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Sampling Rare Events: Efficient Simulation of Fractional Brownian Motion

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Sampling rare events: Efficient simulation of fractional Brownian motion

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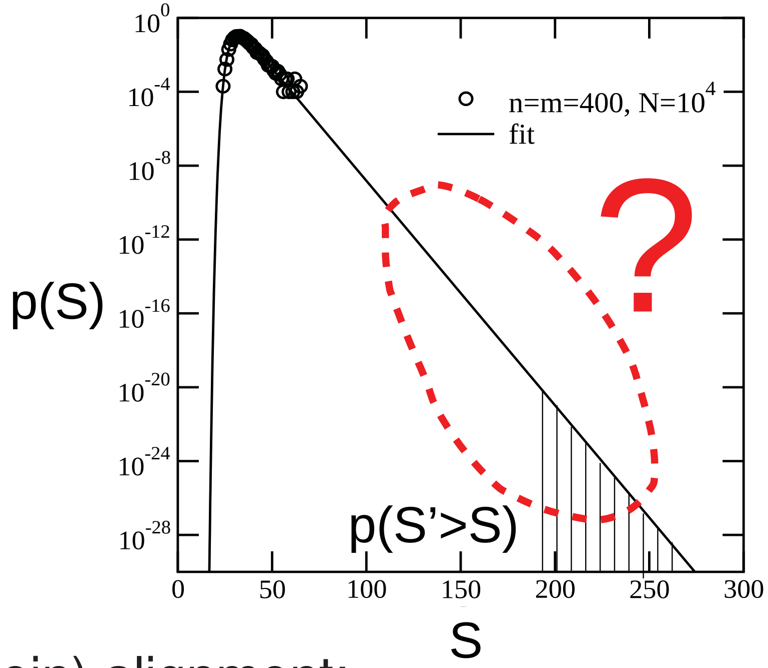
Outline

- Fractional Brownian Motion
- Sampling Algorithm
- Results for $H = 1/2,\ 2/3,\ 1/4$

Large-deviation properties

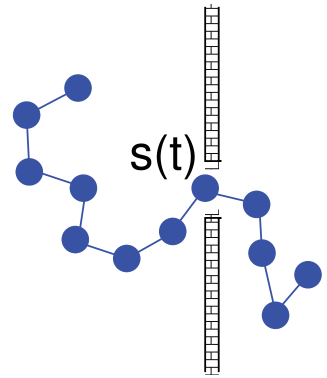
- Typical properties (probabilities $10^{-6}..1$): easy to get by simple sampling simulations
- Sometimes wanted: large deviation properties



- Examples:
  - Biological sequence (protein) alignment: small-probability (significant) scores [AKH, PRE 2001][...]
  - Distribution of ground-state energies of random magnets [M. Körner, H.G. Katzgraber, AKH, JSTAT 2006]
  - Distribution number/size of components of random graphs [A. Engel, R. Monasson, AKH, J. Stat. Phys. 2004][AKH 2011]
  - Calculation of partiction functions in statistical mechanics [AKH, Phys. Rev. Lett. 2005]

Fractional Brownian Motion

- Translocation of polymer through pore:
  viral injection of DNA
  $s(t)$: position of chain at time t
  $s(t > 0) = 0$: absorbing boundary



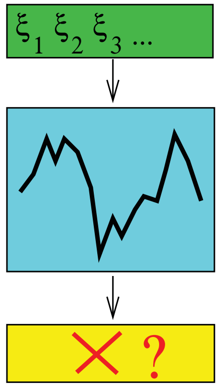
- Proposal [Zoia, Rosso, Majumdar, PRL 2009]:
  Described by fractional Brownian motion = Gaussian process with

$$\langle s(t_1)s(t_2)\rangle \sim t_1^{2H} + t_2^{2H} - |t_1 - t_2|^{2H}$$

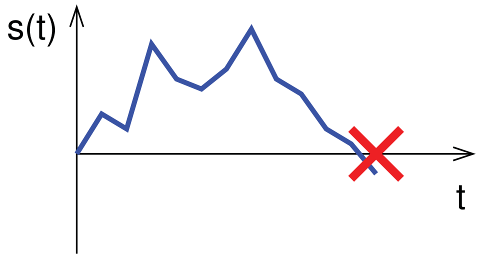
- H: Hurst exponent: $H = 1/2$: Brownian motion,
  $H > 1/2$: correlation, $H < 1/2$: anticorrelation
  ($H = 1/(1-\nu)$, where $R_g \sim N^\nu$ [Chuang, Kantor, Kadar 2001])
- Rescaled variable: $y(t) = s(t)/t^H$
  Prediction for $y \to 0$: $P(y) \sim y^\phi$ with $\phi = (1-H)/H$

Random Walks

- Traditional method for (non-absorbed) walks of length L
  1. Vector ξ of $\tilde{L} \geq L$ Gaussian random numbers ξ_i
  2. For (approximate) correlation: Fourier transform
  3. Create walk $s(t) = \sum_{i<t} \xi_i$
  4. Accept if $s(t) \geq 0$ for all t (non absorbed)



- Problem: Success probability of non absorbance (*persistence*) $\sim t^{-\theta} \quad (\theta = 1 - H)$

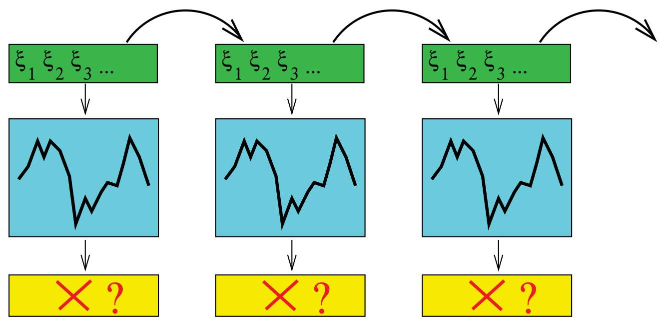


$L =$	10^1	10^3	10^5	10^7
$H = 2/3\ \theta = 1/3$	0.5	0.1	$2 \cdot 10^{-2}$	$5 \cdot 10^{-3}$
$H = 1/2\ \theta = 1/2$	0.3	0.03	$3 \cdot 10^{-3}$	$3 \cdot 10^{-4}$
$H = 1/4\ \theta = 3/4$	0.2	0.006	$2 \cdot 10^{-4}$	$6 \cdot 10^{-6}$

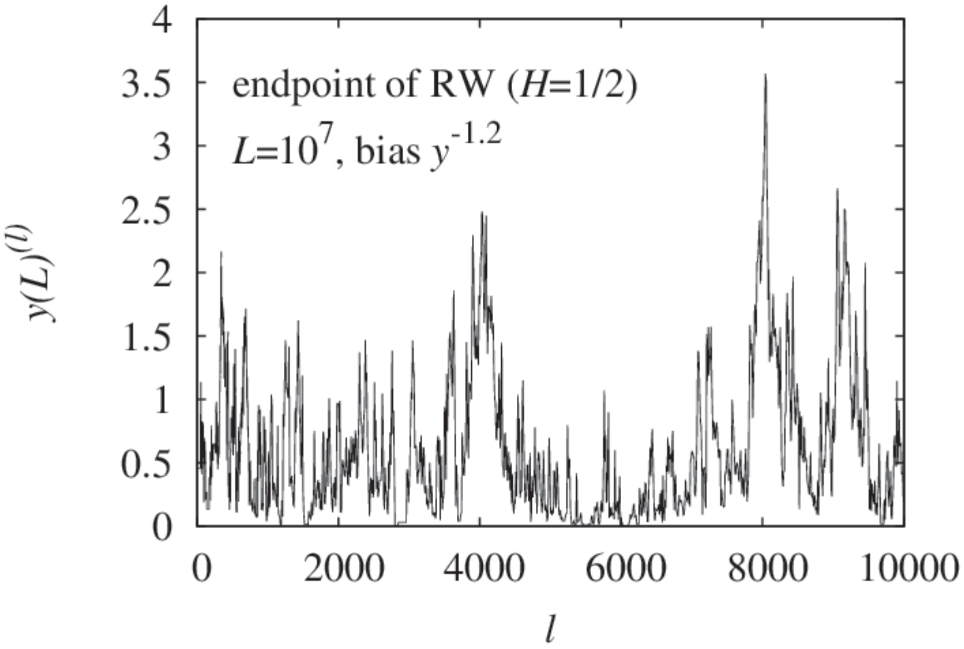
$\rightarrow$ becomes unefficient

Monte Carlo approach

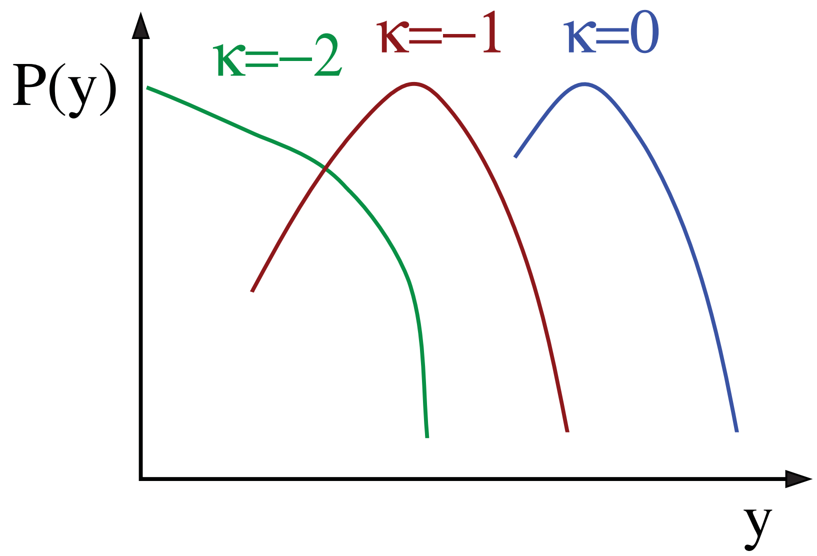
- Basic idea:
  Markov chain of vectors
  $\xi^{(0)} \to \xi^{(1)} \to \xi^{(2)} \to \dots$
  step: change fraction of $\xi^{(l)}$
  accept if walk not absorbed



- Possible: additional reweighting $w \sim y^{\kappa}$ ($\kappa = -\phi \to$ "flat" sampling near $y = 0$)



Distribution of Endpoints



- Raw result $\longrightarrow$ (simple $\leftrightarrow \kappa = 0$) at low κ: small endpoints prefered
- MC moves: $\xi \to \xi'$ change of displacement $\to$ original probability $P_0(\xi)$, additionally: $\Pr(\text{acceptance}) = \min\{1, (y(\xi')/y(\xi))^\kappa\}$
- $\Rightarrow$ equilibrium distribution $Q_\kappa(\xi) = P_0(\xi) y(\xi)^\kappa / Z(\kappa)$

  with $P_0(\xi) =$ Gaussian etc, $Z(\kappa) = \sum_\xi P_0(\xi) y(\xi)^\kappa$

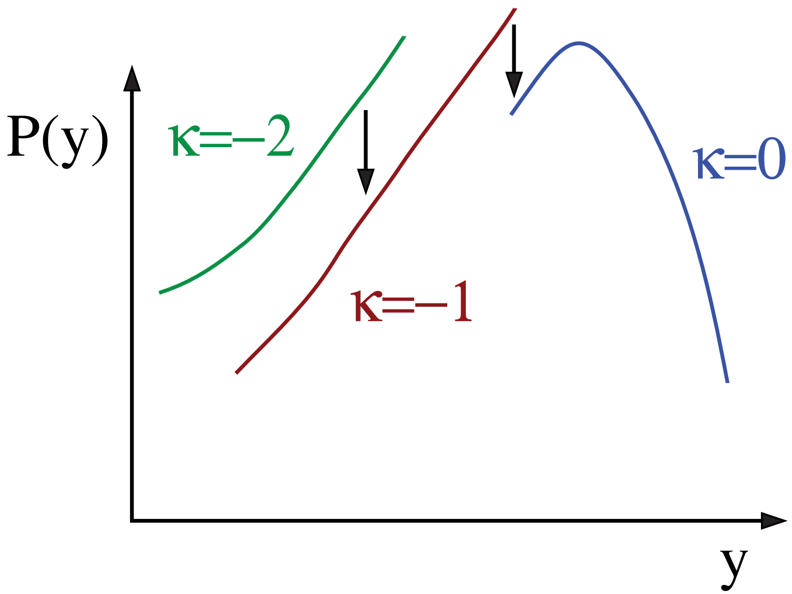
  $\Rightarrow \; p_\kappa(y) = \sum_{\xi, y(\xi)=y} Q_\kappa(\xi) = \frac{y^\kappa}{Z(\kappa)} \sum_{\xi, y(\xi)=y} P_0(\xi)$

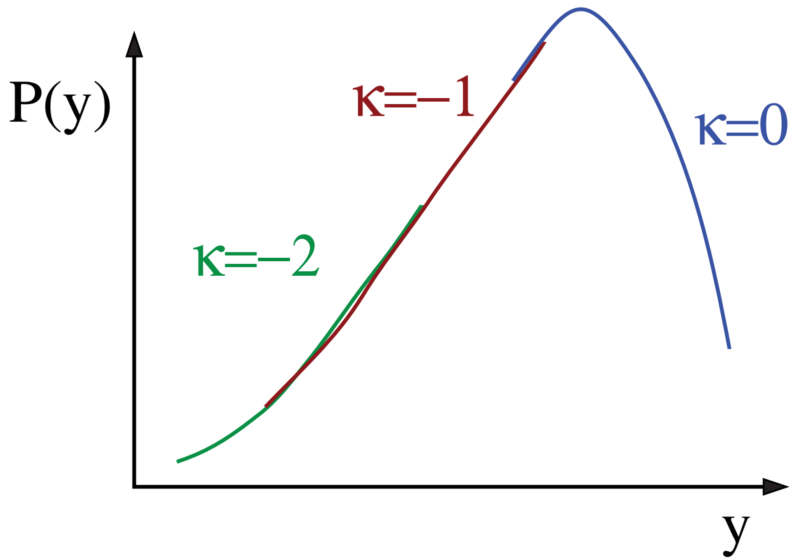
  $\Rightarrow \quad P(y) = p_\kappa(y) Z(\kappa) y^{-\kappa}$ [AKH, PRE 2001]

$$\left[\ P(y) = p_\kappa(y) Z(\kappa) y^{-\kappa})\ \right]$$

rescaling with $y^{-\kappa}$

$Z(\kappa)$ by “matching”



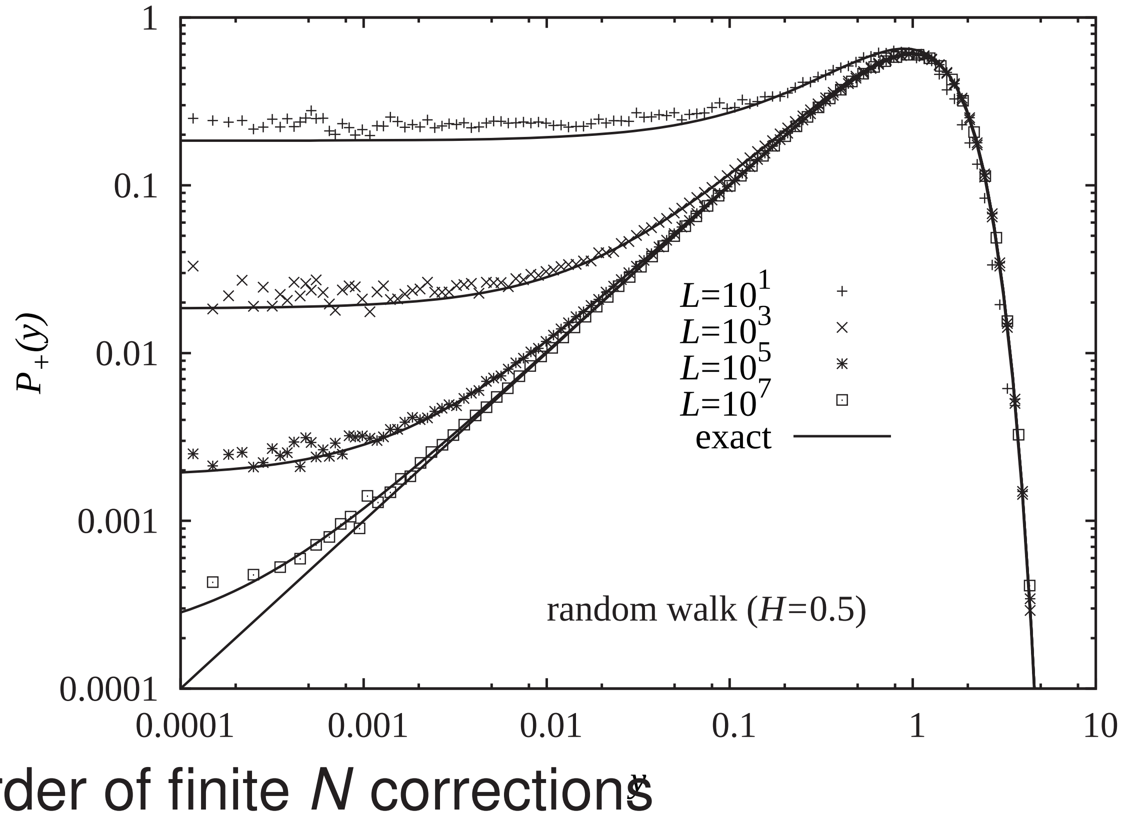


Results

Testcase pure Brownian motion ($H = 0.5$)

$N \to \infty$ distribution known [Zoia, Rosso, Majumdar, PRL 2009]

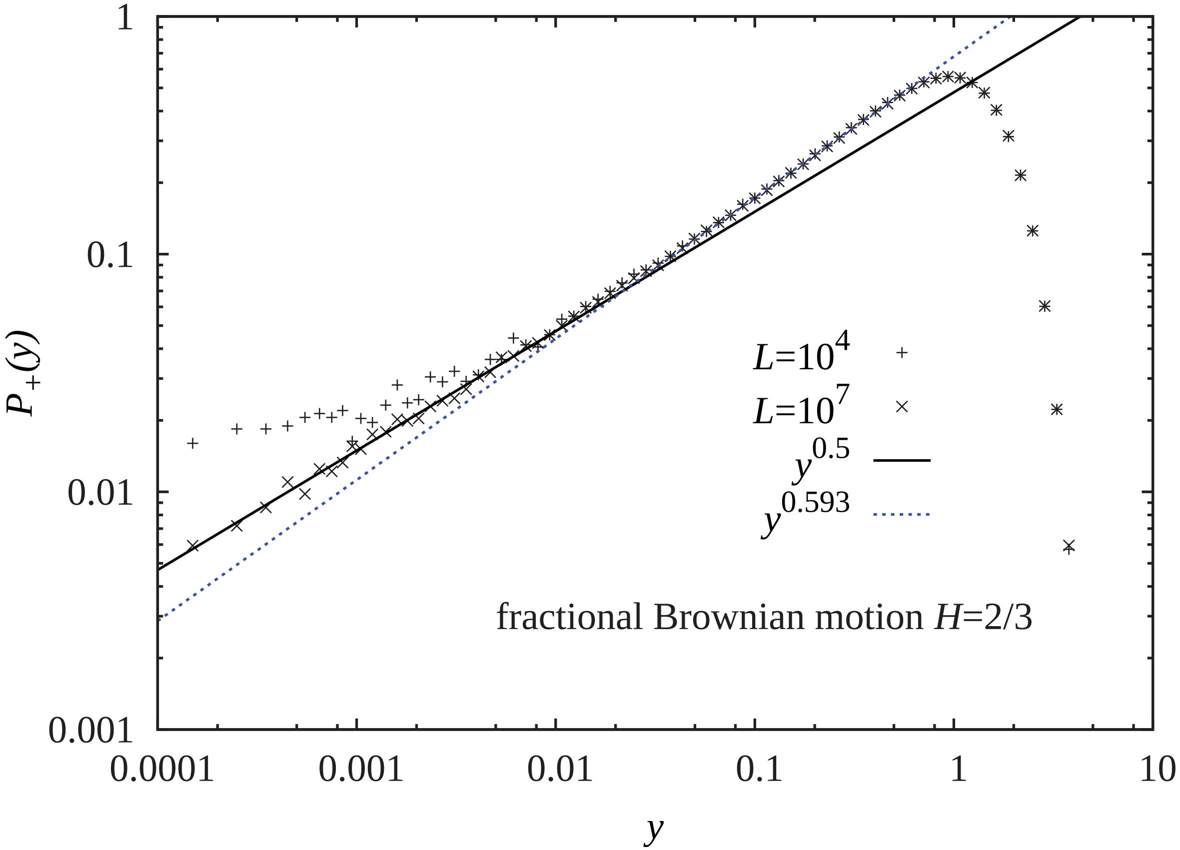
$$P(y) = y \exp(-y^2/2)$$



Leading order of finite N corrections

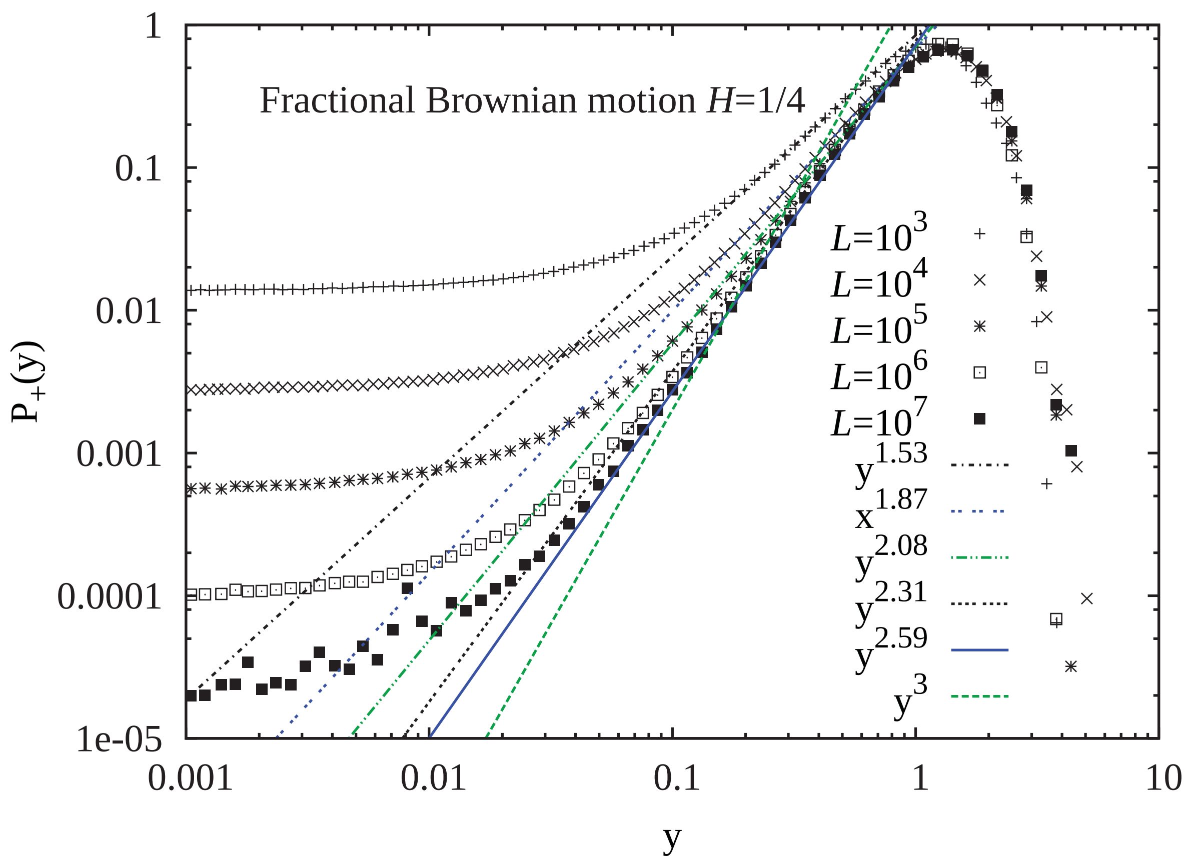
[AKH, S.N. Majumdar, A. Rosso, arXiv:1303.1648]

Superdiffusive case ($H = 2/3$)



$\longrightarrow$ prediction $\phi = (1 - H)/H = 1/2$ well found ($y \to 0$)
confirmed medium-scale behavior y^γ ($\gamma > \phi$)
predicted by [Wiese, Rosso, Majumdar, PRE 2012]

Subdiffusive case ($H = 1/4$)



$\longrightarrow$ strong finite-length effects
converges towards prediction $\phi = (1 - H)/H = 3$ ($y \to 0$)
in contrast to prediction $\phi = 2$ [Amitai, Kantor, Kadar, PRE 2010]
(simulation of effective model for $N = 257$ coupled particles)

Summary

- Large-deviation properties
- Markov chain approach:
  dynamics of walks determined by vector of random numbers
  restricted to region of interest
  focus on low probabilities via reweighting
- Study fractional Brownian motion in high-correlation region for long walks $L = 10^7$

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  A.K. Hartmann, Practical Guide to Computer Simulations (World Scientific, 2009)
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Thank you for your attention !