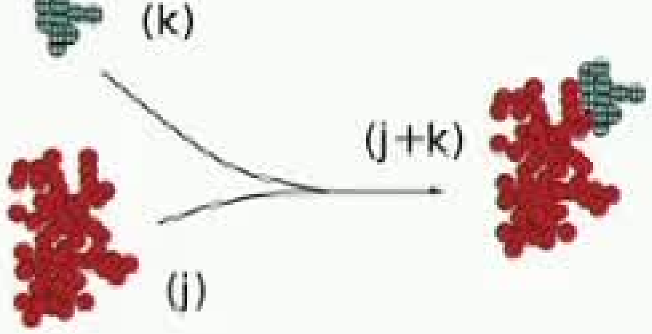
Dynamics in models of coagulation and fragmentation

Bob Pego (Carnegie Mellon)

Dedicated to the memory of Jack Carr

Supported by NSF, Center for Nonlinear Analysis, KI-Net, Simons

Smoluchowski's coagulation equations (1916)



$$(j) + (k) \underset{b_{j,k}}{\overset{a_{j,k}}{\rightleftarrows}} (j+k)$$

Key statistic: Number density $c_j(t)$ of aggregates of size j

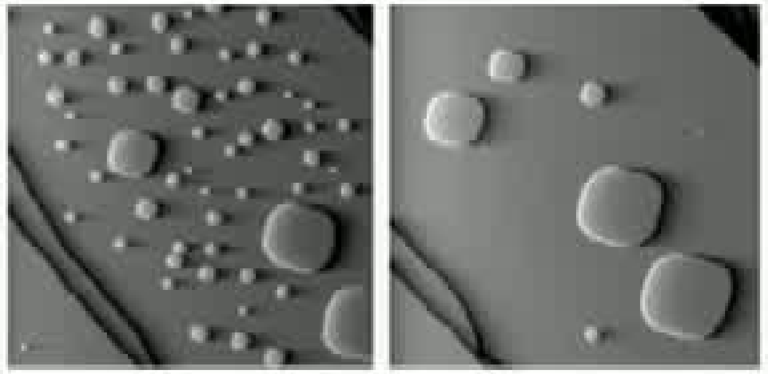
Net rate of aggregation (and binary breakup): $R_{j,k} = a_{j,k}\, c_j c_k - b_{j,k} c_{j+k}$

Rates of gain & loss of j-clusters: $\partial_t c_j(t) = \frac{1}{2}\sum_{k=1}^{j-1} R_{j-k,k} - \sum_{k=1}^{\infty} R_{j,k}$

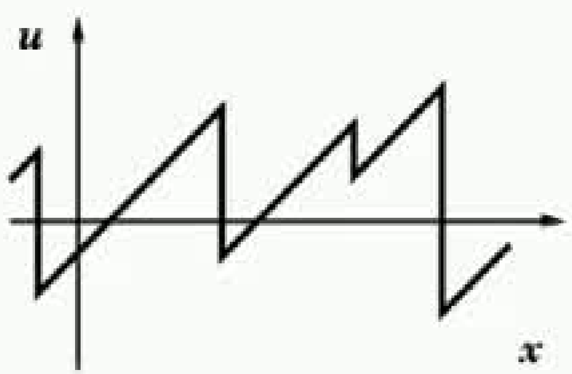
For aggregation of Brownian clusters: $a_{j,k} = (j^{1/3} + k^{1/3})(j^{-1/3} + k^{-1/3})$

Explicit solution for $a_{i,j} = 2$ and monomer initial data

Great variety of scientific applications



- materials science: polymerization, ripening of nanoscale structures
- aerosol physics: formation of clouds, smog, ink fog
- astrophysics: agglomeration of planetesimals, star clusters, galaxies
- probability: random graph growth, random shock-wave clustering
- biology: telomere maintainance, Alzheimer's disease
- population biology: branching of ancestral trees, animal group dynamics

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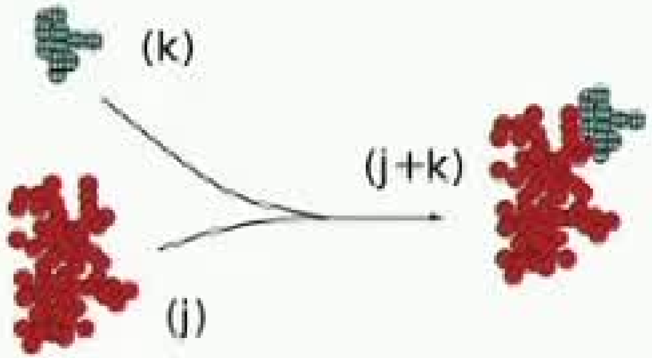

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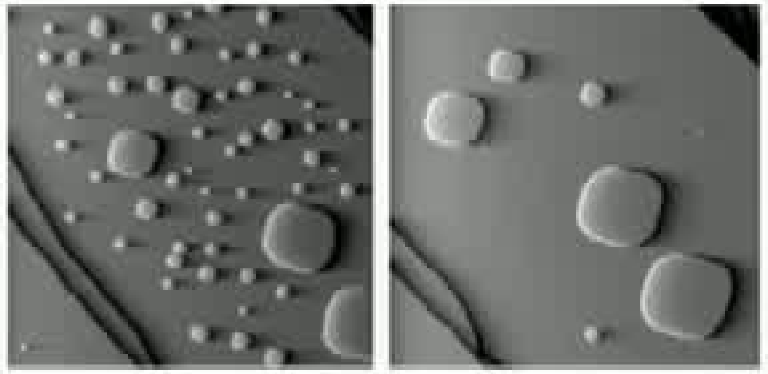

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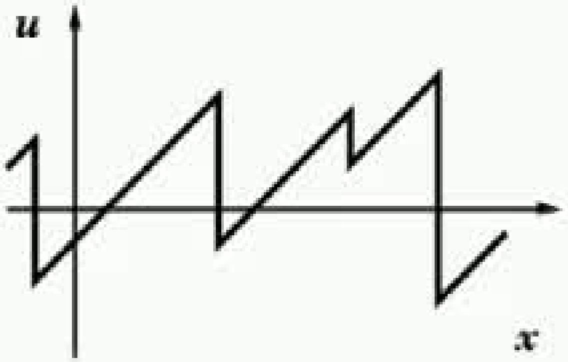

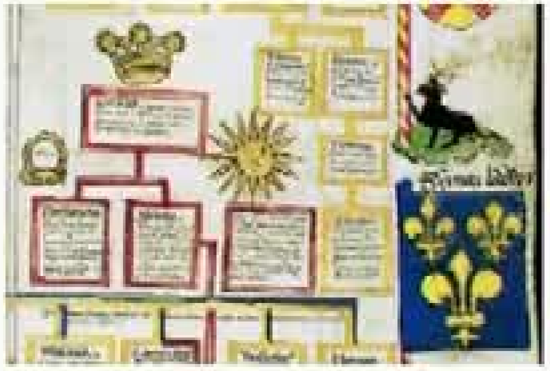

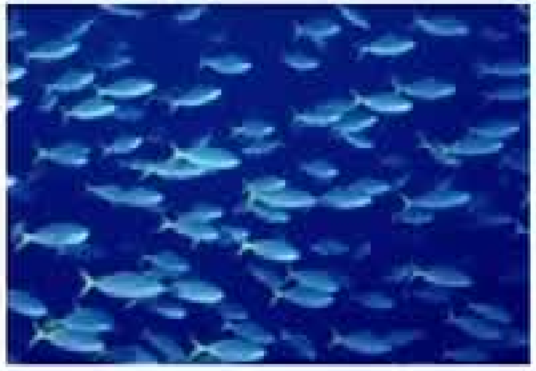

Just another (countable) bunch of ODEs?

- Coagulaton-fragmentation equations:

$$\partial_t c_j(t) = \frac{1}{2}\sum_{k=1}^{j-1} R_{j-k,k} - \sum_{k=1}^{\infty} R_{j,k}, \qquad R_{j,k} = a_{j,k}\, c_j c_k - b_{j,k} c_{j+k}$$

- Navier-Stokes equations in a periodic box

$$\partial_t \hat{\mathbf{u}}_{\mathbf{j}}(t) = -\sum_{\mathbf{k}\in\mathbb{Z}^3} i\,\mathbf{k}\cdot\hat{\mathbf{u}}_{\mathbf{j}-\mathbf{k}}\hat{\mathbf{u}}_{\mathbf{k}} - i\,\mathbf{j}\,\hat{p}_{\mathbf{j}} - \nu|\mathbf{j}|^2\hat{\mathbf{u}}_{\mathbf{j}}, \qquad \mathbf{j}\cdot\hat{\mathbf{u}}_{\mathbf{j}} = 0.$$

- Some coagulation rates $a_{j,k}$ arising in applications:

$$(j^{1/3}+k^{1/3})(j^{-1/3}+k^{-1/3}) \qquad (j^{1/3}+k^{1/3})^2(j^{-1}+k^{-1})^{1/2} \qquad (j^{1/3}+k^{1/3})^3$$

$$(j^{1/3}+k^{1/3})^2|j^{2/3}-k^{2/3}| \qquad (j^{1/3}+k^{1/3})^2|j^{1/3}-k^{1/3}| \qquad (j^{1/3}+k^{1/3})^{7/3}$$

$$(j^{1/3}+k^{1/3})(jk)^{1/2}(j+k)^{-3/2} \qquad (j+c)(k+c) \qquad (j-k)^2(j+k)^{-1}$$

Effects: Brownian motion, shear flow, gravitational settling, turbulence, inertia, large mean-free-path, fractal aggregates.

Dynamical phenomena and issues

- Existence (or not) of unique mass-conserving solutions depends upon growth conditions for rate coefficients, moment conditions for initial data

- Loss of mass to infinite size *(gelation)* can occur:
  - in infinite time (Ball-Carr-Penrose 1986, Becker-Döring over a critical density),
  - in finite time (MacLeod 1962, Jeon 1998, Escobedo etal 2002),
  - instantaneously (Carr-da Costa 1992, Laurençot 1999, Bechor 2017)

- Loss of mass to zero size *(shattering)* occurs in continuous-size models with strong fragmentation

- Scaling dynamics for pure coagulation, continuous-size models:
  - Self-similar solutions often *exist* (Fournier-Laurençot, Escobedo et al 2004)
  - Uniqueness results are rare (see Laurençot 2018 JSP)
  - Convergence to self-similar form is understood only for solvable cases (Menon-P)

- Equilibration for coagulation-fragmentation is analyzed almost exclusively in the case when equilibria have **detailed balance:** $R_{j,k} = a_{j,k}\hat{c}_j\hat{c}_k - b_{j,k}\hat{c}_{j+k} = 0.$

- *Forthcoming book:* 2 volumes by Banasiak, Lamb, Laurençot

Outline of today's talk

- Coagulation-fragmentation dynamics - Prologue.
  Solvable models. Branching, Bernstein functions
- Becker-Döring equations: $\partial_t c_j = R_{j-1,1} - R_{j,1}$. Nature of the semigroup.
  Equilibration rates, cutoff phenomenon, norm-dependent spectrum.
- Animal group size distributions modeled after studies of H.-S. Niwa
  Equilibration without detailed balance
  Self-similar spreading with fat tails
  Role of Bernstein and Pick (Herglotz) functions
  A discrete Pick representation theorem. Hausdorff moment problem.
- A jump-process model of merging-splitting group dynamics
- (Other talk) A coagulation-fragmentation model exhibiting temporal oscillations
- Recurring theme: improvements in math tools, problem-motivated

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Weak form. Solvable cases.

A solution should satisfy a generalized moment identity

$$\partial_t \sum_{i=1}^{\infty} f_i\, c_i(t) = \frac{1}{2} \sum_{j,k=1}^{\infty} (f_{j+k} - f_j - f_k)\,(a_{j,k}\, c_j(t) c_k(t) - b_{j,k} c_{j+k})$$

for all test sequences (f_i) (bounded or c_0, say).

Choosing $f_j = (1 - e^{-qj}) j^p$, for $\varphi(q,t) = \sum_{j=1}^{\infty} (1 - e^{-qj}) j^p c_j(t)$ one finds:

$$\begin{aligned} \partial_t \varphi(q,t) &= -\varphi^2 && \text{for } p = 0,\ a_{j,k} = 2 \\ \partial_t \varphi(q,t) - \varphi\, \partial_q \varphi &= -\varphi && \text{for } p = 0,\ a_{j,k} = j + k \\ \partial_t \varphi(q,t) - \varphi \partial_q \varphi &= 0 && \text{for } p = 1,\ a_{j,k} = jk \end{aligned}$$

Remark: $q \mapsto \varphi(q,t)$ is a *Bernstein function*. (More on this later.)

Solution formulae in contour integrals & series: W.T. Scott 1968 J Atmos Sci

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Branching processes and solvable coagulation equations

Bertoin & Le Gall 2006 – solvable Smoluchowski-like equations for CSBP

Galton-Watson branching process: $X_{n+1} = \sum_{j=1}^{X_n} Y_{j,n}$, $Y_{j,n} \sim \nu_0$ iid on $\mathbb{N}_0$

$X_n \sim C_n(j)$ for a dual merging process on iid sequences $(C_n(1), C_n(2), \ldots)$:

$$C_{n+1}(j) = \sum_{k=1+N_{j-1,n}}^{N_{j,n}} C_n(k), \qquad N_{j,n} - N_{j-1,n} \sim \nu_0 \text{ iid}$$

The law ν_n of $C_n(j)$ or X_n satisfies a discrete, multiple-coagulation equation:

$$\nu_{n+1} - \nu_n = \sum_{k \geq 2} \nu_n^{*k} r_k(\rho_n), \quad \rho_n = \sum_{j>0} \nu_n(j), \; r_k(\rho) = \sum_{m \geq k} \nu_0(m) \binom{m}{k} (1-\rho)^{m-k}$$

- $\hat{\varphi}_n(q) = \sum_{j \geq 1} (1 - e^{-qj}) \nu_n(j)$ satisfies $\hat{\varphi}_{n+1}(q) - \hat{\varphi}_n(q) = -\hat{\Psi}(\hat{\varphi}_n(q))$

In the continuum limit for critical GW branching: $\boxed{\partial_t \varphi(q,t) = -\Psi(\varphi)}$

Bernstein transforms and the topology of Lévy triples

2010 book: *Bernstein Functions*, by Schilling, Song & Vondraček

Defn $\varphi : (0,\infty) \to [0,\infty)$ is *Bernstein* if φ is C^∞ and $\quad \operatorname{sgn} \varphi^{(n+1)} = (-1)^n \quad \forall n$

- **Theorem** φ is Bernstein $\iff$ for some Lévy triple (a_0, a_∞, μ), with

$$a_0,\ a_\infty \geq 0 \quad \text{and} \quad \int_0^\infty (s \wedge 1)\mu(ds) < \infty,$$

we have the representation

$$\boxed{\varphi(q) = a_0 q + a_\infty + \int_0^\infty (1 - e^{-qs})\mu(ds)}$$

- Nice properties: (a) Bernstein functions are stable under pointwise convergence

(b) The composition of Bernstein functions is Bernstein.

(c) If $\psi(q) = \int_0^q \varphi(r)\,dr$ for some Bernstein $\varphi > 0$, then ψ^{-1} is Bernstein.

- Associated κ-*measure* on $[0,\infty]$: $\quad \kappa(ds) = a_0\delta_0 + a_\infty\delta_\infty + (s \wedge 1)\mu(ds)$

Continuity theorem for Bernstein transforms

Let $(a_0^{(n)}, a_\infty^{(n)}, \mu^{(n)})$ be a sequence of Lévy triples, associated with $\varphi^{(n)}$, $\kappa^{(n)}$.

Then the following are equivalent:

(i) $\lim_{n\to\infty} \varphi^{(n)}(q) =: \varphi(q)$ exists for each $q > 0$.

(ii) $\kappa^{(n)}$ converges weak-$\star$ to some measure κ on $[0,\infty]$, meaning

$$\langle f, \kappa^{(n)}\rangle \to \langle f, \kappa\rangle \quad \text{for all } f \in C([0,\infty]).$$

If the conditions hold, φ, κ are associated with a unique Lévy triple (a_0, a_∞, μ):

$$a_0^{(n)}\delta_0 + (s\wedge 1)\mu^{(n)}(ds) + a_\infty^{(n)}\delta_\infty \;\overset{\star}{\rightharpoonup}\; a_0\delta_0 + (s\wedge 1)\mu(ds) + a_\infty\delta_\infty$$

(This is restated from Menon-P 2008; a simple proof is in Leger-Iyer-P 2018)

• Becker-Döring equilibration dynamics

Becker-Döring equations: $\partial_t c_j = R_{j-1,1} - R_{j,1}, \quad R_{j,1} = a_j c_1 c_j - b_{j+1} c_{j+1}.$

Typical assumptions: $\dfrac{a_{j+1}}{a_j} \to 1, \quad \dfrac{b_j}{a_j} \to z_{\text{cr}}, \quad 1 \lesssim a_j, b_j \lesssim j$

Subcritical equilibrium: $\dfrac{\hat{c}_{j+1}}{\hat{c}_j} = \dfrac{b_{j+1}}{a_j \cdot 1}, \quad c_j^{\text{eq}} = \hat{c}_j z^j, \quad c_1^{\text{eq}} = z < z_{\text{cr}}$

- Jabin-Niethammer 2003: $|c_j(0) - c_j^{\text{eq}}| \lesssim e^{-bj} \implies \|c(t) - c^{\text{eq}}\|_{X_1} \lesssim e^{-\lambda t^{1/3}}$
- Cañizo-Lods 2013: Actually $\|c(t) - c^{\text{eq}}\|_{X_1} \lesssim e^{-\lambda t}$ ($\|c\|_{X_k} = \sum_j |j^k c_j|$)

Method: (i) Estimate spectral gap in *self-adjoint* form from detailed balance; (ii) "Lift" the semigroup decay estimate to X_1 (ala Mouhot in kinetic theory)

- Murray-P 2017 (cf. Cañizo-Einav-Lods 2017): For perturbations $c(0) - c^{\text{eq}}$ small in X_k, $\|c(t) - c^{\text{eq}}\|_{X_m} \lesssim (1+t)^{-(k-m-1)}, \quad k - 2 > m > 1$

Method: (i) new (Banach-space) dissipation estimates to prove X_1 stability (ii) interpolation between X_1 and exponentially weighted spaces (ala Engler)

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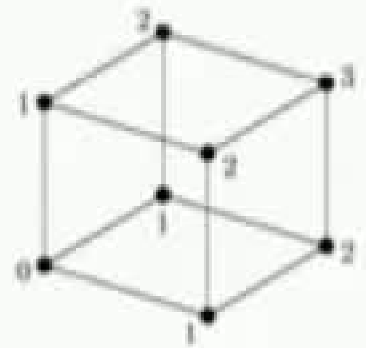
Cutoff phenomenon and card shuffling

For certain Markov chains of size $n \to \infty$: Measured in ℓ^1, equilibration is rapid only after a *time delay*, despite existence of an ℓ^2 *spectral gap*.

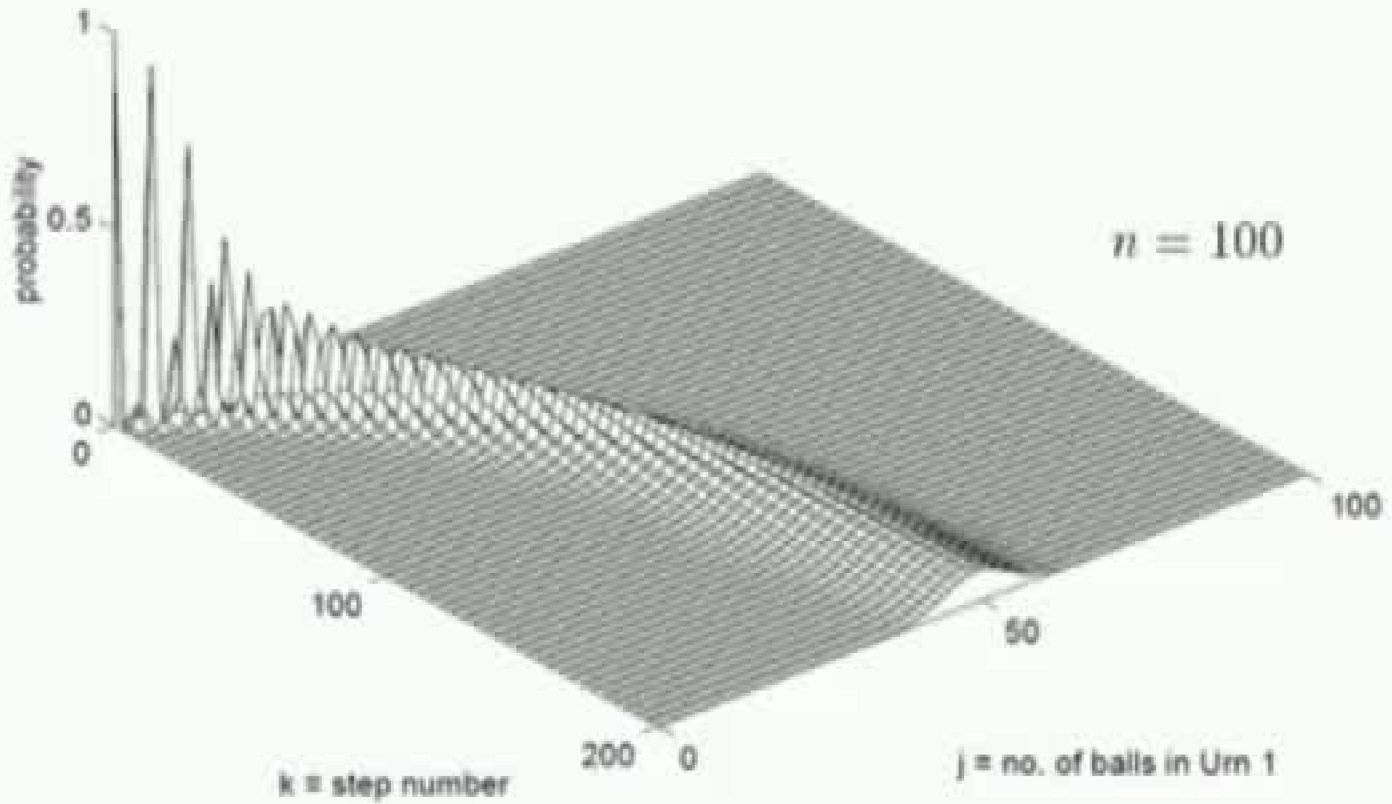
Classic example of Bayer-Diaconis 1992: Shuffling n cards by k riffle shuffles achieves randomization after $k \sim \frac{3}{2}\log_2 n$ shuffles ("7 shuffles suffices")

See discussion in Trefethen & Embree, *Spectra & Pseudospectra*:

Random walk on $\{0,1\}^n$



"A probability wave must propagate from one place to another before convergence can occur."



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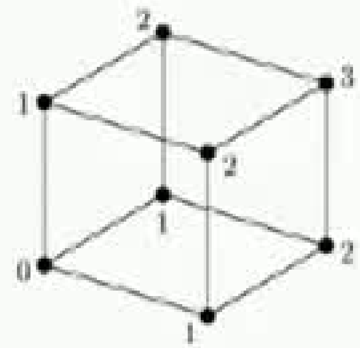

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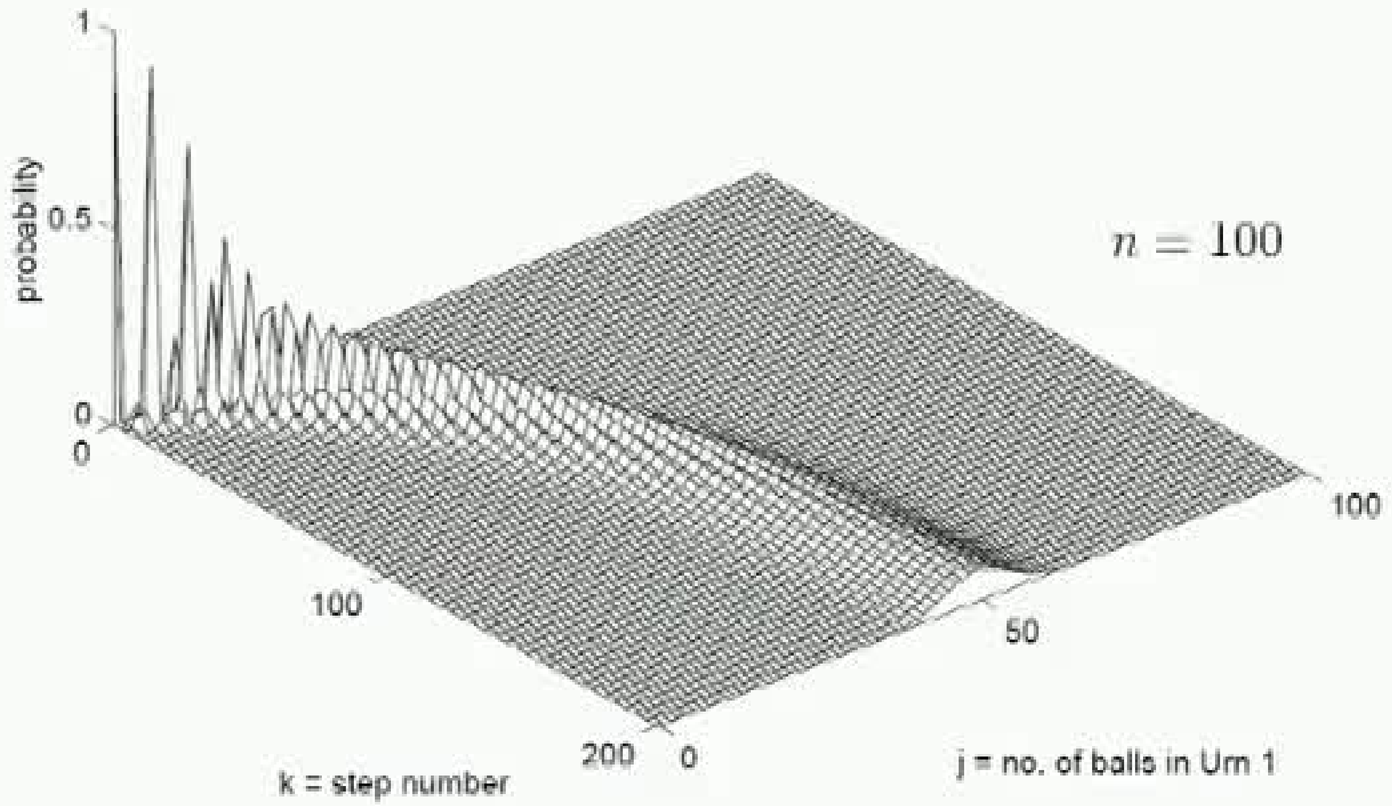


Cutoff phenomenon for Becker-Döring equilibration

Linearized Becker-Döring equilibration in X_k is similarly *delayed by advection*.

Take e.g. $a_j = j^\alpha, \quad b_j = a_j\left(z_{\rm cr} + \gamma/j^{1-\beta}\right), \quad \alpha,\beta \in (0,1)$

Writing $c_j^{\rm eq} = \hat{c}_j z^j, \quad c_j = c_j^{\rm eq}(1+h_j),$ the linearized equations are

$$\partial_t h_j = (Lh)_j = a_j z(h_{j+1} - h_j - h_1) - b_j(h_1 + h_{j-1} - h_j)$$

Lifshitz-Slyozov-like continuum analog:

$$u_t = p(x)u_x + q(x)u_{xx} \qquad \text{with} \quad p(x) \sim (z_{\rm cr} - z)x^\alpha, \quad q(x) \sim x^\alpha$$

Characteristics: $\partial_t Z \sim -(z_{\rm cr} - z)Z^\alpha$ Persistence time: $T \sim \dfrac{Z_0^{1-\alpha}}{(z_{\rm cr} - z)}$

Complications: Linearized mass conservation $\sum c_j^{\rm eq} j h_j = 0$. Coupling to h_1.

Norm-dependence for Becker-Döring equilibration

Write $\|h\|_{X_k} = \sum_j c_j^{\text{eq}} |h_j| j^k$. Compare with $\|h\|_Y^2 = \sum_j c_j^{\text{eq}} |h_j|^2$.

- In Y, Cañizo-Lods show L is self-adjoint with compact resolvent, all eigenvalues are real and negative, and e^{Lt} is analytic with $\|e^{Lt}\|_{\mathcal{L}(Y)} \le Ce^{-at}$.

- In X_k, the resolvent set of L contains $\{\operatorname{Re}\lambda > 0\}$ and $\|e^{Lt}\|_{\mathcal{L}(X_k)} \le C \quad \forall t \ge 0$.

Theorem Assume $a_j \to \infty$ and $|a_j - a_{j-1}| + |b_j - b_{j-1}| \to 0$.
Then the spectrum of L in X_k *contains the entire imaginary axis*.

Theorem Assume $a_j \sim j^\alpha$, $\alpha \in (0,1)$. Then $\forall \varepsilon > 0$, $\exists \delta > 0$ such that for all large enough Z_0, there exists $h^0 \in X_1$ with $h_j^0 = 0 \ \forall j > Z_0$ satisfying

$$(0 < t < \delta Z_0^{1-\alpha}) \ \ 1 - \varepsilon \quad \le \quad \|e^{Lt} h^0\|_{X_1} \quad \le \quad \varepsilon \ \ (t > \delta Z_0).$$

By consequence $\|e^{Lt}\|_{\mathcal{L}(X_1)} \ge 1 \ \ \forall t > 0$

Method of proof: sub/super-solutions for discrete primitives, Duhamel estimates.

Remark: Our results leave room for improvement...

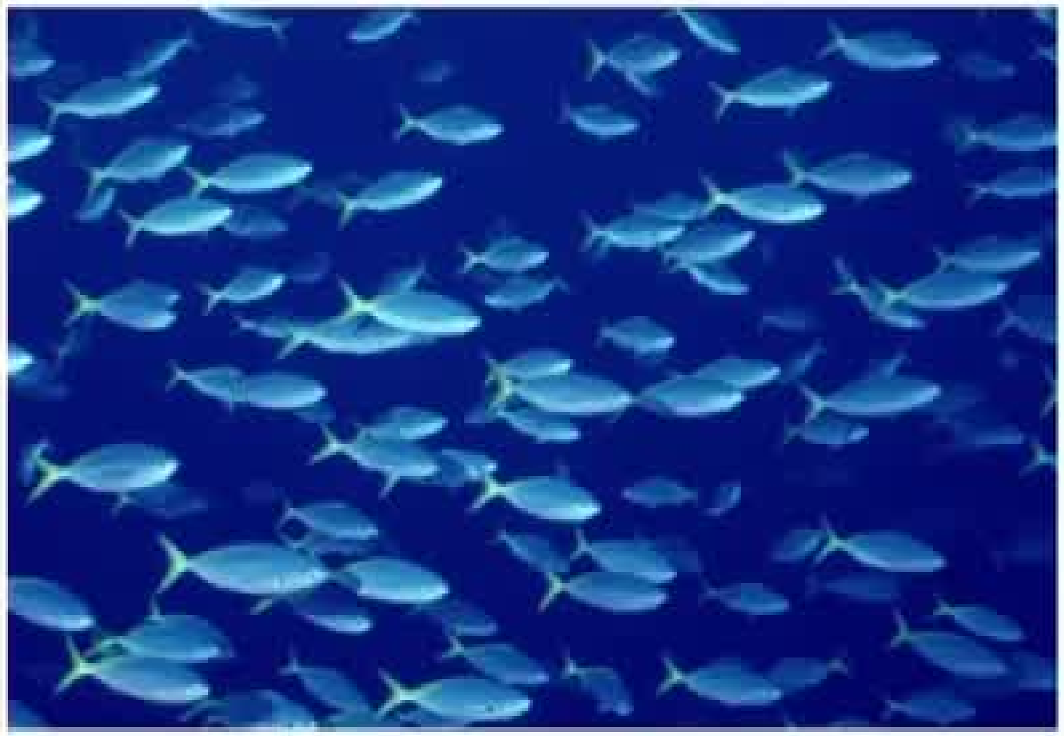
• Animal group size: Universal scaling in fisheries science

H.-S. Niwa (2003 JTB) proposed a simple scaling law for the distribution of group size s:

$$n_{\rm eq}(s) \sim \frac{1}{s_{\rm av}} \Phi\left(\frac{s}{s_{\rm av}}\right)$$

$$s_{\rm av} = \sum s^2 n_{\rm eq}(s) / \sum s n_{\rm eq}(s)$$

= the average group size *experienced by individuals*



- Data analysis for pelagic fish indicate *universal, non-Gaussian* statistics
- SDE model of individual's group size: $dS_t = (\bar{S}_t - S_t)dt + \sigma \exp(S_t/\bar{S}_t)dW$
- Simulated a coagulation-fragmentation process to estimate variance σ
- Solved the SDE to predict: $\Phi(s) = s^{-1} \exp\left(-s + \frac{1}{2} s e^{-s}\right)$

Empirical school-size distribution of pelagic fish

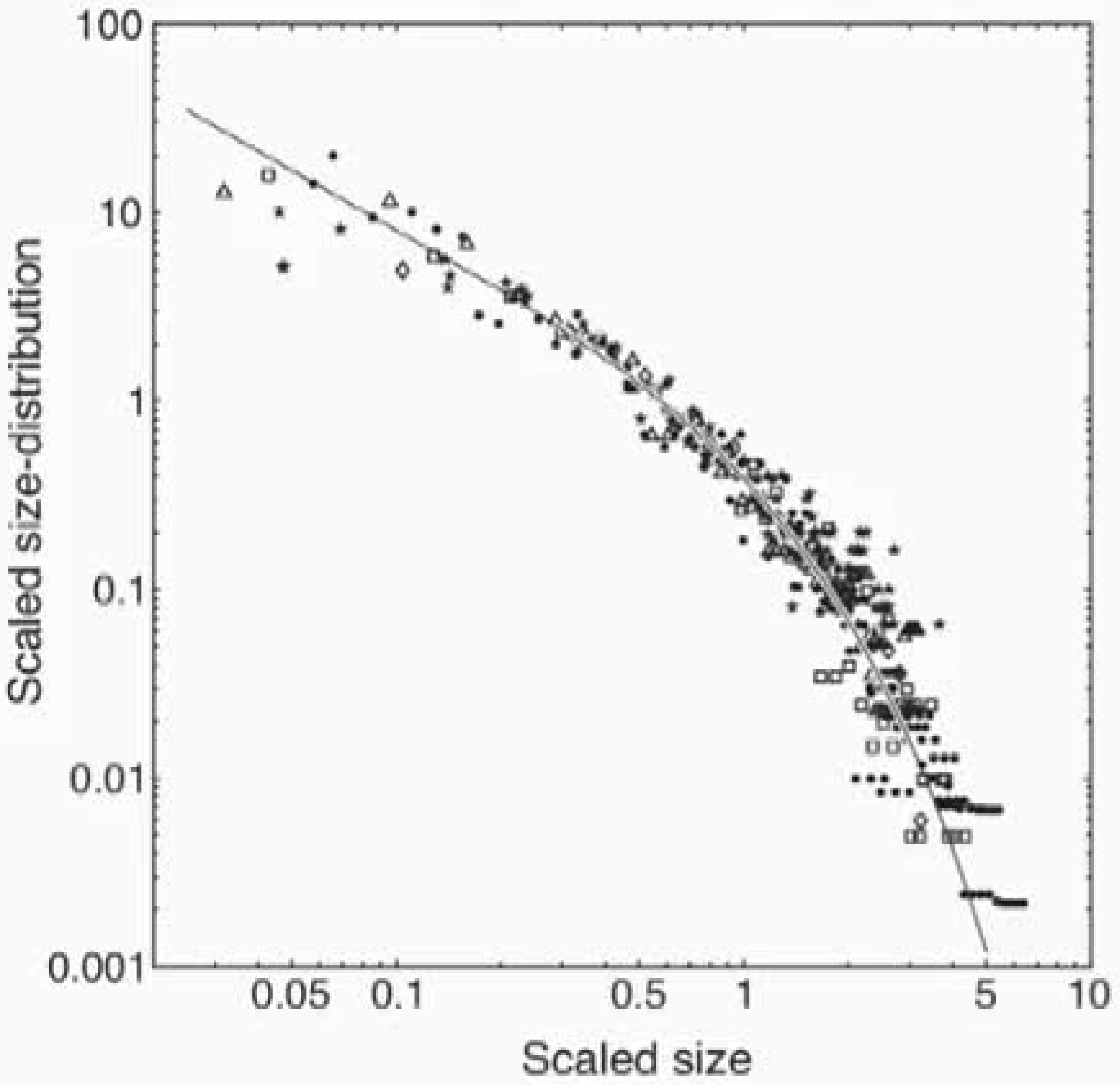


Fig. 5. Empirical school-size distribution of pelagic fishes (the same data sets as Fig. 1). The scaled distributions $W_i\langle N \rangle_P$ are plotted against the scaled school sizes $N_i/\langle N \rangle_P$. The scaled data collapse onto a single curve that corresponds to Eq. (11) with normalization factor Eq. (13).

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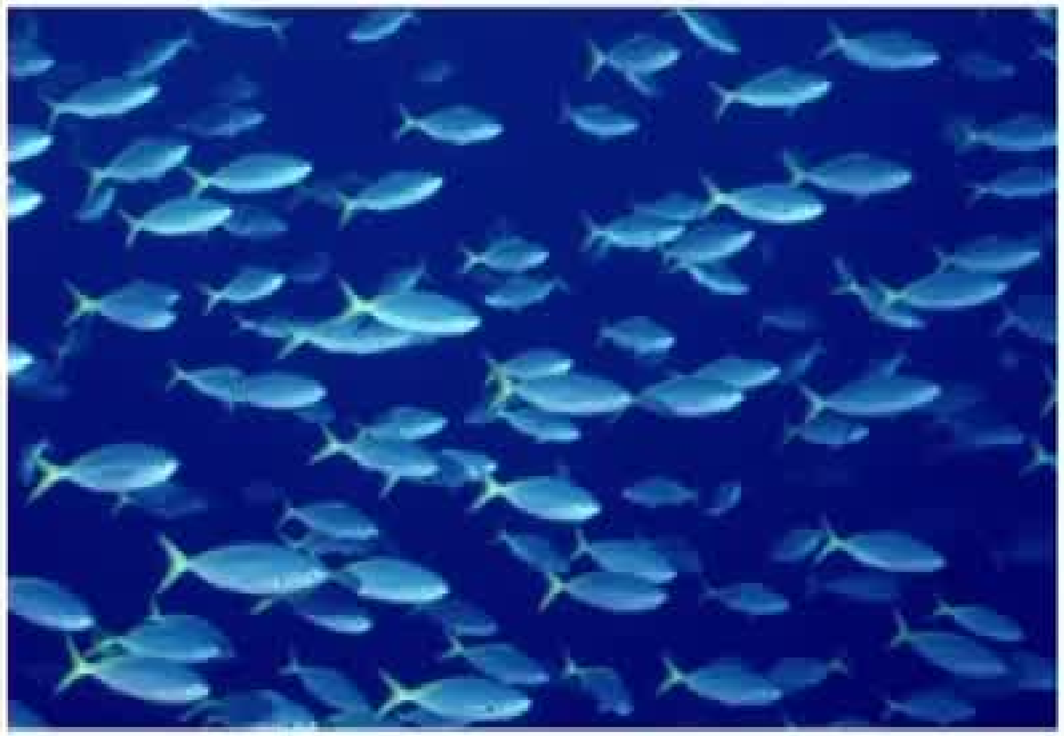

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Empirical school-size distribution of pelagic fish

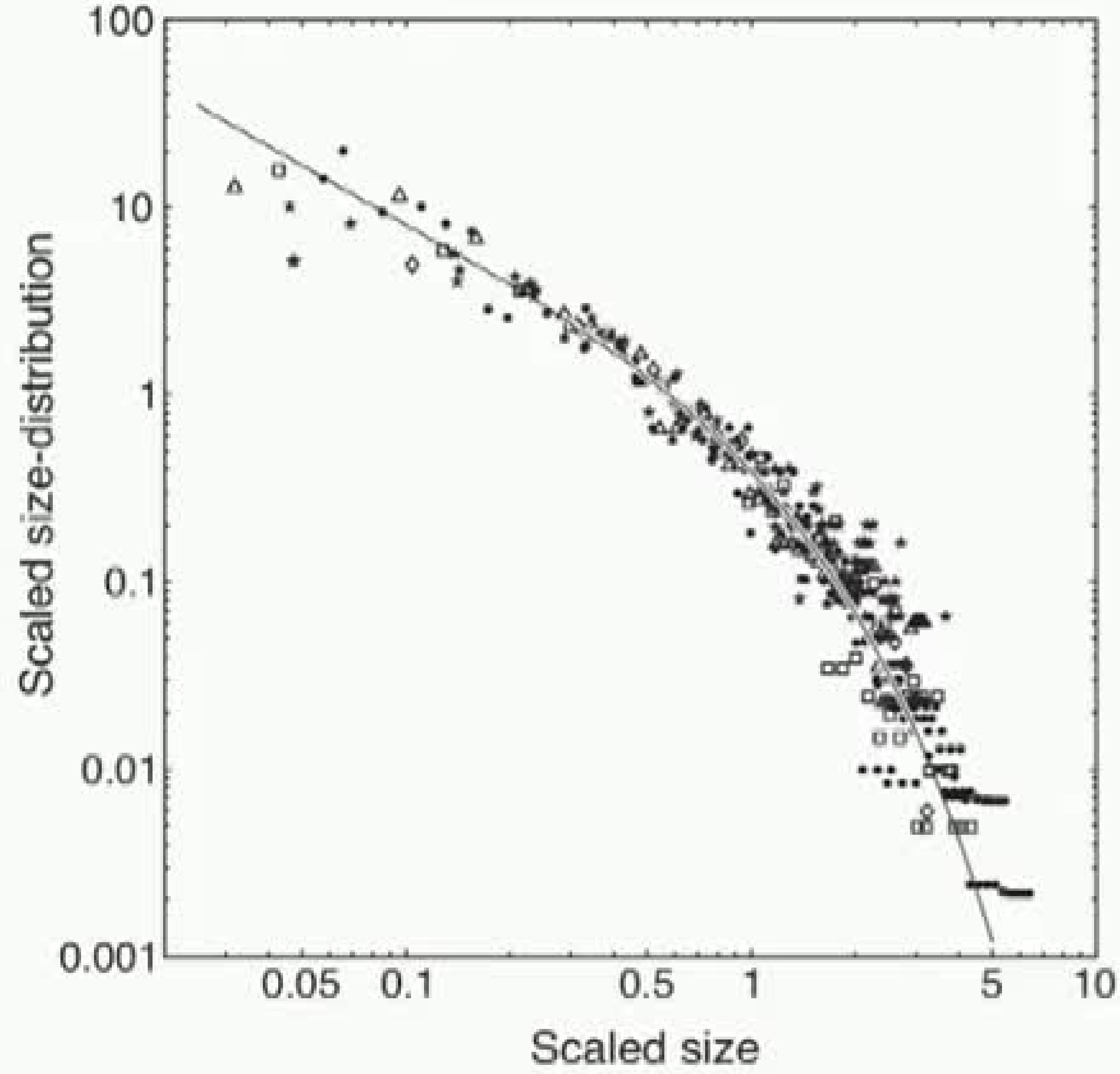


Fig. 5. Empirical school-size distribution of pelagic fishes (the same data sets as Fig. 1). The scaled distributions $W_i\langle N \rangle_P$ are plotted against the scaled school sizes $N_i/\langle N \rangle_P$. The scaled data collapse onto a single curve that corresponds to Eq. (11) with normalization factor Eq. (13).

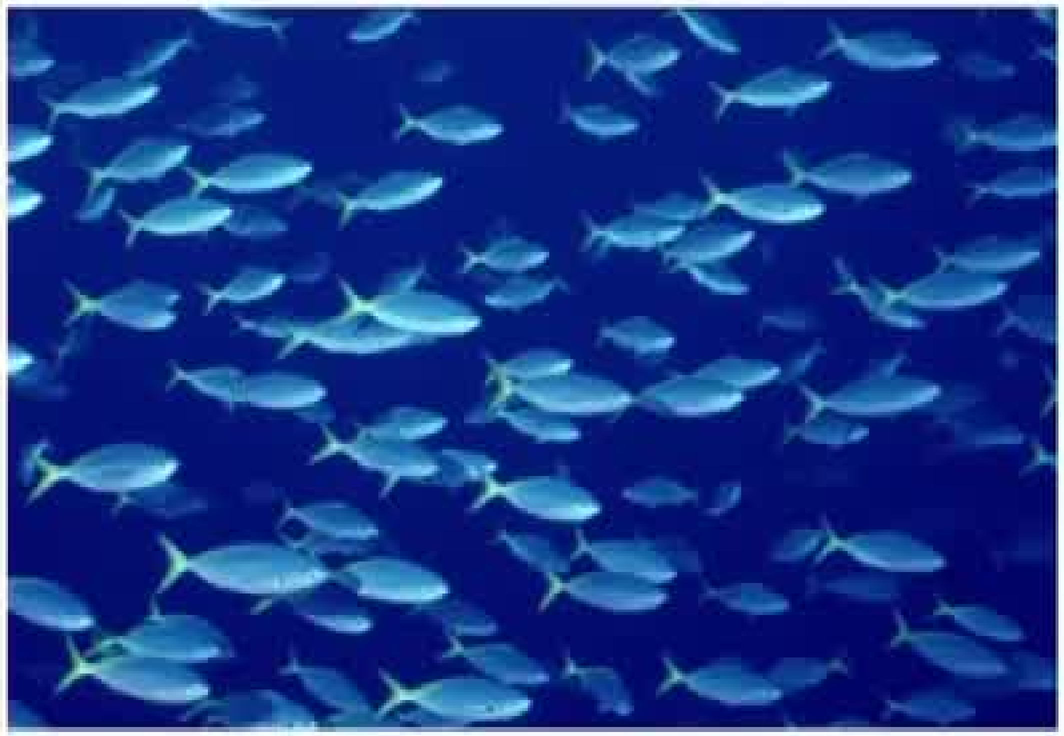
• Animal group size: Universal scaling in fisheries science

H.-S. Niwa (2003 JTB) proposed a simple scaling law for the distribution of group size s:

$$n_{\text{eq}}(s) \sim \frac{1}{s_{\text{av}}} \Phi\left(\frac{s}{s_{\text{av}}}\right)$$

$$s_{\text{av}} = \sum s^2 n_{\text{eq}}(s) / \sum s n_{\text{eq}}(s)$$

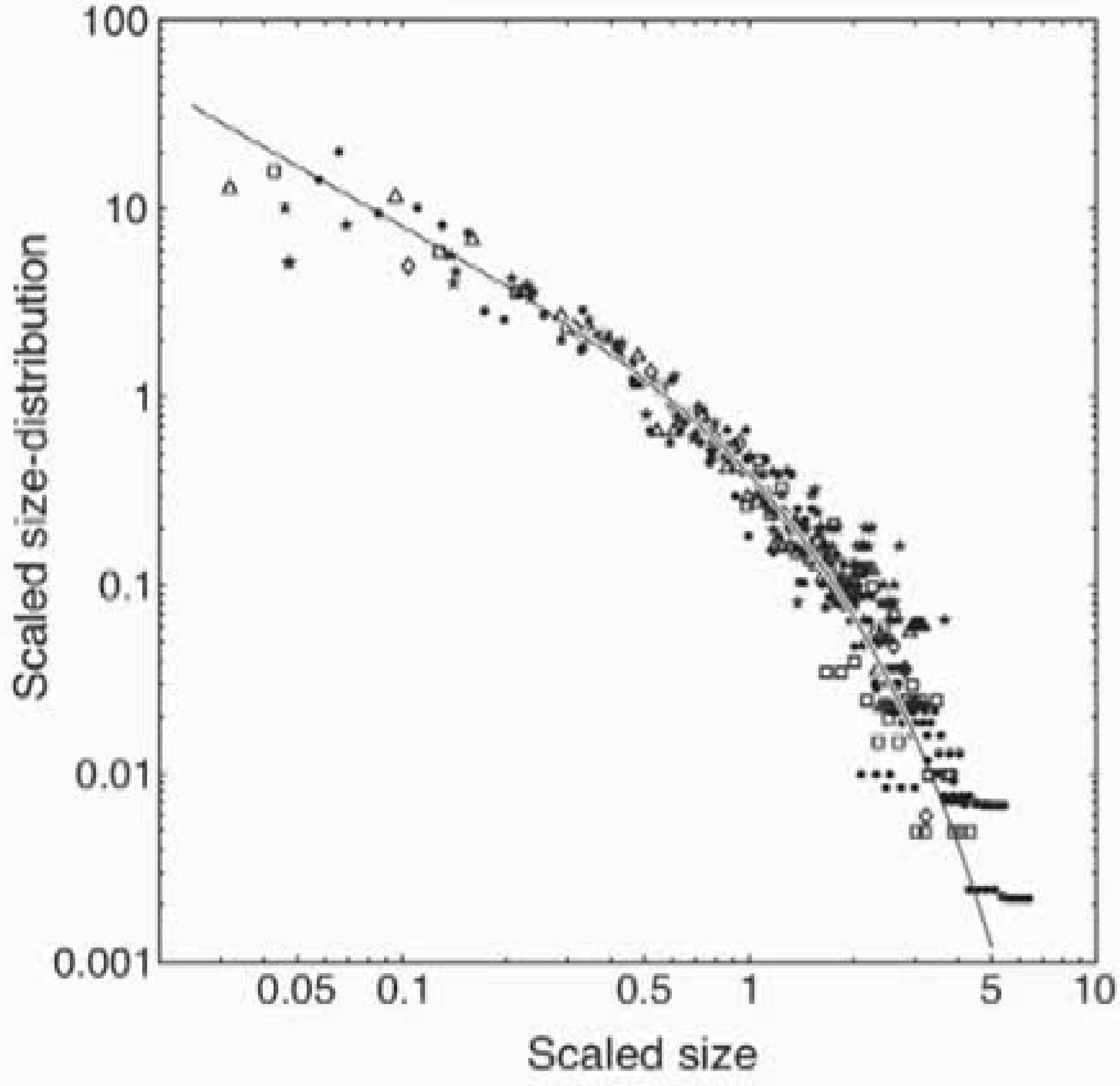
= the average group size *experienced by individuals*



- Data analysis for pelagic fish indicate *universal, non-Gaussian* statistics
- SDE model of individual's group size: $dS_t = (\bar{S}_t - S_t)dt + \sigma \exp(S_t/\bar{S}_t)dW$
- Simulated a coagulation-fragmentation process to estimate variance σ

• Solved the SDE to predict: $\Phi(s) = s^{-1} \exp\left(-s + \frac{1}{2} s e^{-s}\right)$

Empirical school-size distribution of pelagic fish



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Discrete-size coagulation-fragmentation model

(Ma, Johansson, Sumpter 2011)

$$\partial_t c_j(t) = \frac{1}{2}\sum_{k=1}^{j-1} R_{j-k,k} - \sum_{k=1}^{\infty} R_{j,k}, \qquad R_{j,k} = 2c_j c_k - \frac{2c_{j+k}}{j+k-1}$$

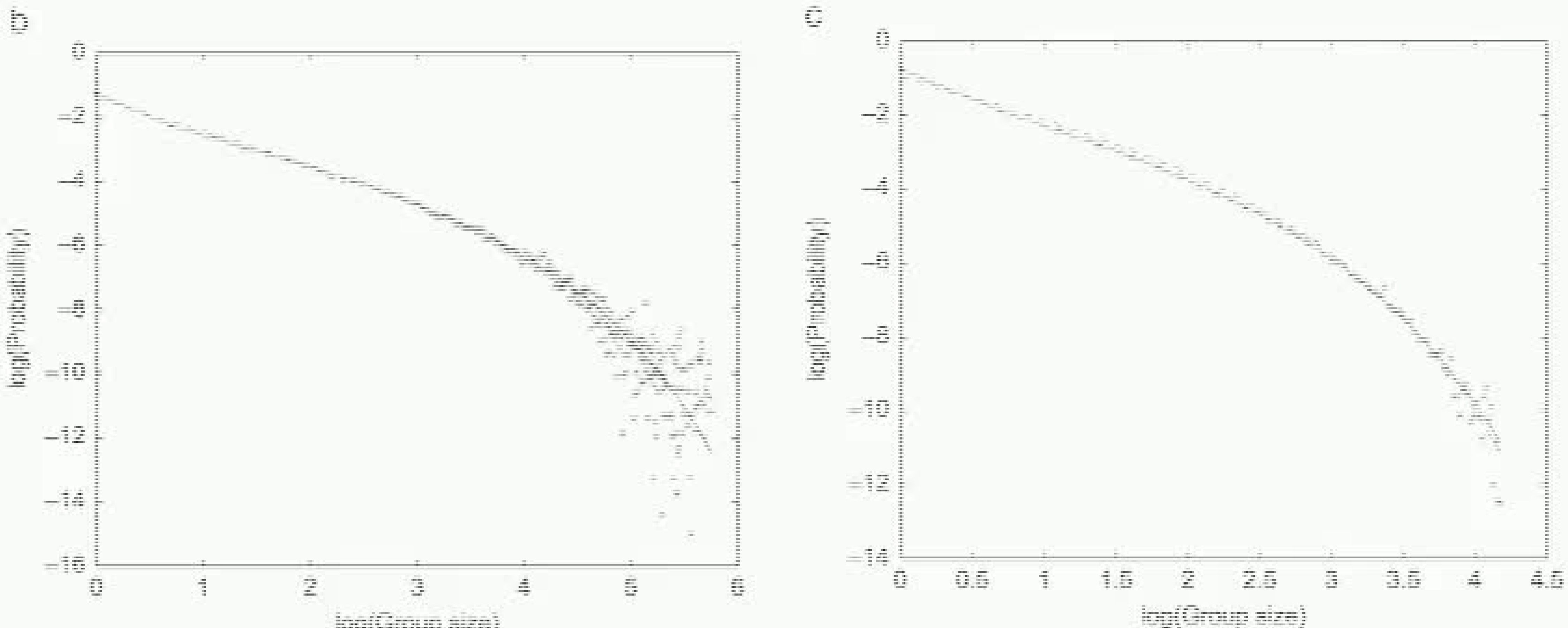


Fig. 2. Comparison of simulated group size distribution (the crosses, with the total population $\Phi = 10\,000$, moving rate $q = 1$, the total number of sites $s = 10\,000$, simulation time step $T = 400\,000$. Every group has size 10 for the initial state), evolution equation iteration (the solid line), and Niwa's distribution as in Eq. (5) (the dashed line). (a) $p = 0.05$, (b) $p = 0.1$, (c) $p = 0.5$, (d) $p = 1$.

The Niwa-MJS model lacks detailed balance–No H-theorem!

- *Open Qs for the Niwa-MJS model:* Unique equilibrium? Stability? $t \to \infty$? (Fournier-Mischler 2004 handle small data)

- Niwa argues explicitly against detailed-balance models of Gueron & Levin (1995)

- An equilibrium $(\hat{c}_j)$ has *detailed balance* if the forward/backward reaction rates balance for each reaction $(j) + (k) \rightleftarrows (j+k)$:

$$0 = R_{j,k} = a_{j,k}\,\hat{c}_j\hat{c}_k - b_{j,k}\,\hat{c}_{j+k}$$

Laurençot-Mischler 2003 (size-continuous models), Cañizo 2008 (size-discrete): If a detailed-balance equilibrium exists, then there is an H-theorem, and all solutions with subcritical mass converge strongly to equilibrium.

Relative free energy $\quad F = \sum_j \hat{c}_j c_1^j (u_j \log u_j - u_j + 1), \qquad u_j = c_j/(\hat{c}_j c_1^j),$

Dissipation $\quad -\partial_t F = D = \sum_j a_{j,1}\hat{c}_j c_1^{j+1}(u_j - u_{j+1})(\log u_j - \log u_{j+1})$

Discrete-size model X (X for Xmas miracle!)

Uniform likelihood among the ~~$j-1$~~ $j+1$ splitting outcomes

$$(0,j),(1,j-1),(2,j-2),\ldots,(j-1,1),(j,0)$$

$$\partial_t c_j(t) = \frac{1}{2}\sum_{k=0}^{j} R_{j-k,k} - \sum_{k=0}^{\infty} R_{j,k}, \qquad R_{j,k} = 2c_j c_k - \frac{2c_{j+k}}{j+k+1}$$

The (discrete) Bernstein transform $\phi(q,t) = \sum_{j=1}^{\infty}(1-e^{-qjh})c_j(t)$ satisfies

$$\partial_t\phi(q,t) = -\phi^2 - \phi + 2A_h(\phi), \qquad A_h(\phi)(q,t) = \frac{h}{1-e^{-qh}}\int_0^q \phi(\hat{q},t)e^{-\hat{q}h}\,d\hat{q}.$$

A nonlocal logistic equation — which transforms exactly to model C below!

In the continuum limit $h \to 0$ we get...

Continuous-size coagulation-fragmentation model C

The distribution $\nu_t(ds) \sim n(s,t)\,ds$ of group size $s \in (0,\infty)$ satisfies $(\forall f)$:

$$\partial_t \int_0^\infty f(s)\,\nu_t(ds) = \int_0^\infty \int_0^\infty \big(f(s+\hat{s}) - f(s) - f(\hat{s})\big)\,\nu_t(d\hat{s})\,\nu_t(ds)$$

$$- \int_0^\infty \int_0^s \,(f(s) - f(s-\hat{s}) - f(\hat{s}))\,\frac{d\hat{s}}{s}\,\nu_t(ds)$$

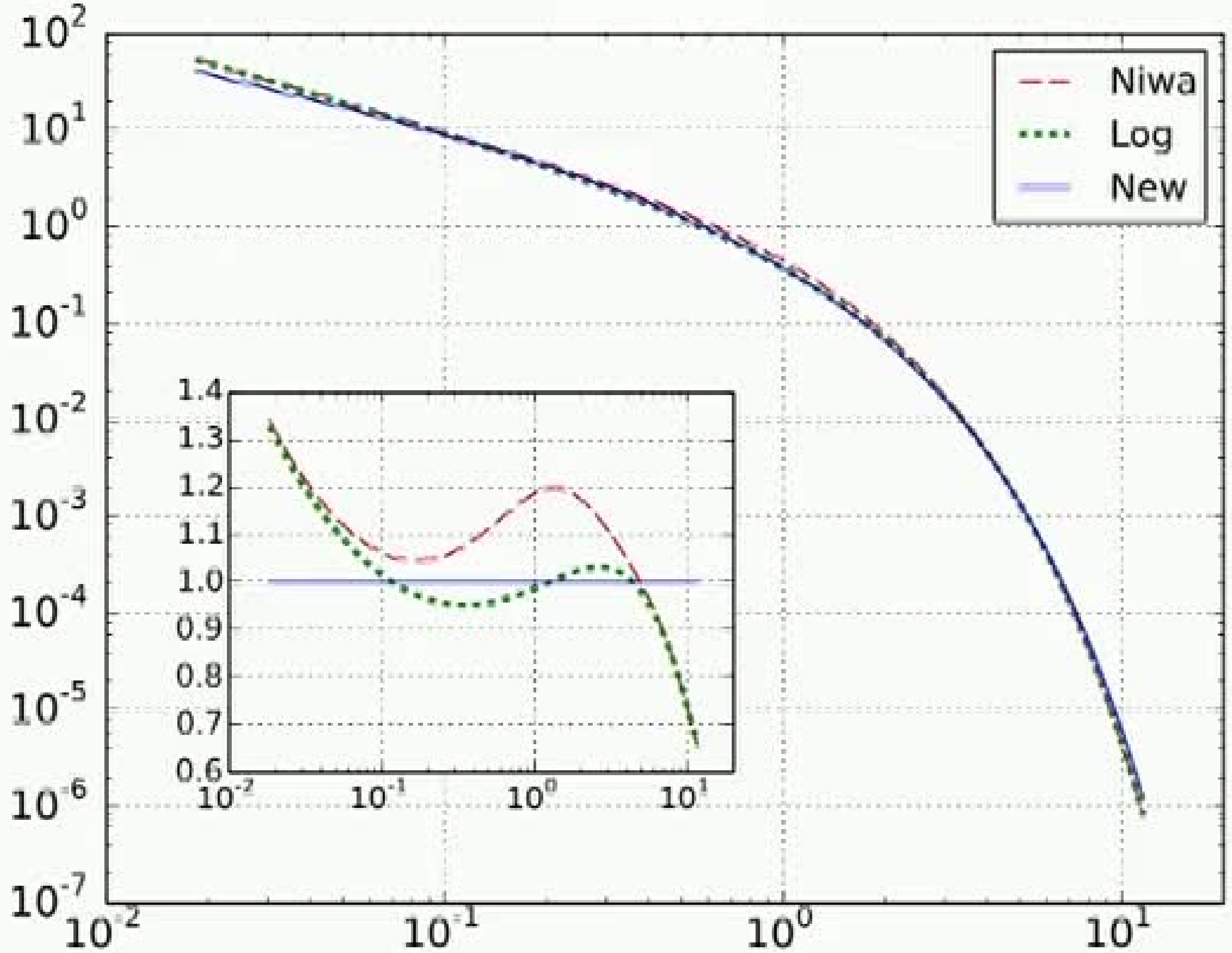
This model has constant coagulation and overall fragmentation rates, with uniform distribution of fragments.

The *Bernstein transform* satisfies a nonlocal logistic equation:

$$\varphi = \int_0^\infty (1-e^{-qs})\nu_t(ds) \quad \Longrightarrow \quad \boxed{\partial_t\varphi = -\varphi^2 - \varphi + \frac{2}{q}\int_0^q \varphi(t,\hat{q})\,d\hat{q}}$$

- *Scaling symmetry:* $\varphi(t,q) \to \varphi(t,Cq)$ leaves the equation invariant.

New universal size-distribution profile



$$n_{\rm eq}(s) = s^{-2/3} \sum_{n=0}^{\infty} \frac{(-1)^n}{3\,\Gamma(\frac{4}{3} - \frac{2}{3}n)} \frac{s^{n/3}}{n!}$$

A theorem from Bernstein function theory, curiously strong

Defn $g : (0,\infty) \to [0,\infty)$ is *completely monotone* if g is C^∞ and

$$\operatorname{sgn} g^{(k)} = (-1)^k \qquad \forall k = 0, 1, 2, \ldots$$

Bernstein's theorem: g is completely monotone $\Leftrightarrow g(s) = \int_0^\infty e^{-sx}\mu(dx)$

CBF Representation Theorem (SSV chap. 6) The following are equivalent:

(i) φ is Bernstein, with $\quad \varphi(q) = a_0 q + a_\infty + \int_0^\infty (1 - e^{-qs})\, \gamma(s)\, ds$

where $a_0, a_\infty \geq 0$ and the density γ is *completely monotone.*

(ii) φ is Bernstein, and holomorphically extends globally to $\mathbb{C} \setminus (-\infty, 0]$, mapping the upper half-plane to itself: $\operatorname{Im} \varphi(q) \geq 0$ for $\operatorname{Im} q \geq 0$.

Remark: (ii) means φ is a *Pick function* analytic and nonnegative on $(0,\infty)$.

Equilibrium states for the continuous-size model C

- **Theorem** For fixed finite $m_1 = \int_0^\infty s\,\nu_t(ds)$ (scaled to $= 1$),

there is a unique equilibrium, having a very nice density:

$$\nu_{\text{eq}}(ds) = n_{\text{eq}}(s)\,ds = \gamma(s)\exp\left(\frac{-4s}{27}\right)ds$$

where γ is *completely monotone* and satisfies

$$\gamma(s) \sim \frac{1}{3\,\Gamma(4/3)}\,s^{-2/3} \qquad \text{as } s \to 0,$$

$$\gamma(s) \sim \frac{9}{8\,\Gamma(1/2)}\,s^{-3/2} \qquad \text{as } s \to \infty.$$

Long-time behavior of Model C

- **Theorem** (i) Suppose $\int_0^\infty s\,\nu_0(ds) = 1$. Then (weakly-$\star$ on $[0,\infty]$)

$$(s\wedge 1)\nu_t(ds) \stackrel{\star}{\rightharpoonup} (s\wedge 1)\nu_{\mathrm{eq}}(ds) \qquad \text{as } t\to\infty.$$

(ii) Suppose $\int_0^\infty s\,\nu_0(ds) = \infty$. Then (weakly-$\star$ on $[0,\infty]$)

$$(s\wedge 1)\nu_t(ds) \stackrel{\star}{\rightharpoonup} \delta_\infty \qquad \text{as } t\to\infty.$$

Method of proof: Prove $\varphi(q,t)\to\varphi_{\mathrm{eq}}(q)$, using comparison principles

$$\varphi(q,t_0)\le\hat\varphi(q,t_0) \implies \varphi(q,t)\le\hat\varphi(q,t)$$

Invoke Bernstein-transform continuity theorem.

Scaling limits with fat tails

(with J.-G. Liu and B. Niethammer, in preparation)

- **Theorem** (Self-similar spreading solutions for model C)

For each $\alpha \in (0,1)$ model C admits a *unique self-similar solution*

$$\nu_t(ds) = \hat{\nu}_\alpha(e^{-\beta t}ds) \quad \text{with} \quad \int_0^s z\,\hat{\nu}_\alpha(dz) \sim \frac{s^{1-\alpha}}{1-\alpha} \ (s \to \infty).$$

The measure $\hat{\nu}_\alpha$ has a *completely monotone density* f_α satisfying

$$f_\alpha(s) \sim s^{-\alpha-1} \ (s \to \infty), \qquad \hat{c}_\alpha s^{-\hat{\alpha}} \ (s \to 0).$$

- **Theorem** (Large-t behavior with algebraic tails) Suppose the initial data

$$\int_0^s z\,\nu_0(dz) \sim \int_0^s z\,\hat{\nu}_\alpha(dz) \quad (s \to \infty).$$

Then on $[0,\infty]$ we have $\quad \nu_t(e^{\beta t}ds) \xrightarrow{\star} \hat{\nu}_\alpha(ds), \quad t \to \infty.$

Discrete analog of the CBF representation theorem

Definition $c = (c_n)_{n=0}^{\infty}$ is a completely monotone sequence if its differences alternate sign: $\forall k, \quad \operatorname{sgn}(S-I)^k c_j = (-1)^k, \quad (Sc)_j = c_{j+1}$.

- **Theorem** (Hausdorff) c is completely monotone $\iff$ $c_n = \int_0^1 t^n \, d\mu(t)$ for some finite measure $d\mu$ on $[0,1]$.
- **Theorem** (Liu-Pego) Let $c = (c_n)_{n=0}^{\infty}$ be a bounded real sequence, and

$$F(z) = \sum_{n=0}^{\infty} c_n z^n, \qquad F_1(z) = zF(z) = \sum_{n=0}^{\infty} c_n z^{n+1}.$$

Then the following are equivalent:

(i) c is completely monotone

(ii) F is a Pick function analytic and nonnegative on $(-\infty, 1)$

(iii) F_1 is a Pick function analytic on $(-\infty, 1)$

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Infinite divisibility, convolution groups

• **Theorem** If (c_j) is a probability distribution on $\mathbb{N}_0$ and (c_j) is completely monotone, then (c_j) is *infinitely divisible.*

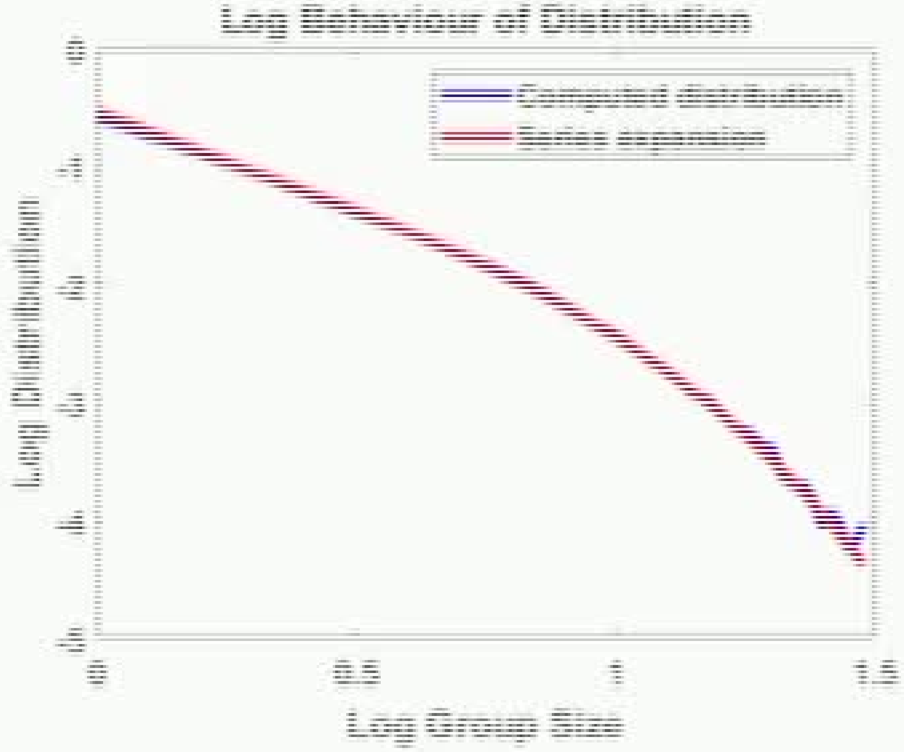
Proof: For any $n \in \mathbb{N}$, c can be expressed as an n-fold convolution $c = a^{*n}$ of the sequence $a = (a_j)$ with generating function $A(z) = F(z)^{1/n}$.

Because $z \mapsto z^{1/n}$ is a Pick function and F is Pick and nonnegative on $(-\infty, 1)$, the composition A is Pick and nonnegative on $(-\infty, 1)$.

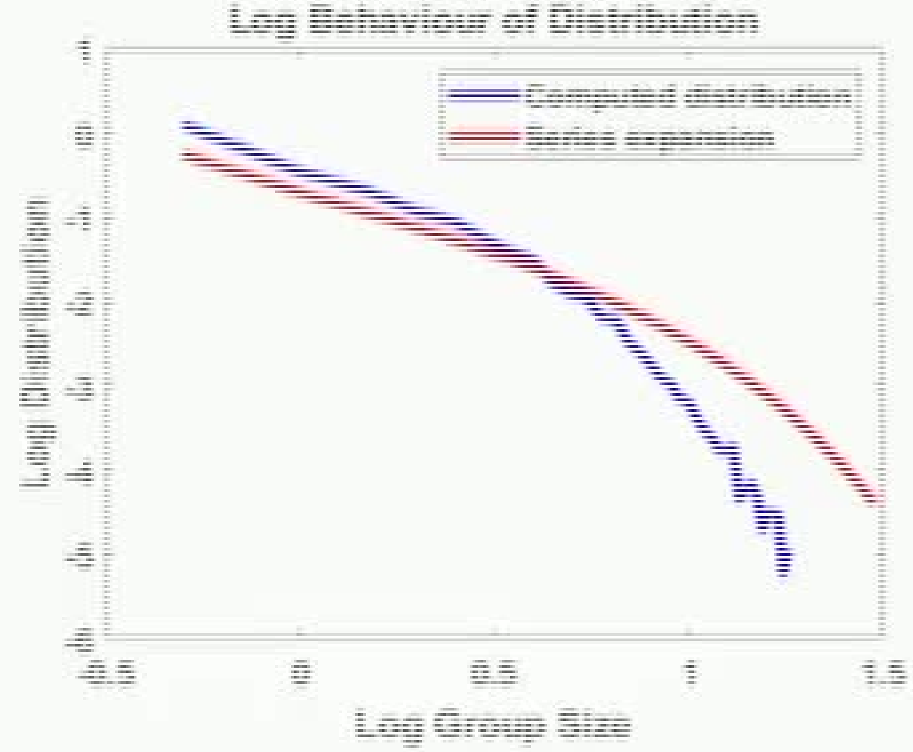
• The map $t \mapsto F(z)^t$ $(t \in \mathbb{R})$ determines a *convolution group* of sequences $a^{(t)}$ with generating functions $A^{(t)}$ satisfying

$$A^{(t)}(z) = F(z)^t, \quad a^{(t)} * a^{(s)} = a^{(t+s)}.$$

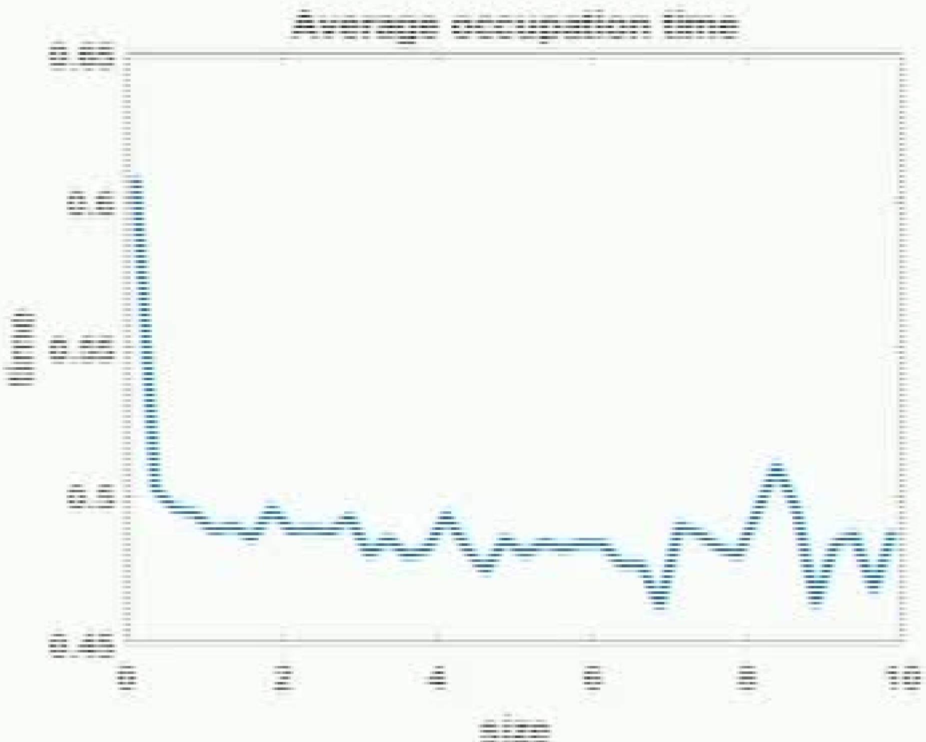
• Li-Liu 2018, Li-Liu-Feng-Xu 2018:
– structure theorem for the deconvolving sequence $a^{(-1)}$.
– desingularized Caputo fractional derivative with Gronwall estimates



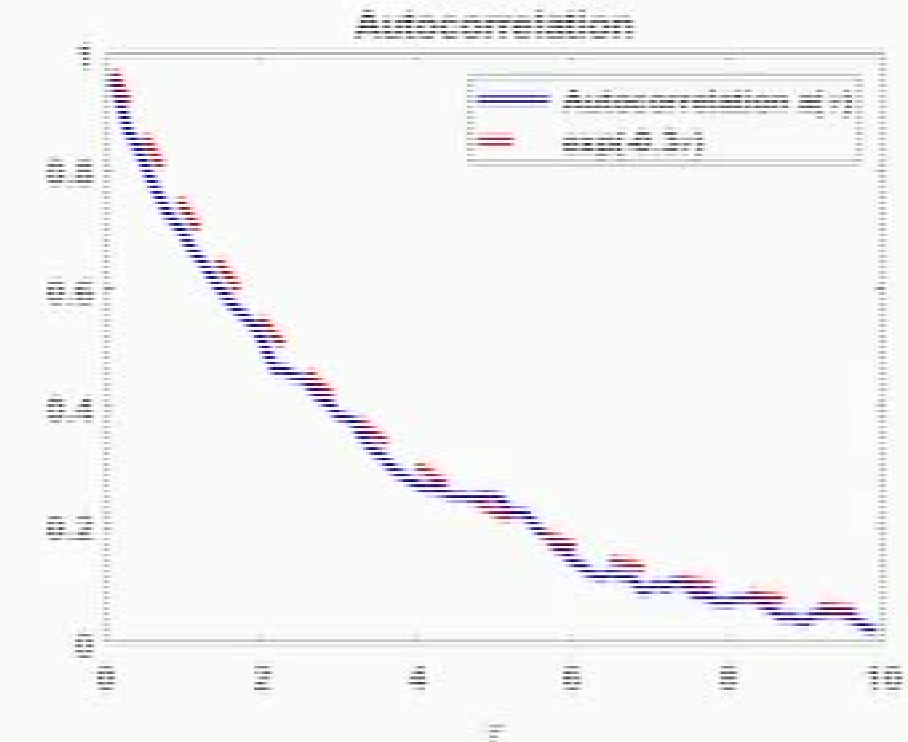
(a) Compare series, $N = 10^4$, $t = 20$



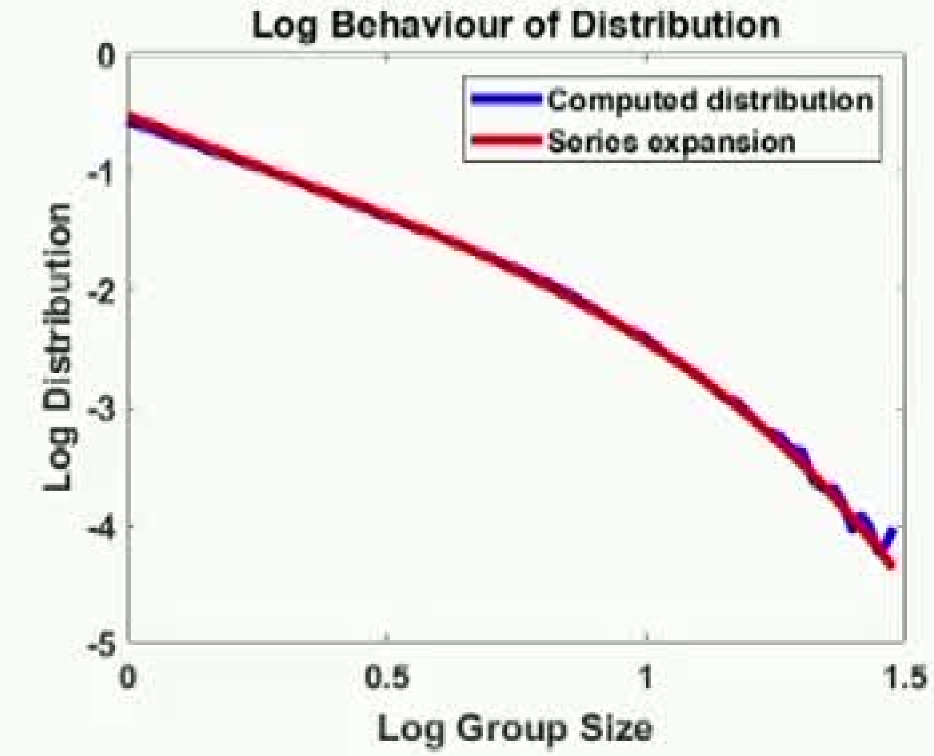
(b) Random rates, $N = 2 \cdot 10^4$, $t = 20$



(c) Occupation time, $t \in [0, 10^7]$



(d) Autocorrelation, $N = 10^7$



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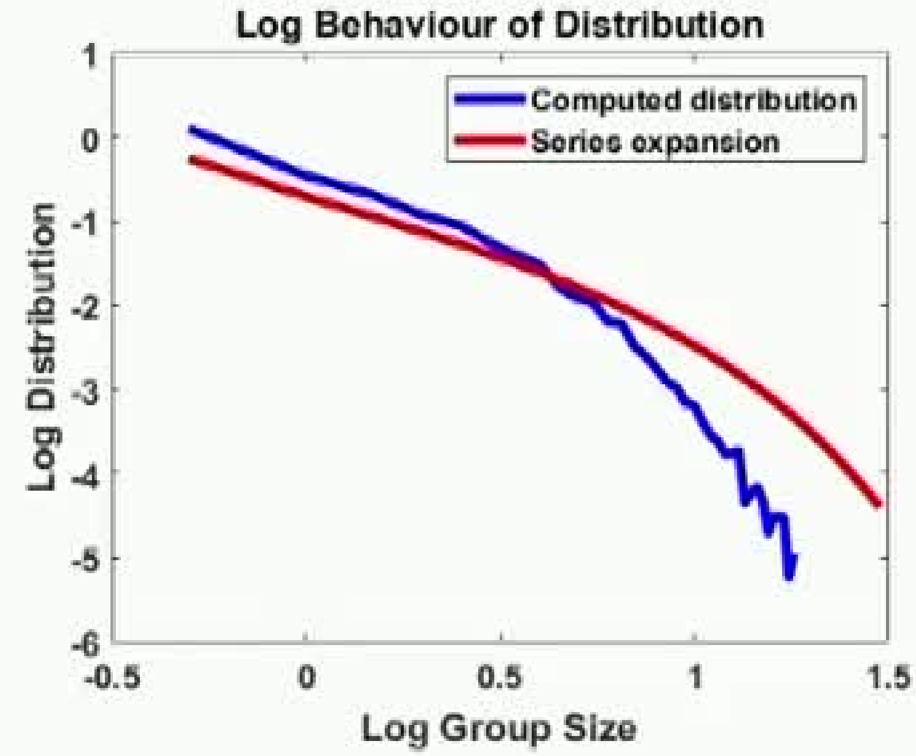

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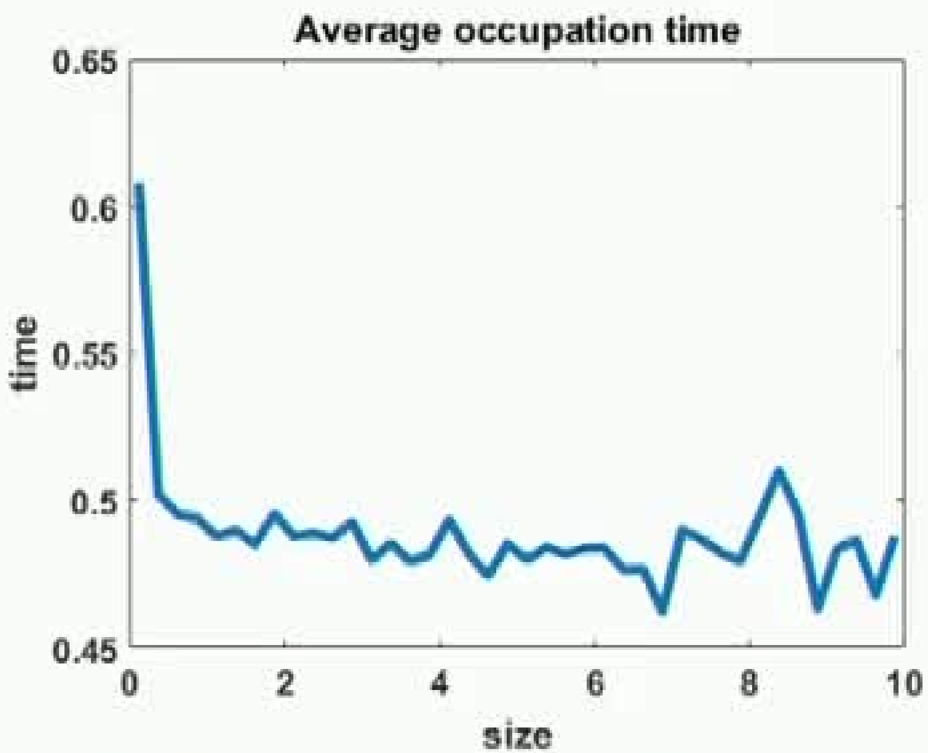
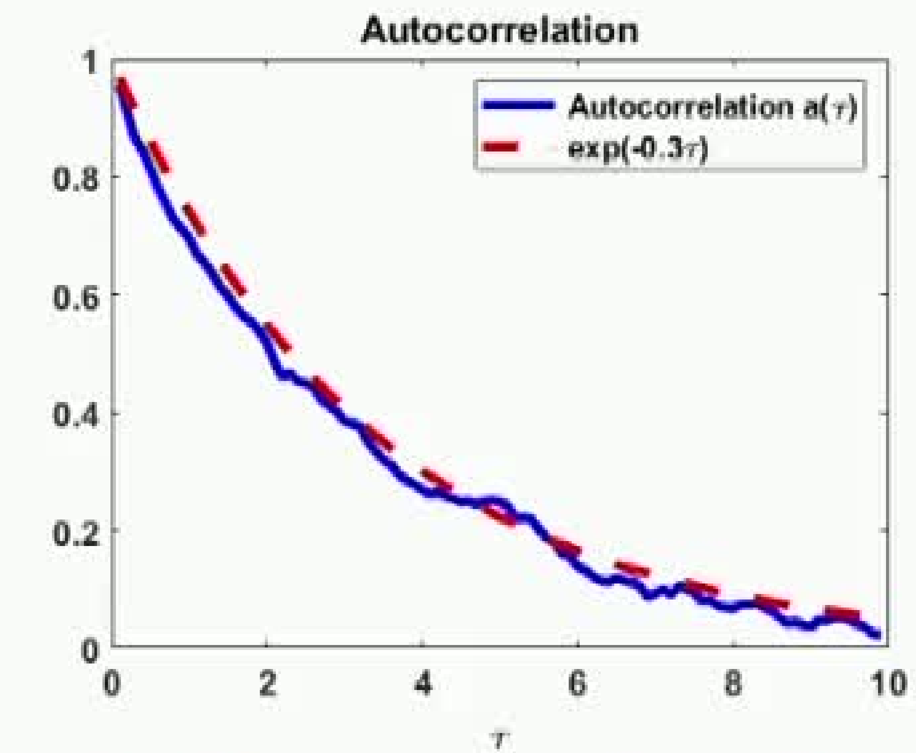


(c) Occupation time, $t \in [0, 10^5]$



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