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Residence time and collision number statistics: a Feynman-Kac approach

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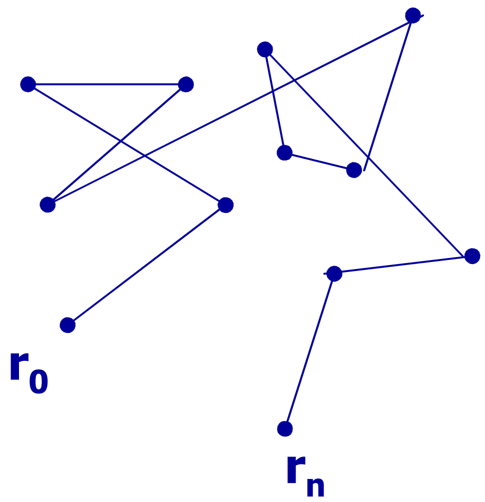
Outline

- Introduction
- Stochastic transport: random flights
  - Collision number statistics and diffusion limit
  - Exponential flights and residence time statistics
- Conclusions

- Foreword*: joint work with* Eric Dumonteil *and* Alain Mazzolo *at* LTSD *laboratory, CEA/Saclay*

Stochastic transport

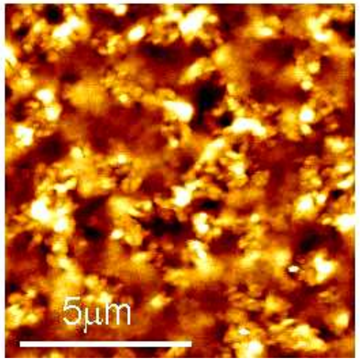
- **Random flights** (Pearson's random walk, 1905)
  - Straight line 'flights' (random length)
  - Collisions
    - Scattered with probability p
    - Absorbed with probability 1-p



- **Renewal** process with reorientation and reward
- Deceivingly simple: many open questions…

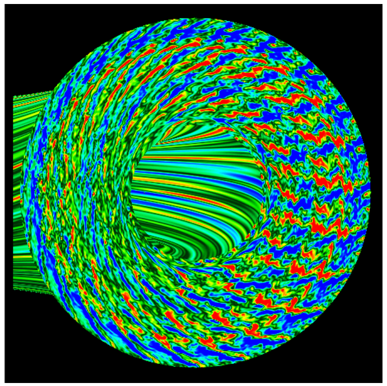
Examples of random flights

Neutron/photon flux

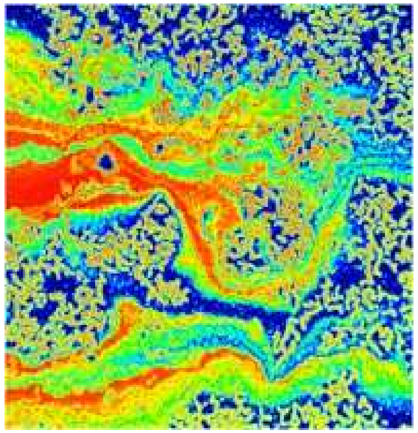


Charge transport

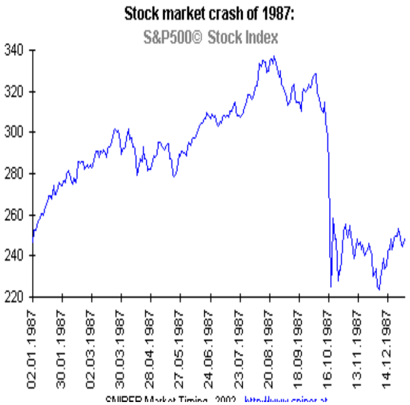
Search strategies



Plasmas



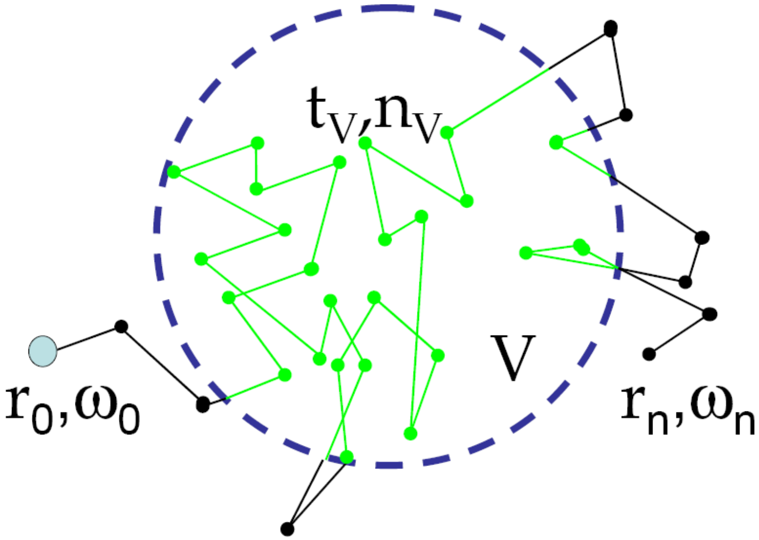
Porous media



Finance

General framework

- Collision number $\mathbf{n_V}$ and residence time $\mathbf{t_V}$ in a region **V**



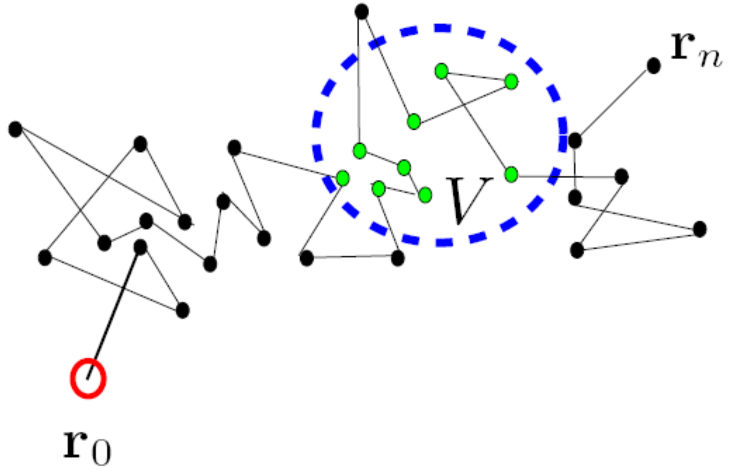
- **Mean**: average particle concentration in V
- **Variance**: uncertainty

- Applications in **reactor physics**: neutrons or photons
  - power deposition and/or atomic displacements in a volume
  - theory of Monte Carlo estimators: “collision” ($\mathbf{n_V}$) and “track length” ($\mathbf{t_V}$)

- **Hypotheses**: iid flights, single speed, isotropic scattering

Collision statistics

- Statistics of collision number $\mathbf{n_V} \leq$ n in a volume **V**



- **Distribution**: $\mathcal{P}(n_{\mathcal{V}}|\mathbf{r}_0)$

- Key of our analysis: **moments**

$$\langle n_{\mathcal{V}}^m \rangle(\mathbf{r}_0) = \sum_{n_{\mathcal{V}}=1}^{+\infty} n_{\mathcal{V}}^m \mathcal{P}(n_{\mathcal{V}}|\mathbf{r}_0)$$

- d-dimensional setup (dependence on $\mathbf{r_0}$)

Key ingredients

- Isotropic point source: $\delta(\mathbf{r}-\mathbf{r_0})$
- The **propagator** $\Psi(\mathbf{r},n|\mathbf{r_0})$ is the probability density of finding a particle in **r** entering the n-th collision, starting from $\mathbf{r_0}$ (*)
- Let $\pi(\mathbf{r},\mathbf{r}')$ be the probability density of performing a **flight** from **r'** to **r**
- Define the **transport** operator $$\pi[f](\mathbf{r}) = \int_{\mathcal{V}} \pi(\mathbf{r},\mathbf{r}') f(\mathbf{r}') d\mathbf{r}'$$
- If we define the **n**-iterated transport operator

$$\pi^n[f](\mathbf{r}) = \int_{\mathcal{V}} \int_{\mathcal{V}} \pi(\mathbf{r},\mathbf{r}_n) ... \pi(\mathbf{r}_2,\mathbf{r}_1) f(\mathbf{r}_1) d\mathbf{r}_1 ... d\mathbf{r}_n$$

it follows then $$\Psi(\mathbf{r},n|\mathbf{r}_0) = p^{n-1}\pi^n[\delta](\mathbf{r},\mathbf{r}_0)$$

(*) The propagator depends on **boundary conditions**

Collision statistics

- Define the **collision density** $\Psi(\mathbf{r}|\mathbf{r_0})$

$$\Psi(\mathbf{r}|\mathbf{r}_0) = \lim_{N\to\infty} \sum_{n=1}^{N} \Psi(\mathbf{r}, n|\mathbf{r}_0)$$

Equilibrium (limit) distribution

- Then we have the **moments**

$$\langle n_{\mathcal{V}}^m \rangle(\mathbf{r}_0) = \frac{1}{p} \sum_{k=1}^{m} s_{m,k} p^k \mathcal{C}_k(\mathbf{r}_0)$$

Kac integrals $\mathcal{C}_k(\mathbf{r}_0) = k! \int_{\mathcal{V}} d\mathbf{r}_k ... \int_{\mathcal{V}} d\mathbf{r}_1 \Psi(\mathbf{r}_k|\mathbf{r}_{k-1})...\Psi(\mathbf{r}_1|\mathbf{r}_0)$

Stirling numbers of the second kind $s_{m,k} = \frac{1}{k!} \sum_{i=0} (-1)^i \binom{k}{i} (k-i)^m$

- Link between Ψ_V and $\mathbf{n_V}$

Applications

- Moment formula $$\langle n_{\mathcal{V}}^{m} \rangle(\mathbf{r}_0) = \frac{1}{p} \sum_{k=1}^{m} s_{m,k} p^k \mathcal{C}_k(\mathbf{r}_0)$$

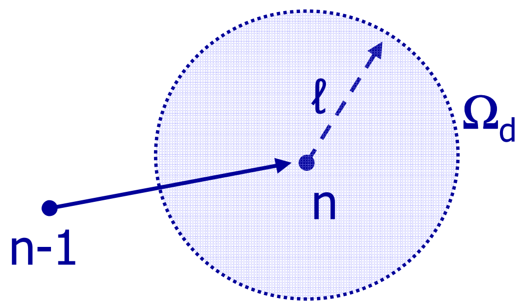
- **Numerical** integration for arbitrary $\pi(\mathbf{r},\mathbf{r}')$

- **Analytical** calculations for simple geometries and propagators

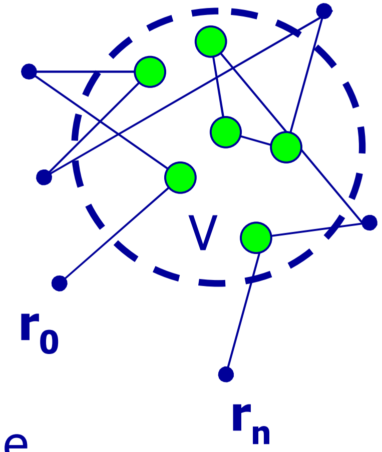
- Example. d-dimensional "**Gamma flights**" in spherical geometries: random flights with Gamma-distributed lengths $\ell^{\alpha-1}\exp(-\ell)/\Gamma(\alpha)$

$$\pi(\mathbf{r},\mathbf{r}') = \pi(\ell = |\mathbf{r}-\mathbf{r}'|)$$

$$\pi(\ell) = \ell^{\alpha-d}\exp(-\ell)/\Omega_d\Gamma(\alpha),\ \alpha > 0$$



Example 1



- Gamma flights: d=3, α=2, p=1, "transparent" boundaries

$$\pi(\ell) = \ell^{\alpha-d}\exp(-\ell)/\Omega_d\Gamma(\alpha),\ \alpha > 0$$

- V is a sphere with radius **R**; walks can start inside or outside

- Collision density $\Psi(\mathbf{r}|\mathbf{r}_0) = \dfrac{1}{4\pi|\mathbf{r}-\mathbf{r}_0|}$

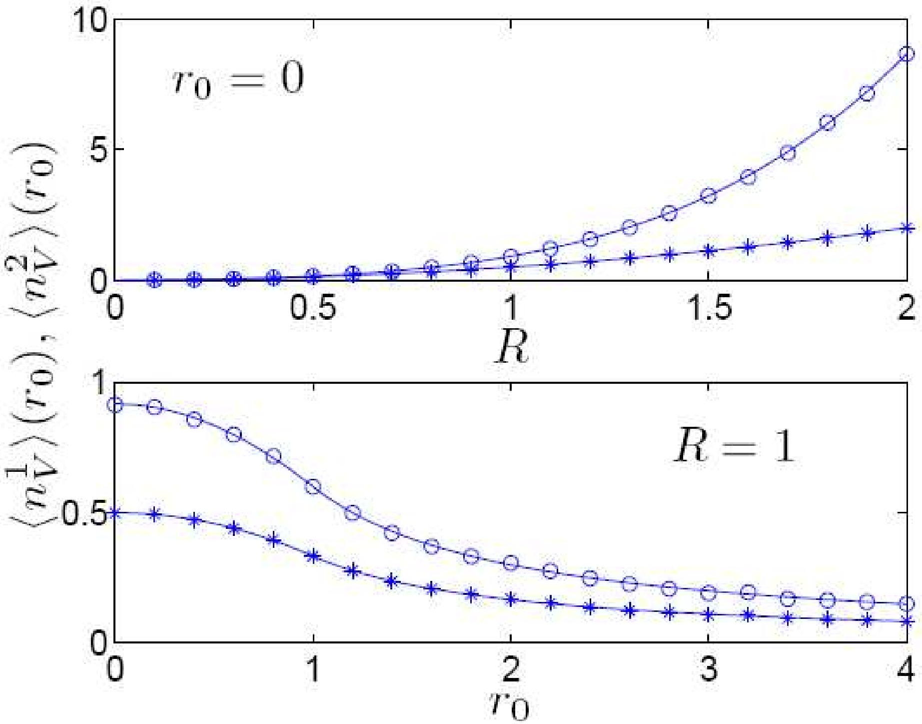
- Moments: $\langle n^1_{\mathcal{V}}\rangle(\mathbf{r}_0) = \begin{cases} \frac{3R^2-r_0^2}{6} & r_0 < R \\ \frac{R^3}{3r_0} & r_0 \geq R \end{cases}$

and

$$\langle n^2_{\mathcal{V}}\rangle(\mathbf{r}_0) = \begin{cases} \frac{25R^4-10R^2r_0^2+r_0^4}{60} + \langle n^1_{\mathcal{V}}\rangle(\mathbf{r}_0) & r_0 < R \\ \frac{4}{15}\frac{R^5}{r_0} + \langle n^1_{\mathcal{V}}\rangle(\mathbf{r}_0) & r_0 \geq R \end{cases}$$

Example 1

- Gamma flights: d=3, α=2, p=1
- Monte Carlo simulation (symbols), analytical curves (solid lines)



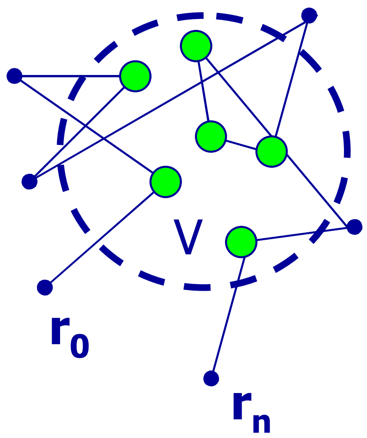
- Fixed r_0, varying R
- Fixed R, varying r_0

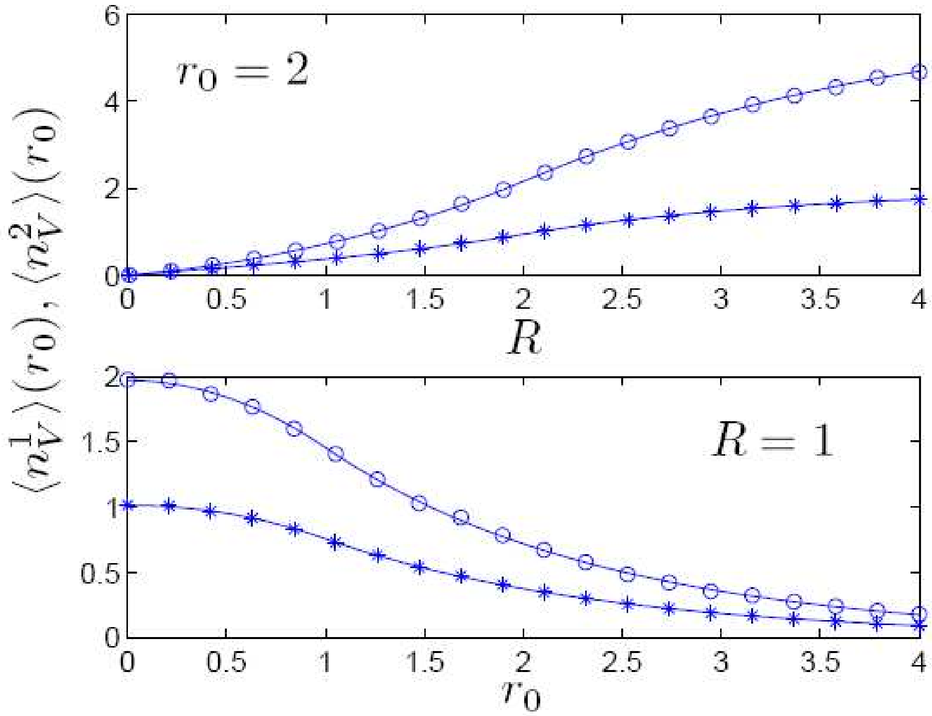
Example 2

- Gamma flights: d=1, α=1, p=0.5, transparent boundaries

$$\pi(\ell) = \ell^{1-d}\exp(-\ell)/\Omega_d$$

Exponential flights: α=1





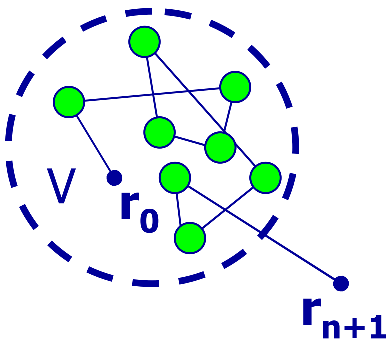
- V is a "sphere" with radius **R**; walks can start inside or outside

- Collision density

$$\Psi(\mathbf{r}|\mathbf{r}_0) = \frac{e^{-\sqrt{1-p}|\mathbf{r}-\mathbf{r}_0|}}{2\sqrt{1-p}}$$

- Omitted formulas

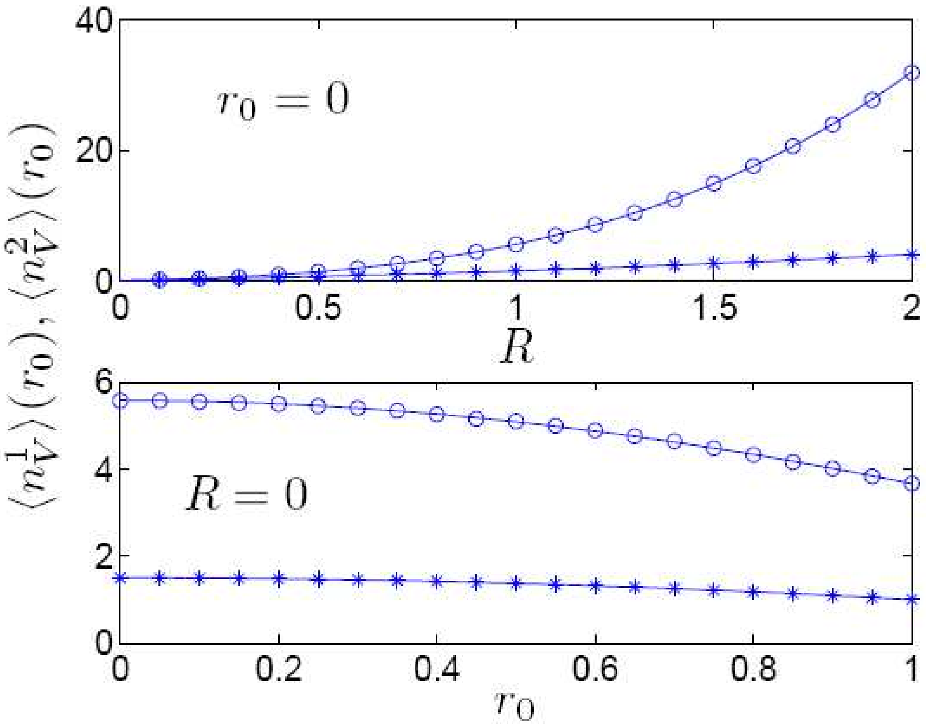
Example 3



- Gamma flights: d=1, α=1, p=1, **leakage** boundaries

$$\pi(\ell) = \ell^{1-d}\exp(-\ell)/\Omega_d$$

Exponential flights: α=1



- Collision density

$$\Psi(\mathbf{r}|\mathbf{r}_0) = \frac{|r_0\mathbf{r}/r_e - r_e\mathbf{r}_0/r_0| - |\mathbf{r}-\mathbf{r}_0|}{2}$$

$$r_e = R + 1$$

- Method of images

- Omitted formulas

Why? Proof (1)

- Formal relation $\mathcal{P}(n_{\mathcal{V}}|\mathbf{r}_0) = \int_{\mathcal{V}} d\mathbf{r}\Psi(\mathbf{r}, n_{\mathcal{V}}|\mathbf{r}_0) - \int_{\mathcal{V}} d\mathbf{r}\Psi(\mathbf{r}, n_{\mathcal{V}}+1|\mathbf{r}_0)$
- **Survival** probability
- Recall that $\langle n_{\mathcal{V}}^m \rangle(\mathbf{r}_0) = \sum_{n_{\mathcal{V}}=1}^{+\infty} n_{\mathcal{V}}^m \mathcal{P}(n_{\mathcal{V}}|\mathbf{r}_0)$
- Then, from $\Psi(\mathbf{r}, n|\mathbf{r}_0) = p^{n-1}\pi^n[\delta](\mathbf{r}, \mathbf{r}_0)$

we have $\langle n_{\mathcal{V}}^m \rangle(\mathbf{r}_0) = \frac{1}{p}\int_{\mathcal{V}} d\mathbf{r}\,\mathrm{Li}_{-m}(p\pi)(1-p\pi)[\delta](\mathbf{r}, \mathbf{r}_0)$

where $\mathrm{Li}_s(x) = \sum_{k=1}^{\infty} x^k/k^s$ **Polylogarithm** (Jonquière function)

Rational function: $\mathrm{Li}_{-m}(x) = \sum_{k=0}^{m} k!\, s_{m+1,k+1} \left(\frac{x}{1-x}\right)^{k+1}$

for non-negative integer -m

Proof (2)

- Define the operator $\Psi[f](\mathbf{r}) = \int_{\mathcal{V}} \Psi(\mathbf{r}|\mathbf{r}')f(\mathbf{r}')d\mathbf{r}'$
- Recall that $\Psi(\mathbf{r}|\mathbf{r}_0) = \lim_{N\to\infty} \sum_{n=1}^{N} \Psi(\mathbf{r}, n|\mathbf{r}_0)$ and $\Psi(\mathbf{r}, n|\mathbf{r}_0) = p^{n-1}\pi^n[\delta](\mathbf{r}, \mathbf{r}_0)$
- Apply formal **Neumann** series $\sum_{n=1}^{\infty} p^{n-1}\pi^n[f](\mathbf{r}) = \frac{\pi}{1-p\pi}[f](\mathbf{r})$
- Then $\Psi[f](\mathbf{r}) = \frac{\pi}{1-p\pi}[f](\mathbf{r})$ and $\Psi(\mathbf{r}|\mathbf{r}_0) = \Psi[\delta](\mathbf{r}, \mathbf{r}_0)$
- From $\mathrm{Li}_{-m}(x) = \sum_{k=0}^{m} k!s_{m+1,k+1}\left(\frac{x}{1-x}\right)^{k+1}$

  we can rewrite $\langle n_{\mathcal{V}}^m\rangle(\mathbf{r}_0) = \frac{1}{p}\int_{\mathcal{V}} d\mathbf{r}\,\mathrm{Li}_{-m}(p\pi)(1-p\pi)[\delta](\mathbf{r}, \mathbf{r}_0)$

  as $\langle n_{\mathcal{V}}^m\rangle(\mathbf{r}_0) = \frac{1}{p}\int_{\mathcal{V}} d\mathbf{r} \sum_{k=1}^{m} k!s_{m,k}p^k\Psi^k[\delta](\mathbf{r}, \mathbf{r}_0)$

Proof (3)

- We have $$\langle n_{\mathcal{V}}^m \rangle(\mathbf{r}_0) = \frac{1}{p}\int_{\mathcal{V}} d\mathbf{r} \sum_{k=1}^{m} k! s_{m,k} p^k \Psi^k[\delta](\mathbf{r}, \mathbf{r}_0)$$
- We can identify $$\mathcal{C}_k(\mathbf{r}_0) = k! \int_{\mathcal{V}} d\mathbf{r}_k ... \int_{\mathcal{V}} d\mathbf{r}_1 \Psi(\mathbf{r}_k|\mathbf{r}_{k-1})...\Psi(\mathbf{r}_1|\mathbf{r}_0)$$

  with $$\mathcal{C}_k(\mathbf{r}_0) = k! \int_{\mathcal{V}} d\mathbf{r} \Psi^k[\delta](\mathbf{r}, \mathbf{r}_0)$$
- It follows finally $$\langle n_{\mathcal{V}}^m \rangle(\mathbf{r}_0) = \frac{1}{p} \sum_{k=1}^{m} s_{m,k} p^k \mathcal{C}_k(\mathbf{r}_0)$$
- Remark the **recursion** property $$\mathcal{C}_{k+1}(\mathbf{r}_0) = (k+1)\Psi[\mathcal{C}_k](\mathbf{r}_0)$$

Large n_V behavior

- Discrete **moment generating function** G(z|**r₀**)
- Relation to the distribution $\mathcal{P}(n_\mathcal{V}|\mathbf{r}_0) = \frac{1}{n_\mathcal{V}!}\frac{\partial^{n_\mathcal{V}}}{\partial z^{n_\mathcal{V}}} G(\log(z)|\mathbf{r}_0)|_{z=0}$
- Moments expansion $G(z|\mathbf{r}_0) = \sum_{m=0}^{\infty} \langle n_\mathcal{V}^m \rangle(\mathbf{r}_0) \frac{z^m}{m!}$

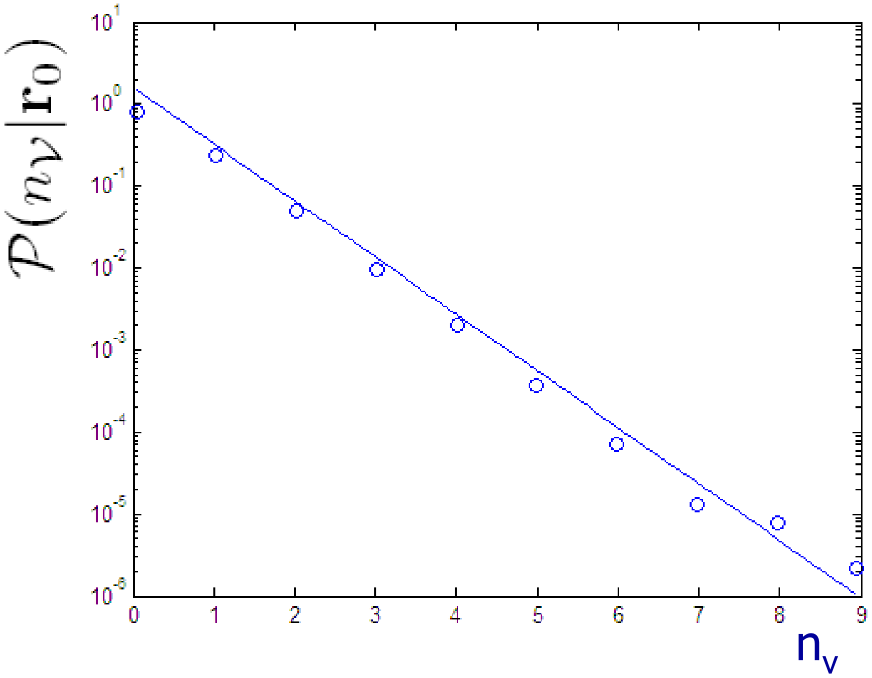
$$G(z|\mathbf{r}_0) = \sum_{k=0}^{\infty} \int_\mathcal{V} d\mathbf{r} e^{kz} (p\pi)^k (1-p\pi)[\delta](\mathbf{r},\mathbf{r}_0) = \frac{1}{p} \int_\mathcal{V} d\mathbf{r} \frac{1-p\pi}{1-e^z p\pi}[\delta](\mathbf{r},\mathbf{r}_0)$$

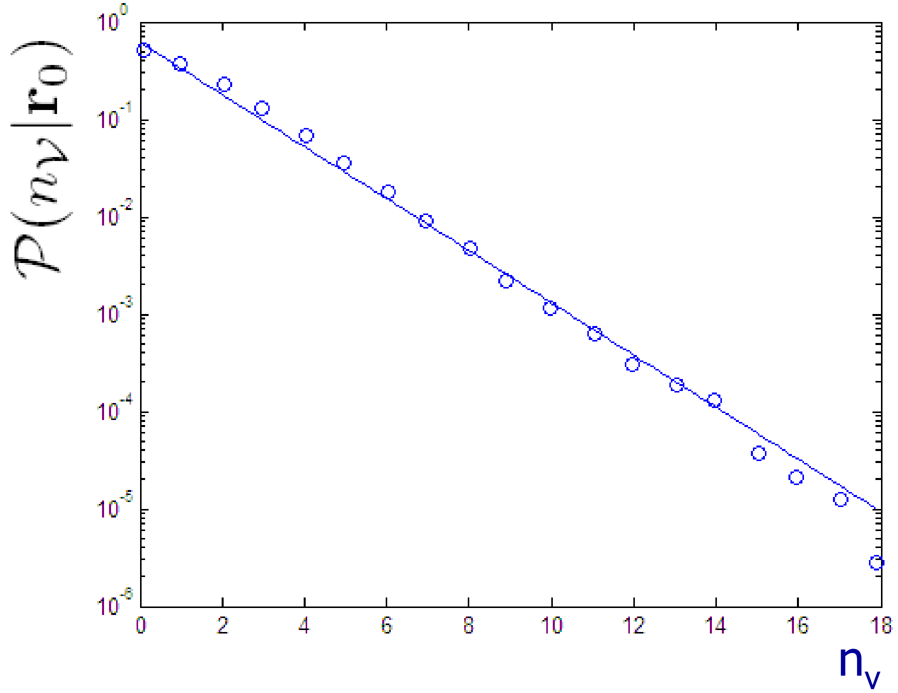
- It follows the **small-z** behavior $G(z|\mathbf{r}_0) \simeq 1 + z \int_\mathcal{V} d\mathbf{r} \Psi[\delta](\mathbf{r},\mathbf{r}_0)$
- Hence from **Tauberian** theorems $\mathcal{P}(n_\mathcal{V}|\mathbf{r}_0) \simeq e^{-n_\mathcal{V}/\langle n_\mathcal{V}^1 \rangle(\mathbf{r}_0)}$

Simulations

- **Exponential** decay of the distribution: simulations (circles) and log-lin fit (solid line)

$$\mathcal{P}(n_\mathcal{V}|\mathbf{r}_0) \simeq e^{-n_\mathcal{V}/\langle n^1_\mathcal{V}\rangle(\mathbf{r}_0)}$$





- 3d Gamma flights (α=2)
- 3d exponential flights

Discussion: existence of $C_k(\mathbf{r}_0)$

- Convolution Kac integrals $$\mathcal{C}_k(\mathbf{r}_0) = k! \int_{\mathcal{V}} d\mathbf{r}_k ... \int_{\mathcal{V}} d\mathbf{r}_1 \Psi(\mathbf{r}_k|\mathbf{r}_{k-1}) ... \Psi(\mathbf{r}_1|\mathbf{r}_0)$$
- Recursion $$\mathcal{C}_{k+1}(\mathbf{r}_0) = (k+1)\Psi[\mathcal{C}_k](\mathbf{r}_0)$$
- Hence the existence of $C_k(\mathbf{r}_0)$ depends on $$\Psi(\mathbf{r}|\mathbf{r}_0) = \lim_{N\to\infty} \sum_{n=1}^{N} \Psi(\mathbf{r}, n|\mathbf{r}_0)$$
- $\Psi(\mathbf{r}|\mathbf{r}_0)$ depends on boundary conditions, p, and dimension **d**
- Worst case (transparent boundaries and p=1): **d>2**
  - **Recurrent** and **transient** walks: Polya's theorem
- Remark that we have $$\langle n_{\mathcal{V}}^1 \rangle(\mathbf{r}_0) = \int_{\mathcal{V}} d\mathbf{r} \Psi(\mathbf{r}|\mathbf{r}_0)$$

Use and abuse of the formula

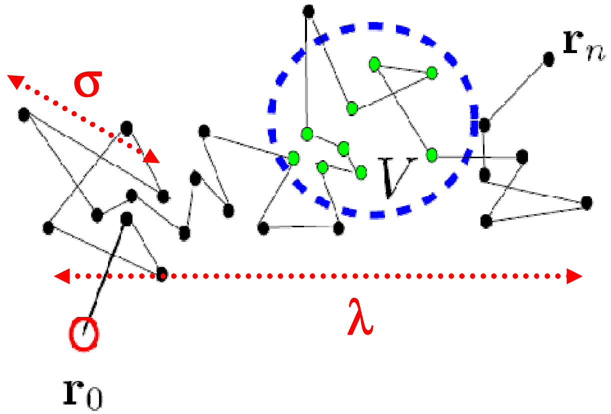
$$\langle n_{\mathcal{V}}^{m} \rangle(\mathbf{r}_0) = \frac{1}{p} \sum_{k=1}^{m} s_{m,k} p^k \mathcal{C}_k(\mathbf{r}_0)$$

+

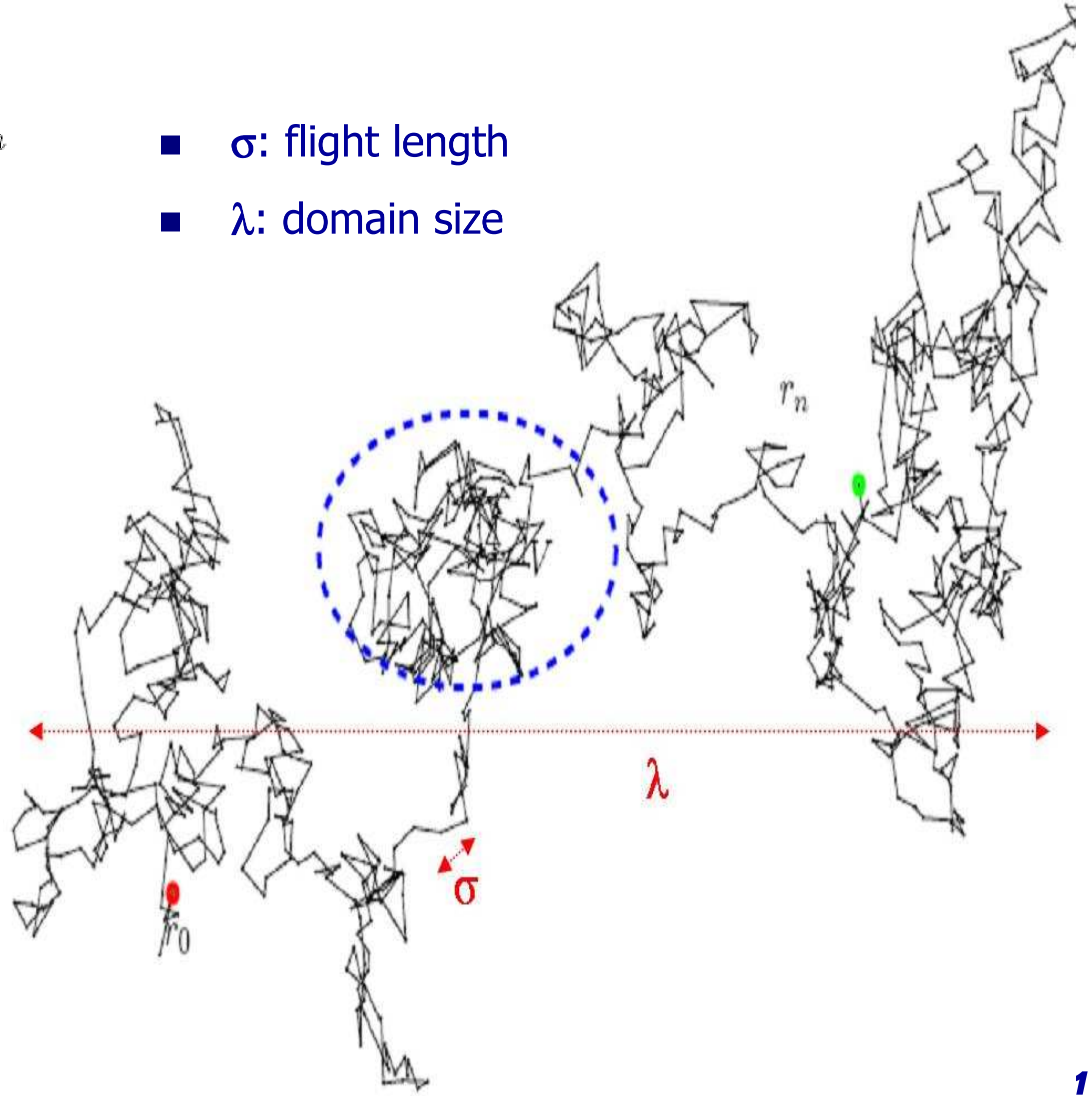
$$\mathcal{C}_k(\mathbf{r}_0) = k! \int_{\mathcal{V}} d\mathbf{r}_k ... \int_{\mathcal{V}} d\mathbf{r}_1 \Psi(\mathbf{r}_k|\mathbf{r}_{k-1}) ... \Psi(\mathbf{r}_1|\mathbf{r}_0)$$

- **Direct** approach: from equilibrium distribution to moments
  - Knowledge of the process allows assessing collision statistics
  - Example: neutron or photon transport
- **Inverse** approach: from moments to equilibrium distribution
  - Knowledge of the moments allows assessing features of underlying process
  - Example: biology or economics
- Warning: it is a **difficult** problem!

Diffusion limit



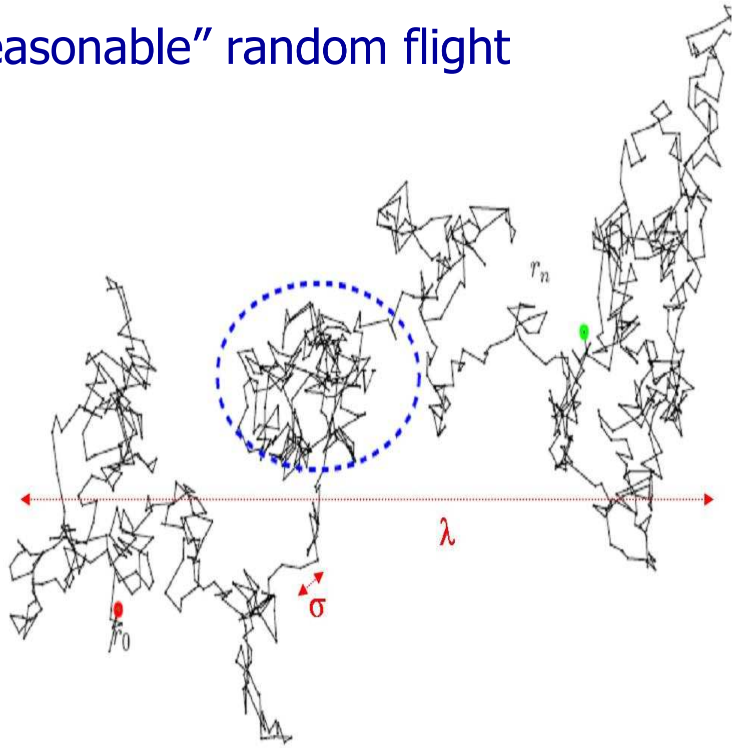
- σ: flight length
- λ: domain size



- Choose σ « λ

Brownian functionals

- Central Limit Theorem: when $\sigma \ll \lambda$, every "reasonable" random flight $\mathbf{r}_n$ *converges* to **Brownian motion** $\mathbf{B}_n$
- Analogously, $F[\mathbf{r}_n]$ converges to $F[\mathbf{B}_n]$
- What happens to $F = \langle n_{\mathcal{V}}^m \rangle (\mathbf{r}_0)$ → ?
- When $\sigma \ll \lambda$, n_V explodes
- We need a **rescaling**: the natural candidate is the **time** $t = n\,(\sigma / v)$

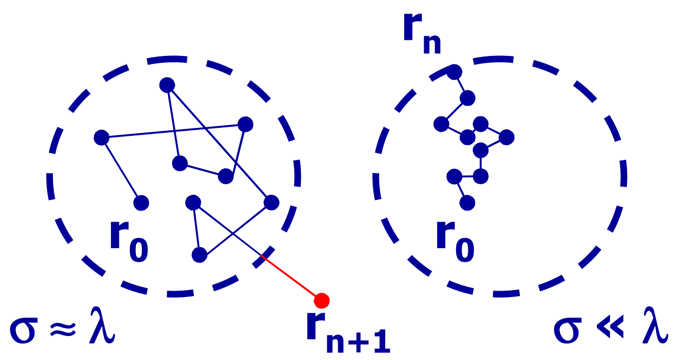


Diffusion limit (1)

- Finite speed v (neglect absorption)
- Isotropy: $\pi(\mathbf{r},\mathbf{r}') = \pi(\ell = |\mathbf{r}-\mathbf{r}'|)$
- Identically distributed **flight times** $t_i = |\mathbf{r}_i - \mathbf{r}_{i-1}|/v$

  $w(t_i) = \Omega_d \int \ell^{d-1}\pi(\ell)\delta(t_i - \ell/v)d\ell$
- **Diffusion limit**: small σ, which implies small $\tau = \langle t_i \rangle$, and $n_{\mathcal{V}} \to \infty$

  We impose a finite ratio $D = \sigma^2/\tau$
- **Residence time** in V: $t_{\mathcal{V}} = \sum_{i=1}^{n_{\mathcal{V}}} t_i$
- Effects of **boundary conditions**



Diffusion limit (2)

- Introduce the distribution $\mathcal{Q}(t_{\mathcal{V}}|\mathbf{r}_0)$ of $t_{\mathcal{V}} = \sum_{i=1}^{n_{\mathcal{V}}} t_i$
- In **Laplace** space the distribution of the sum is

$$\mathcal{Q}(s|\mathbf{r}_0) = \int \exp(-st_{\mathcal{V}})\mathcal{Q}(t_{\mathcal{V}}|\mathbf{r}_0)dt_{\mathcal{V}} = w(s)^{n_{\mathcal{V}}}$$

- For any "reasonable" w(t), we have $w(s) \simeq 1 - s\tau$ when $\tau \to 0$
- Then, $\mathcal{Q}(s|\mathbf{r}_0) \simeq e^{-n_{\mathcal{V}}s\tau}$

  which implies $\mathcal{Q}(t_{\mathcal{V}}|\mathbf{r}_0) \simeq \delta(t_{\mathcal{V}} - n_{\mathcal{V}}\tau)$
- Hence, $\langle t_{\mathcal{V}}^m \rangle(\mathbf{r}_0) \simeq \tau^m \langle n_{\mathcal{V}}^m \rangle(\mathbf{r}_0)$

Diffusion limit (3)

- We can combine $\langle t_{\mathcal{V}}^m \rangle(\mathbf{r}_0) \simeq \tau^m \langle n_{\mathcal{V}}^m \rangle(\mathbf{r}_0)$

  with $\langle n_{\mathcal{V}}^m \rangle(\mathbf{r}_0) = \frac{1}{p} \sum_{k=1}^{m} s_{m,k} p^k \mathcal{C}_k(\mathbf{r}_0)$ (p=1)

- Rescale **r** by σ: each term in the sum gives σ^{-2k}
- Only the leading order m survives

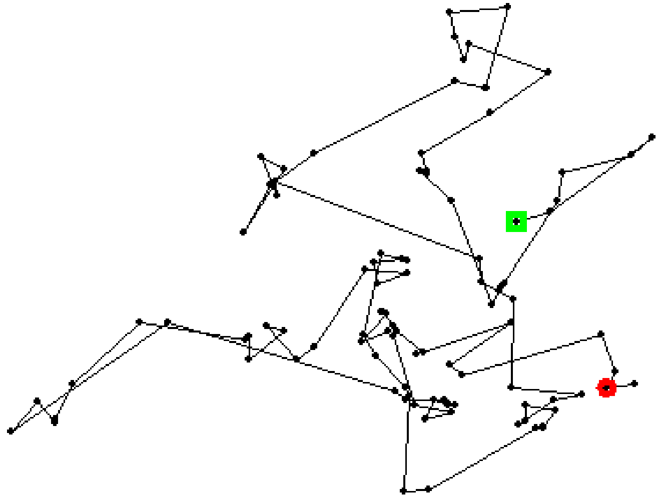
- We finally obtain the celebrated **Kac formula** $\langle t_{\mathcal{V}}^m \rangle(\mathbf{r}_0) \simeq \frac{\mathcal{C}_m(\mathbf{r}_0)}{D^m}$

  which is known for **Brownian motion**

- Moreover, we have the recursion property

$$D\langle t_{\mathcal{V}}^{m+1} \rangle(\mathbf{r}_0) = (m+1)\Psi[\langle t_{\mathcal{V}}^m \rangle](\mathbf{r}_0)$$

Exponential flights



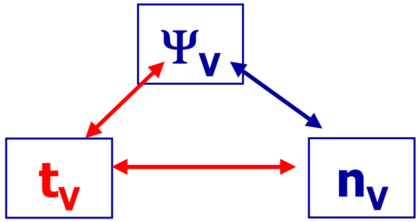
- Random flights with jump lengths

  $$\varphi(\ell) = \sigma_t e^{-\ell\sigma_t}$$

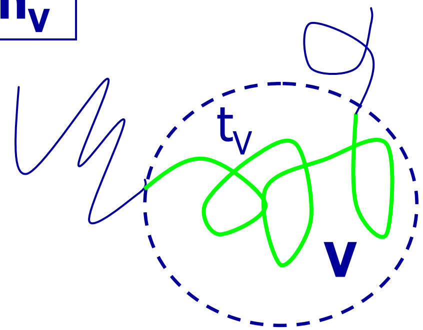
- Physical meaning: **homogeneous** scattering centers
- Defining **time**: t=ℓ/v
- **Markovian** (memoryless) $\mathbf{z}_t = \{\mathbf{r}_t, \omega_t\}$
- Chapman-Kolmogorov: $$\frac{\partial}{\partial t}\Psi(\mathbf{r}, \omega, t|\mathbf{r}_0, \omega_0) = \mathcal{L}\Psi(\mathbf{r}, \omega, t|\mathbf{r}_0, \omega_0)$$
  - Forward transport operator $$\mathcal{L} = -\mathbf{v}\cdot\nabla_{\mathbf{r}} + \frac{1}{\tau_s\Omega_d}\int d\omega - \frac{1}{\tau_t}$$
- Collision density: $$\Psi(\mathbf{r}, \omega|\mathbf{r}_0, \omega_0) = \frac{1}{\tau_t}\int_0^{+\infty}\Psi(\mathbf{r}, \omega, t|\mathbf{r}_0, \omega_0)dt$$

Residence times of exponential flights

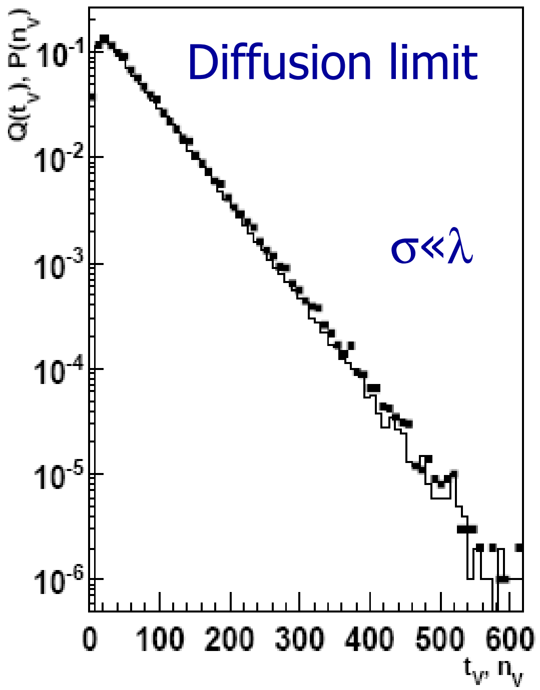
- Understanding the relation between

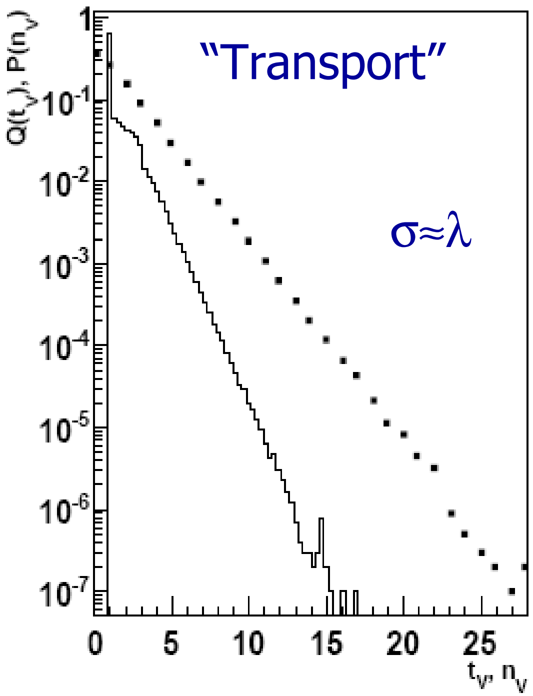


$t_V(t) \leq t$



- **Residence time** $t_V(t) = \int_0^t \chi[\mathbf{z}(t')]dt'$





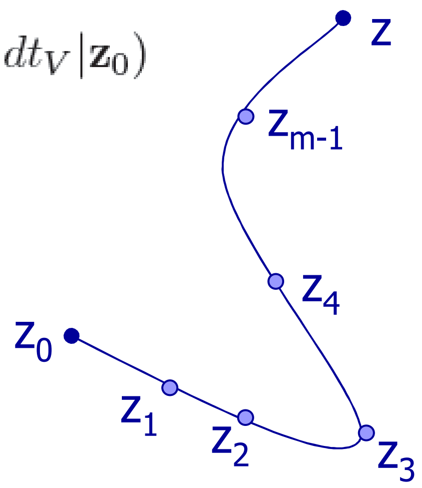
- Collisions: dots
- Residence time: solid line

Kac moment formula

- Moments $$\langle t_V^m \rangle(\mathbf{r}_0, \omega_0) = \int_0^{+\infty} t_V^m \mathcal{Q}(t_V|\mathbf{r}_0, \omega_0) dt_V$$

$$\mathcal{Q}(t_V|\mathbf{z}_0)dt_V = \int d\mathbf{z}\Psi(\mathbf{z}, t_V|\mathbf{z}_0) - \int d\mathbf{z}\Psi(\mathbf{z}, t_V + dt_V|\mathbf{z}_0)$$

$$\langle t_V^m \rangle(\mathbf{z}_0) = m \int_0^{+\infty} t_V^{m-1} \int d\mathbf{z}\Psi(\mathbf{z}, t_V|\mathbf{z}_0) dt_V$$



- **Markovian**: partition trajectory over z_i

$$\mathbf{z}_0, \mathbf{z}_1, \mathbf{z}_2, ..., \mathbf{z}_m = \mathbf{z}$$

$$t_0 = 0, t_1, t_2, ..., t_m = t_V$$

- **Convolutions** in phase space: $\Psi(z_0 \rightarrow z) = \Psi(z_0 \rightarrow z_1) * \Psi(z_1 \rightarrow z_2) * \ldots * \Psi(z_{m-1} \rightarrow z)$

Kac moment formula

- We have then the convolution products

$$\langle t_V^m \rangle(\mathbf{z}_0) = m! \int d\mathbf{z}_m \int_0^{+\infty} dt_m ... \int_0^{t_2} dt_1 \Psi(\mathbf{z}_m, t_m - t_{m-1} | \mathbf{z}_{m-1}) * ... * \Psi(\mathbf{z}_1, t_1 | \mathbf{z}_0)$$

$$\Psi(\mathbf{z}_{i+1}, t_{i+1} - t_i | \mathbf{z}_i) * \Psi(\mathbf{z}_i, t_i - t_{i-1} | \mathbf{z}_{i-1}) = \int d\mathbf{z}_i \Psi(\mathbf{z}_{i+1}, t_{i+1} - t_i | \mathbf{z}_i) \Psi(\mathbf{z}_i, t_i - t_{i-1} | \mathbf{z}_{i-1})$$

  - Fubini's theorem $m \int_0^{+\infty} t_m^{m-1} ... dt_m = m! \int_0^{+\infty} dt_m ... \int_0^{t_2} dt_1$

- **Moment formula** $$\frac{\langle t_V^m \rangle(\mathbf{z}_0)}{\tau_t^m} = m! \int d\mathbf{z}_m \Psi(\mathbf{z}_m | \mathbf{z}_{m-1}) * ... * \Psi(\mathbf{z}_1 | \mathbf{z}_0)$$

  - Collision density $\Psi(\mathbf{z}_{i+1} | \mathbf{z}_i) = \frac{1}{\tau_t} \int_0^{+\infty} \Psi(\mathbf{z}_{i+1}, t | \mathbf{z}_i) dt$

Some calculations

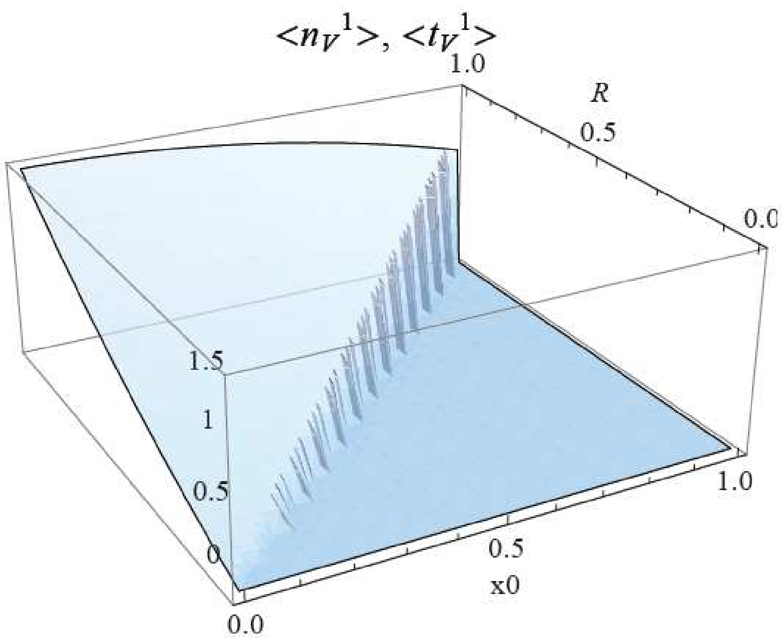
- Exponential flights in **1d** ("rod model")
- Oversimplified model, but captures essential transport features
- Analytical results: compare the moments of $\mathbf{n_V}$ and $\mathbf{t_V}$

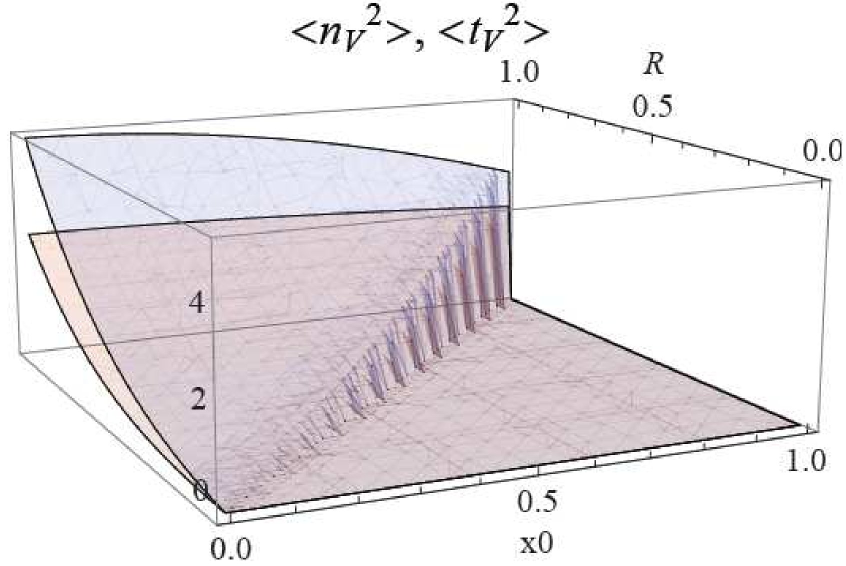
- Two cases:
  - **Leakage** boundary conditions and pure scattering (homogeneous finite-size medium V surrounded by vacuum: first-passage problem)
  - **Transparent** boundaries and absorption (homogeneous infinite medium: observe statistics on a finite-size domain V)

- Set v=1, and rescale r=r/σ (equal average flight time and flight length)
  - Directly compare the moments of $\mathbf{n_V}$ and $\mathbf{t_V}$

Leakage boundaries

- Moments for isotropic source: depend on x_0 and R



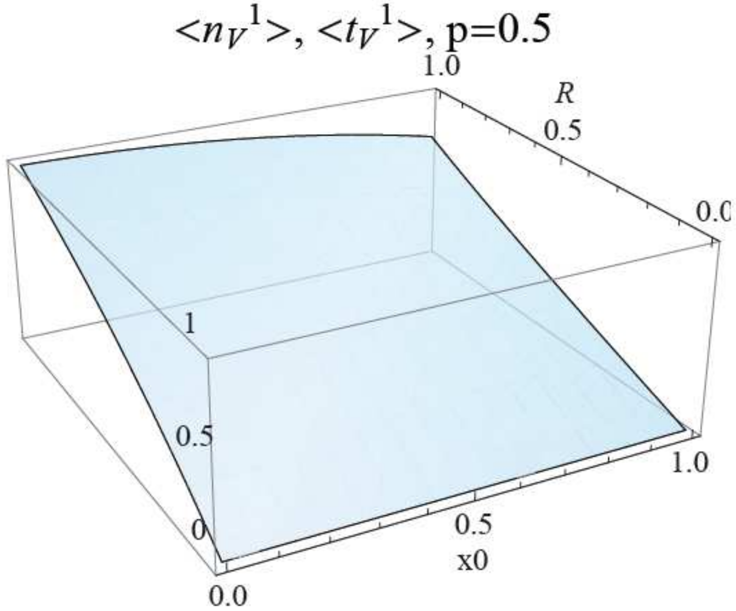


Average n_V and t_V **unbiased** to each other

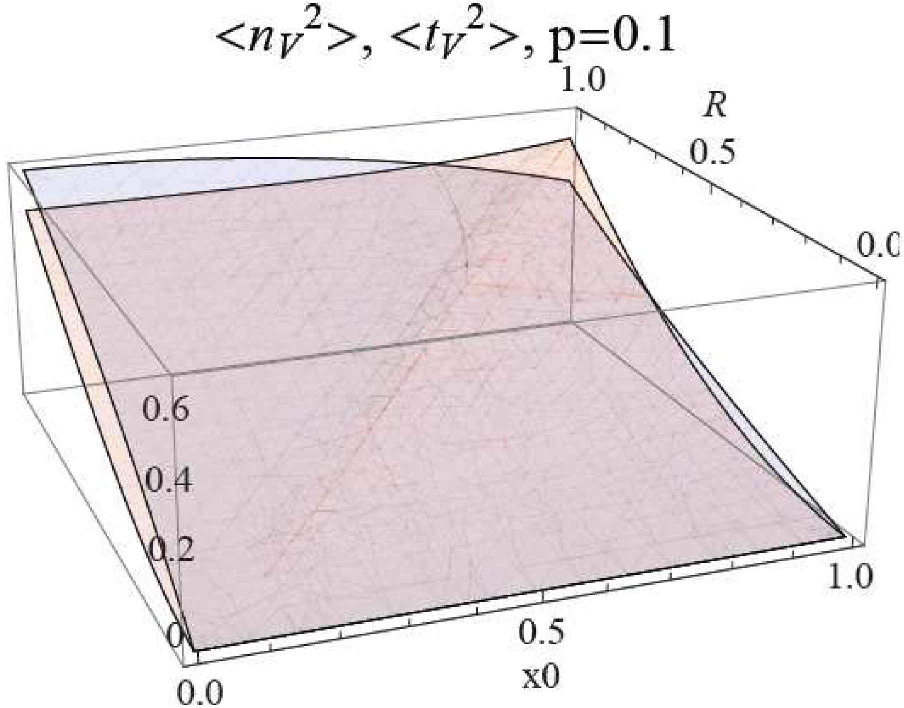
… but have different variances

Transparent boundaries

- Moments for isotropic source: depend on x_0, R and p



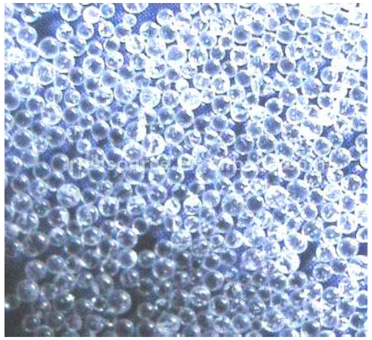
Average n_V and t_V **unbiased** (for any p)



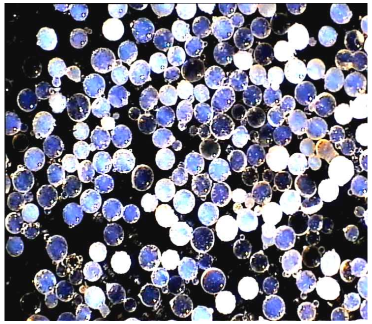
… but have different variances

Conclusions and perspectives

- General mathematical framework for random flights
- Collision statistics and equilibrium distribution
- Exponential flights as a particular case: time statistics



- Strong hypothesis: **single** space scale
  - Adequate model for '**homogeneous**' media
  - In the diffusion limit, converges to Brownian motion



- Transport in **disordered** (heterogeneous/anisotropic) media
  - Coexistence of **many** space **scales**
  - Converges to **anomalous diffusion** (?)

Thank you

- Questions?
- References [ArXiv]
  - A. Zoia, E. Dumonteil, A. Mazzolo, *Collision densities and mean residence times for d-dimensional exponential flights,* Phys. Rev. E **83**, 041137 (2011).
  - A. Zoia, E. Dumonteil, A. Mazzolo, *Collision number statistics for transport processes,* Phys. Rev. Lett. **106**, 220602 (2011).
  - A. Zoia, E. Dumonteil, A. Mazzolo, *Residence time and collision statistics for exponential flights: the rod problem revisited*, Phys. Rev. E **84**, 021139 (2011).
  - A. Zoia, E. Dumonteil, A. Mazzolo, *Collision statistics for random flights with anisotropic scattering and absorption*, in preparation.

Feynman-Kac formulae

- Kac functional $F(t,s|\mathbf{z}_0) = \langle e^{-st_V(t)} \rangle$

$$\frac{\partial}{\partial t} F(t,s|\mathbf{z}_0) = \mathcal{L}^* F(t,s|\mathbf{z}_0) - s\chi[\mathbf{z}_0] F(t,s|\mathbf{z}_0) \qquad \mathcal{L}^* = \mathbf{v}_0 \cdot \nabla_{\mathbf{r}_0} + \frac{1}{\tau_s}\int d\omega_0 - \frac{1}{\tau_t}$$

$$\boxed{\langle t_V^m \rangle(\mathbf{z}_0, t) = (-1)^m \frac{\partial^m}{\partial s^m} F(t,s|\mathbf{z}_0)|_{s=0}}$$

- **Recursion** for the moments

$$\frac{\partial}{\partial t}\langle t_V^m \rangle(\mathbf{z}_0, t) = \mathcal{L}^* \langle t_V^m \rangle(\mathbf{z}_0, t) + m\chi[\mathbf{z}_0]\langle t_V^{m-1} \rangle(\mathbf{z}_0, t)$$

- Infinite observation time: $\boxed{\mathcal{L}^* \langle t_V^m \rangle(\mathbf{z}_0) = -m\chi[\mathbf{z}_0]\langle t_V^{m-1} \rangle(\mathbf{z}_0)}$

$$t_V(\mathbf{z}_0) = \lim_{t\to+\infty} t_V(\mathbf{z}_0, t)$$