sup_x \int_{||y-x|| \leq 1} \frac{V_0(dy)}{|y-x|^{d-2+\beta}} < \infty \quad \text{(DC)}
\]

guarantees the existence of

- collision time, $\Gamma^V_t (w)$, between a Brownian particle and the catalyst, $V_0$, which controls the branching rate of the particle,
- the existence of a “non-trivial” solutions to (LLE)
- the existence of a non-trivial catalytic branching process.

Lemma: (DC) is satisfied if the Hausdorff dimension of support of $V_0$ is at least $d - 2 + \beta$, $\beta > 0$.

Theorem. The random measure $U_t$ has a density iff

\[
\frac{\partial u}{\partial t} = \frac{1}{2} (\Delta u - V_0 u^2)
\]

has a fundamental solution.

2.8.1 Example: Single Point Catalyst in $R^1$

\[ V_0 = \delta_0 \]

- $\Gamma^V_t$ is Brownian local time and the \( R^V_t (\{0\}, ds) = \text{occupation density of } \{0\} \) is a singular measure on \([0, \infty]\).
Super-Brownian Catalyst

Let

\[ V_t = \text{SBM in } \mathbb{R}^d \]

**Theorem.** Existence of catalytic SBM in a super-Brownian catalyst in dimensions \( d \leq 3 \).

[D-Fleischmann 1997]

**Laplace Functional Characterization**

\[
E(\exp -\int \phi(x)U(t, dx)) = \exp(-\int u(t,x)U(0, dx))
\]

**First Approach: Analytical**

\[
\frac{\partial u(t,x)}{\partial t} = \frac{1}{2} \Delta u(t,x) - V_t(dx)u^2(t,x)
\]

**Second Approach:** Existence of collision time and Dynkin’s function space approach

\[ u_s(t,x) = P_s[x \phi(w_t) - \int_s^t u^2(r, \rho, w_r) \Gamma^V_r (d\rho)] \]

### 2.8.2 Mutually Catalytic Branching

Formally the Continuum model is given by the pair of nonlinear SPDE:

\[
\begin{align*}
\frac{\partial U}{\partial t}(t,x) &= \frac{1}{2} \Delta U(t,x) + \sqrt{\gamma UV(t,x)B^1}(t,x) \\
\frac{\partial V}{\partial t}(t,x) &= \frac{1}{2} \Delta V(t,x) + \sqrt{\gamma UV(t,x)B^2}(t,x)
\end{align*}
\]

**Heuristics:**

From the (one-way) catalytic results we expect that if \( d \geq 2 \),

1. \( U_t(dx) \ll dx \) on \( \text{supp } (V_t)^c \)
2. \( \text{supp}(U_t) \cap \text{supp}(V_t) \) is Leb. null
3. \( U_t(dx) \ll dx, \ V_t(dx) \ll dx \) off this interface
For the moment let’s return to the lattice:

2.8.3 Uniqueness for the Lattice System.

Self-Duality (Mytnik): $X = U = V, \ Y = U - V$

\[
\Phi(x,y) = e^{-x+iy} \\
< X, \bar{X} > := \sum X(k)\bar{X}(k)
\]

\[
\begin{align*}
\Phi(< X_t, \bar{X}_0 >, < Y_t, \bar{Y}_0 >) \\
& \quad - \Phi(< X_0, \bar{X}_0 >, < Y_0, \bar{Y}_0 >) \\
& = \int_0^t [- < X_s, \Delta \bar{X}_0 > + i < Y_s, \Delta \bar{Y}_0 > \\
& \quad + \frac{1}{4} < X_s^2 - Y_s^2, \bar{X}_0^2 - \bar{Y}_0^2 >] \\
& \quad \times \Phi(< X_s, \bar{X}_0 >, < Y_s, \bar{Y}_0 >)ds + M_t
\end{align*}
\]

Since this is symmetric in $((X_s, Y_s), (\bar{X}_0, \bar{Y}_0)), (X, Y)$ is self dual and

\[
\begin{align*}
E(\Phi(< X_t, \bar{X}_0 >, < Y_t, \bar{Y}_0 >)) \\
& = E(\Phi(< X_0, \bar{X}_t >, < Y_0, \bar{Y}_t >)
\end{align*}
\]

Therefore existence proves uniqueness!
2.8.4 The One Dimensional Case

**Theorem (DP)** In the case $d = 1$ there exist solutions to the SPDE which are unique in law and such that for $\lambda > 0, q > 0$,

$$\sup_{r \leq 1} P \left( \int (u_r(x)^q + v_r(x)^q)e^{-\lambda|x|}dx \right) < \infty$$

2.8.5 The Two Dimensional Case

Define the rescaled lattice system:

$$U^{(K)}(A) : = \frac{1}{K} \sum_{x} U_{Kl}(x) \mathbb{1}_{K \uplus A}(x)$$

$$V^{(K)}(A) : = \frac{1}{K} \sum_{x} V_{Kl}(x) \mathbb{1}_{K \uplus A}(x)$$
Theorem (D-E-F-P-X) If \(d = 2\) and \(\gamma < \gamma_0\) then (a) the rescaled lattice systems converge weakly to a solution to the mutually catalytic martingale problem.

(b) any solution satisfies:

1. \(U_t(dx) = u_t(x)dx, \quad V_t(dx) = v_t(x)dx\)
2. \(\int u_t(x)v_t(x)dx = 0\) a.s. \(\forall t > 0\)
3. \(P((u_t(x), v_t(x)) \in Q) = P_{u,v}(B_T \in Q)\) where \(B_t\) is planar Brownian motion and
   \[T := \inf\{t : B^1_tB^2_t = 0\}\]
4. If \((U_0, V_0) = (dx, dx)\), then \((U, V)\) is self-similar
   \[(U_K(\sqrt{K}), V_K(\sqrt{K})) \equiv K(U(\cdot), V(\cdot))\]

Remarks and Open Questions:

1. The condition on \(\gamma\) should not be needed.
2. There is a Lebesgue null “interface” and densities away from the interface.
   Also we have no mass on the interface.

2.9 Long-time Behaviour for Lattice Systems

2.9.1 Case 1. Finite Initial Conditions

Assume \(0 < U_0(1), V_0(1) < \infty\). Then \((U_t(1), V_t(1)) \equiv B(A_t)\) where

\[A_t = \int_0^t \sum U_s(k)V_s(k)ds\]

and \(B\) is planar Brownian motion.

By MCT

\[(U_t(1), V_t(1)) \overset{a.s.}{\rightarrow} (U_\infty(1), V_\infty(1))\]

Let

\[T := \inf\{t : B^1_tB^2_t = 0\},\]

Theorem 1.

(a) In dimensions \(d = 1, 2\),

\[A_t \to \infty, \text{ on } \{U_\infty(1)V_\infty(1) > 0\}.\]
Corollary

\[ U_\infty(1)V_\infty(1) = 0, \text{ a.s.} \]

In the case \( d = 1, 2 \) one type dies out with probability one. Mueller and Perkins have shown that either finite time extinction, \( \{T < \infty\} \), or only ultimate extinction can occur depending on the nature of the i.c.

**Theorem 2.** In dimensions \( d \geq 3 \),

\[ E(A_\infty) < \infty \]

and

\[ P(U_\infty(1)V_\infty(1) > 0) > 0 \]

In this case co-existence can occur.

### 2.9.2 Case 2. Uniform Initial Conditions

**Theorem (DP).** Consider nearest neighbour RW in \( d \geq 3 \), \( U_0, V_0 \) are uniform measures. Then

\[ P((U_t, V_t) \in \cdot) \Rightarrow P_{\text{equil}} \]

where \( P_{\text{equil}} \) is a translation invariant equilibrium measure that preserves the initial intensity.

### 2.9.3 Local Segregation in the Recurrent Case

In the case \( d \leq 2 \), let \( U_0, V_0 \) be uniform measures.

As \( t \to \infty \), locally see one predominant type near 0. How big are “one type blocks” for \( t \) large? Let \( \beta > 0 \).

Define

\[ U_t^{(K)}(A) = K^{-\beta d} \sum_x U(K)(x)1_{A_K^d}(x) \]
\[ V_t^{(K)} = K^{-\beta d} \sum_x V(K)(x)1_{A_K^d}(x) \]

**Theorem (Dawson-Cox-Perkins)**

\( m = \) Lebesgue measure

(a) \( \beta > \frac{1}{2}, (U^{(K)}, V^{(K)}) \to (um, vm) \) as \( K \to \infty \).

(b) \( d = 1, \beta < \frac{1}{2} \), \( (U^{(K)}, V^{(K)}) \to m(B_1^d, B_2^d) \).

This means that Unitype Blocks at time \( t = K \) are of size \( O(K^{1/2}) \).

**Theorem.** (Cox-Klenke)

Let \( (u', v') \in R^2 \) and
\hat{\alpha}'(k) = u' \forall k.

Then with probability one the limit points of \{(u_n, v_n) : n \in N\} include both \((\hat{\alpha}', \hat{0})\) and \((\hat{0}, \hat{\alpha}')\).

**Remark.** This means that the predominant type near zero changes infinitely often as \(t \to \infty\).
2.10 Summary

- Catalytic and mutually catalytic branching leads to highly clumped spatial distributions of reactants
- The methodology of measure-valued processes provides a unified framework for the study of particle systems, lattice approximations and continuum limits.

2.11 Open Problems

1. Determination of rates of product formation
2. Higher dimensional continuum mutually catalytic branching
3. Hypercyclic catalytic branching
2.12 References


