Field Theoretic Approach

to

Reaction-Diffusion Problems

at the

Upper Critical Dimension

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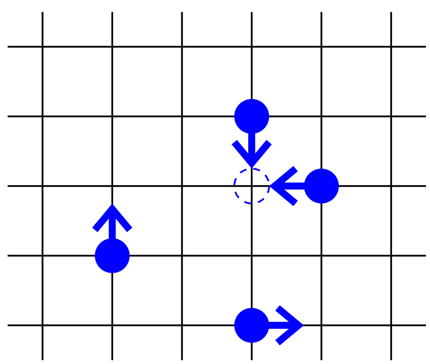
- Reaction-Diffusion Models
  - ◇ Doi "Second Quantized" Representation
  - ◇ Field Theory
- $3A \to (\emptyset, A, 2A)$ Reactions in One Dimension
  - ◇ Renormalization Group Calculation
  - ◇ Smoluchowski Theory
  - ◇ Simulations
- Summary

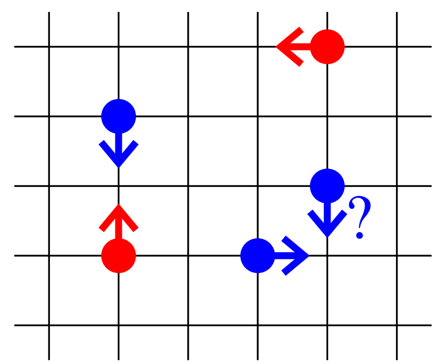
Reaction-Diffusion Models

- classical particles hop randomly on lattice
- one-species or multi-species
- react when occupying the same site

$\mathrm{A+A \rightarrow A}$



$\mathrm{A+B \rightarrow \varnothing}$



Reaction-Diffusion Models

- classical particles hop randomly on lattice
  - short- and long-range hops (diffusion vs. Levy flights)
  - quenched disorder
  - varying lattices, networks, continuum

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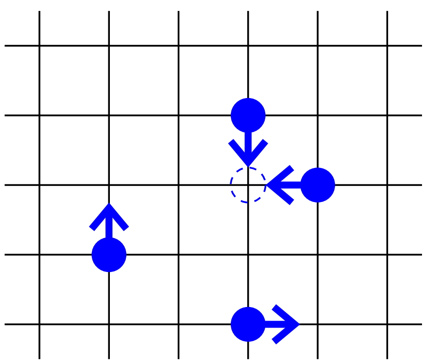

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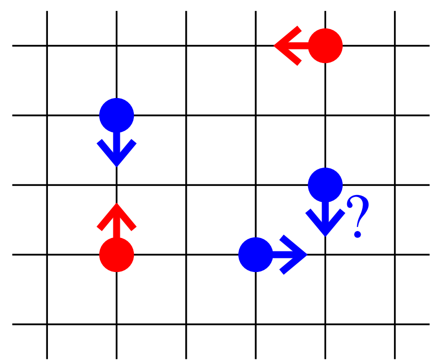

Reaction-Diffusion Models

- classical particles hop randomly on lattice
- one-species or multi-species
  - ◇ general one-species decay: $kA \to \ell A$
  - ◇ reversible: $A + B \leftrightarrow C$
  - ◇ directed percolation: $A + A \leftrightarrow A$ and $A \to \emptyset$
  - ◇ $A + B \to \emptyset$ conserves $n_A - n_B \Rightarrow$ slow mode

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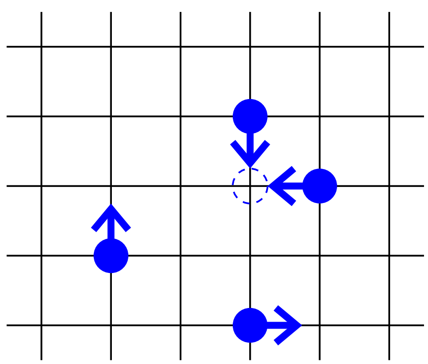

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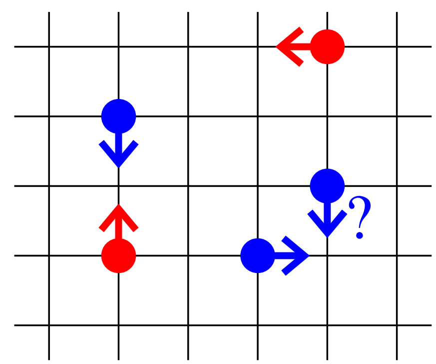

Reaction-Diffusion Models

- classical particles hop randomly on lattice
- one-species or multi-species
- react when occupying the same site
  - ◇ reaction rate or probability
  - ◇ capture radius (continuum)
  - ◇ site occupancy restrictions

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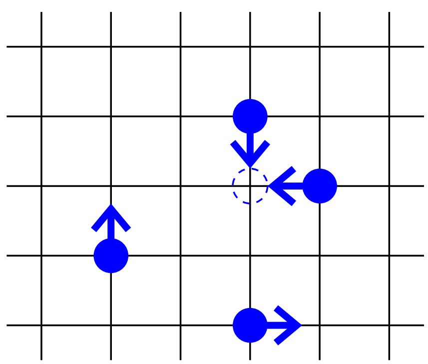

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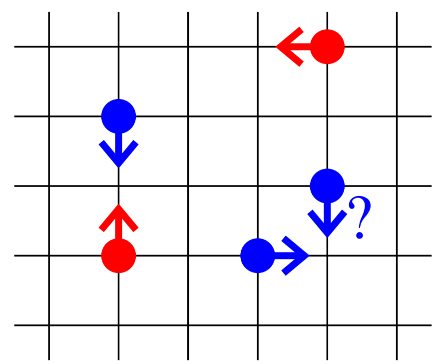

Master Equation

$$\frac{\partial}{\partial t} P(\alpha, t) = \sum_{\beta} \Big[w_{\beta \to \alpha} P(\beta, t) - w_{\alpha \to \beta} P(\alpha, t) \Big]$$

- α, β specified by occupation numbers $\{n\} = (n_1, n_2, \ldots)$
- rates $w_{\alpha \to \beta}$ for states connected by hops and reactions
- Poisson initial conditions

Diffusion

$$\partial_t P(\{n\},t) = \frac{D}{h^2} \sum_{\langle ij \rangle} \Big[(n_i+1)\, P(n_i+1, n_j-1, t) - n_i\, P$$
$$+ (n_j+1)\, P(n_i-1, n_j+1, t) - n_j\, P \Big]$$

$A + A \to 0$ Reaction

$$\partial_t P(n,t) = \lambda \Big[(n+2)(n+1)\, P(n+2,t) - n(n-1)\, P(n,t) \Big]$$

Diffusion

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Yuck!

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  - ◇ Doi "Second Quantized" Representation
  - ◇ Field Theory
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Doi Representation

- introduce $\hat{a}$, $\hat{a}^\dagger$ at each site with $[\hat{a}_i, \hat{a}_j^\dagger] = \delta_{ij}$
- occupation state $|\{n\}\rangle = \prod_i (\hat{a}_i^\dagger)^{n_i} |0\rangle$

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- define nonequilibrium state vector

$$|\phi(t)\rangle = \sum_{\{n\}} P(\{n\}, t)\,|\{n\}\rangle$$

- master equation becomes $\partial_t|\phi(t)\rangle = -\hat{H}|\phi(t)\rangle$

Doi Hamiltonian $\hat{H} = \hat{H}_D + \hat{H}_R$

- Diffusion: $\hat{H}_D = \frac{D}{h^2} \sum_{\langle ij \rangle} (\hat{a}_i^\dagger - \hat{a}_j^\dagger)(\hat{a}_i - \hat{a}_j)$

- Reaction:

  $A + A \to \emptyset$: $\hat{H}_R = \lambda(\hat{a}^{\dagger 2}\hat{a}^2 - \hat{a}^2)$

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$A + B \to C$: $\hat{H}_R = \lambda(\hat{a}^\dagger \hat{b}^\dagger \hat{a}\hat{b} - \hat{c}^\dagger \hat{a}\hat{b})$

[compare to master equation]

Expectation Values

- Formal solution $|\phi(t)\rangle = e^{-\hat{H}t}|\phi(0)\rangle$
- Nonequilibrium averages

$$\overline{Q(t)} = \sum_{\{n\}} Q(\{n\})P(\{n\},t) = \langle\cdot|\hat{Q}|\phi(t)\rangle$$

- Requires projection state $\langle\cdot| = \langle 0|e^{\sum_i a_i}$

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- Requires projection state $\langle \cdot | = \langle 0 | e^{\sum_i a_i}$
- Probability conservation: $1 = \langle \cdot | e^{-\hat{H}t} | \phi(0) \rangle$
  $\Rightarrow \quad \langle \cdot | \hat{H} = 0.$

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Coherent State Representation [Peliti '85]

- Coherent states: $\hat{a}|z\rangle = z|z\rangle$, complex z
- Identity operator: $\mathbf{1} = \int \frac{d^2z}{\pi} |z\rangle\langle z|$
- Divide into $N = t/\Delta t$ time slices:

$$\overline{Q} = \langle \cdot | \hat{Q}(e^{-\hat{H}\Delta t}) \ldots (e^{-\hat{H}\Delta t}) | \phi(0) \rangle$$

- Insert identity at each site between each slice: $z_{i,t} \longrightarrow \phi(x,t)$

Field Theory for $kA \to \ell A$ [BPL '94]

- Complex fields ϕ and $\phi^* \to 1 + \bar{\phi}$
- Expectation value: $\overline{Q} = \frac{1}{\mathcal{N}} \int \mathcal{D}(\phi, \bar{\phi})\, Q(\phi) e^{-S[\phi,\bar{\phi}]}$

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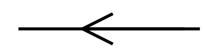
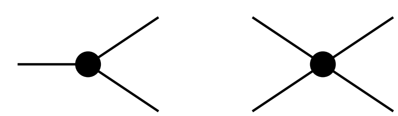
Action $S = S_D + S_R - \int d^dx\, n_0 \bar{\phi}_{t=0}$

- $S_D = \int d^dx\, dt\, \bar{\phi}(\partial_t - D\nabla^2)\phi$



- $S_R = \int d^dx\, dt\, \sum_{i=1}^{k} \lambda_0 c_i \bar{\phi}^i \phi^k$



- $c_k = 1$, c_i depend only on k, ℓ

Why is this Field Theory Useful?

- Apply RG to extract universal quantities
  - ◇ asymptotic late times, small currents
  - ◇ noneq critical points, e.g. directed percolation
- No *ad hoc* assumptions, as in Langevin equations
- Flexible: can handle many generalizations

Review Article

U.C. Täuber, M. Howard, and BPV-L, J. Phys. A, R79 (2005).

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Rate Equations Assume particles remain randomly distributed

- $A + B \to \emptyset$ reaction: $\frac{\partial}{\partial t}a = \frac{\partial}{\partial t}b = -\Gamma ab$
- $kA \to \ell A$ reaction: $\frac{\partial}{\partial t}a = -\Gamma a^k$

$$\Rightarrow \quad a \sim (\Gamma t)^{-1/(k-1)} \sim \begin{cases} 1/t & 2A \to (\emptyset, A) \\ 1/t^{1/2} & 3A \to (\emptyset, A, 2A) \end{cases}$$

Valid for single-species when $d > d_c = 2/(k-1)$

One-Species Reactions with $d \le d_c$:

- particles become anti-correlated, slower decay:

$$a \sim \begin{cases} A(Dt)^{-d/2} & d < d_c \\ \tilde{A}(\ln t / Dt)^{d_c/2} & d = d_c = \begin{cases} 2 & 2A \to \ell A \\ 1 & 3A \to \ell A \end{cases} \\ \text{const.}\, t^{-d_c/2} & d > d_c \end{cases}$$

- decay amplitudes A and $\tilde{A}$ are universal, as demonstrated by RG calculations [BPL '94]

Tests of RG Predictions

- $\tilde{A} = 1/4\pi$ for $A + A \to A$ in $d_c = 2$ matches exact solution [Bramson and Griffeaths '80]

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- $\tilde{A} = \left(\frac{\sqrt{3}}{4\pi(3-\ell)}\right)^{1/2}$ for $3A \to \ell A$ in $d_c = 1$ $\simeq (0.21, 0.26, 0.37)$ for $\ell = (0, 1, 2)$

  - ◇ Simulations give (0.26, 0.76, 0.93)

  - ◇ $3A \to \emptyset$ data matches Smoluchowski Theory

[Oshanin, *et al.* '95, ben-Avraham '93]

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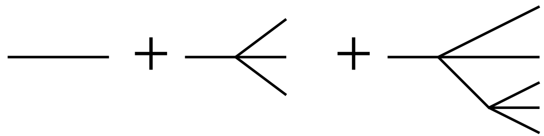
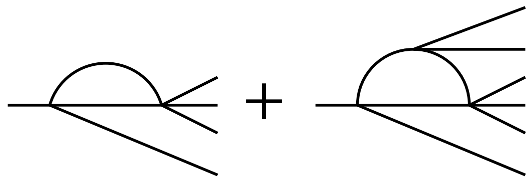
Loop Expansion for Density

- Tree level:  $+\cdots$
- One-loop:  $+\cdots$
- Renormalization: $n_0 \to \infty$, $\lambda_0 \to \lambda_R \sim \frac{2\pi}{\sqrt{3}\ln(t/\tau)}$

Result

$$n(t)(Dt)^{1/2} \sim \tilde{A}\sqrt{\ln(t/\tau)} + \tilde{B} + \tilde{C}\frac{1}{\sqrt{\ln(t/\tau)}} + \ldots$$

Universal Leading Corrections!

Since $\sqrt{\ln(t/\tau)} = \sqrt{\ln t} + \frac{\ln \tau}{2} \frac{1}{\sqrt{\ln t}} + \dots$

$\Rightarrow n(t)(Dt)^{1/2} \sim \tilde{A}\sqrt{\ln t} + \tilde{B} +$ nonuniversal

- $\tilde{B} = \frac{9\sqrt{2\pi}(2+\ell)}{128}$
- Corrections large ($\sim 50\%$) for accessible simulation range
- Does not happen for $2A \longrightarrow (\emptyset, A)$, which has $\ln(t/\tau)$ instead of $\sqrt{\ln(t/\tau)}$

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Smoluchowski Theory

- Correlation function mean-field theory: gets correct exponents for $2A \to (\emptyset, A)$!
- Two different generalizations to $3A \to \ell A$, both find log corrections, different amplitudes [Krapivsky '94, Oshanin *et al.* '95]
- Both missed various factors. When corrected

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- Two different generalizations to $3A \to \ell A$, both find log corrections, different amplitudes [Krapivsky '94, Oshanin *et al.* '95]
- Both missed various factors. When corrected . . . both agree with RG for $\tilde{A}$
- but Smoluchowksi theory has $\tilde{B} = 0$

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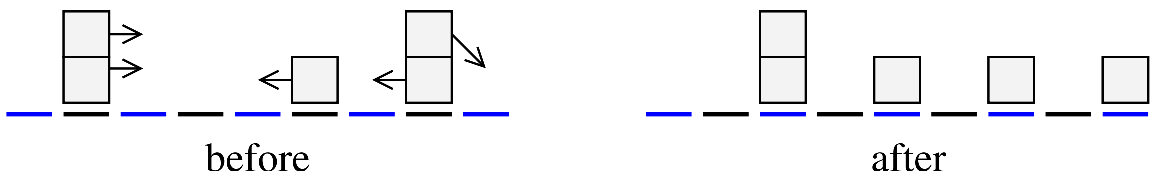
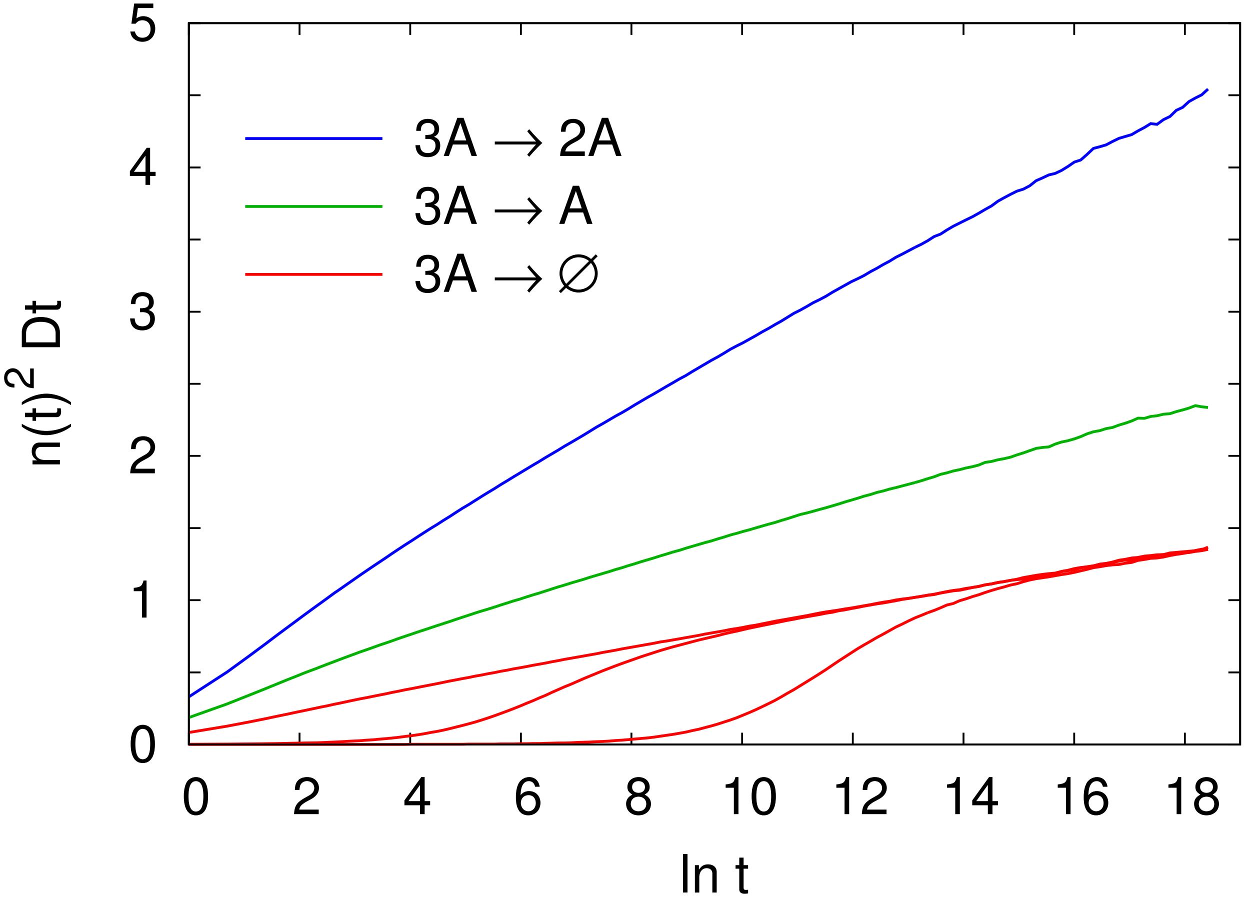
Simulation Technique

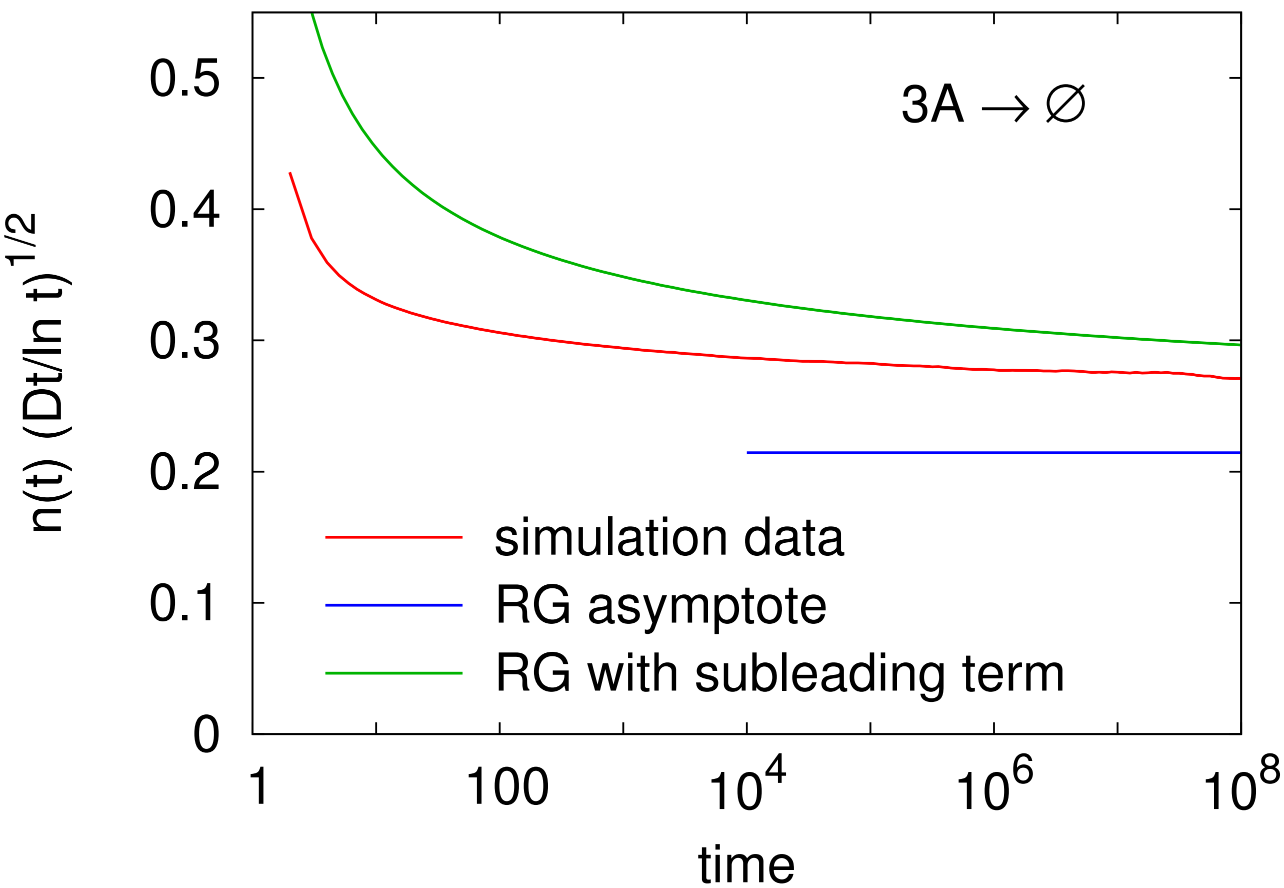
- 1d lattice, $2^{23} \simeq 8.4 \times 10^6$ sites, 10^8 time steps
- synchronous dynamics ($D = 1/2$):



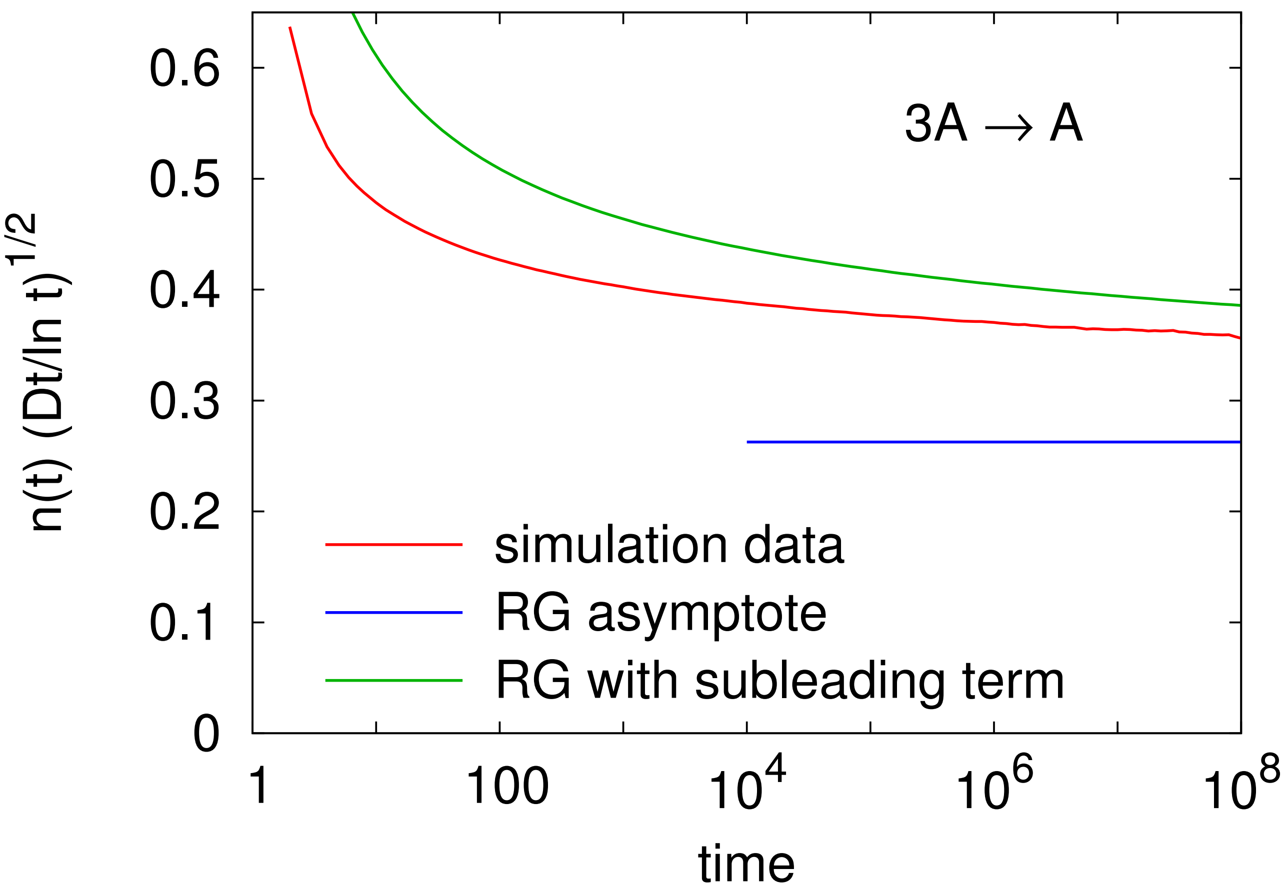
- linked list of particle sites $\Rightarrow$ efficient update
- 10 to 20 independent runs for each reaction

RG: $n \sim \tilde{A}\sqrt{\ln t / Dt}$ Rate Eq: $n \sim 1/t^{1/2}$

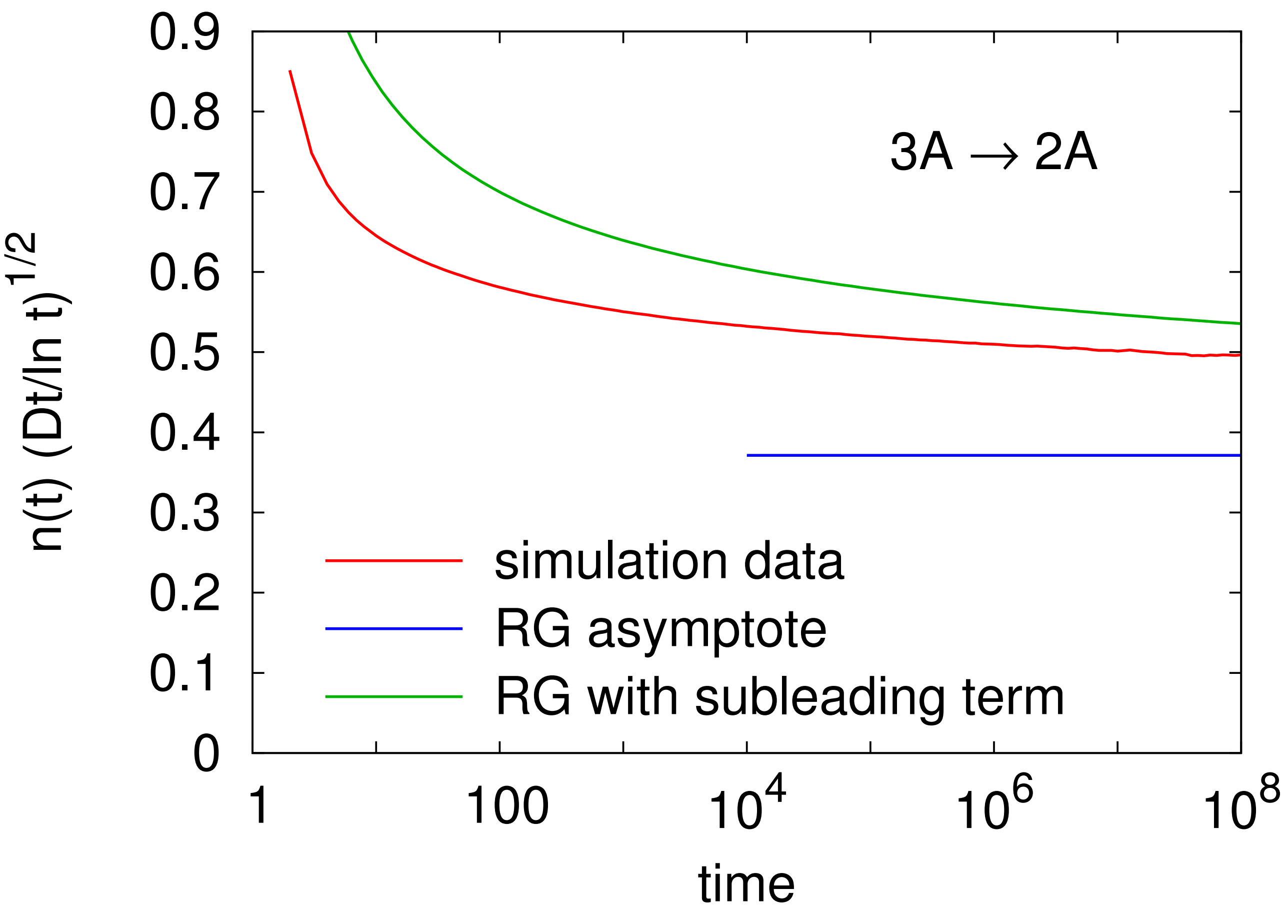




Data consistent with Oshanin *et al.* '95



Data not consistent with ben-Avraham '93



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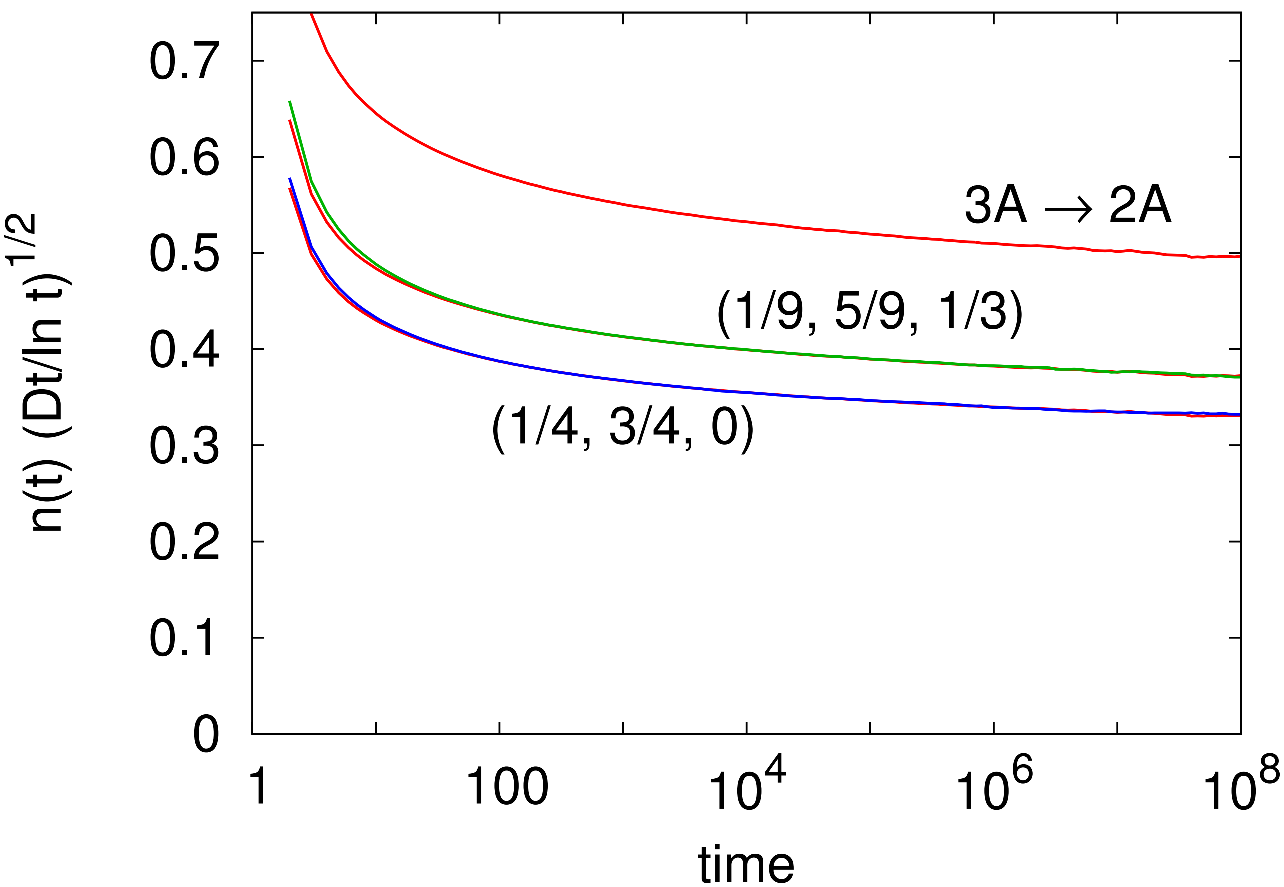
Rescaling Symmetry

- rescaling $\phi \longrightarrow b\phi$, $\bar{\phi} \longrightarrow b^{-1}\phi$ changes only c_i
- density for different reactions related by rescaling to all orders in $1/\sqrt{\ln(t/\tau)}$
- mixed reactions: (p_0, p_1, p_2) related to $3A \longrightarrow 2A$

Mixed $3A \rightarrow (\emptyset, A, 2A)$ with rates (p_0, p_1, p_2)



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