Numerical Methods for Langevin Equations

with applications to gravitational systems

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Recall simplest case: Stoke's law for a particle in fluid,

$$dv(t) = -\gamma\ v(t)\ dt$$

where

$$\begin{aligned} \gamma &= \frac{6\pi r}{m}\eta, \\ \eta &= \text{viscosity coefficient.} \end{aligned}$$

Langevin's idea: small particles bounced around by fluid molecules,

$$dv(t) = -\gamma\ v(t)\ dt + \sigma\ dw(t), \qquad \text{(LE)}$$

$w(t) =$ Brownian motion, $\gamma =$ Stoke's coefficient.
$\sigma^2 = \frac{2kT\gamma}{m}$ =Diffusion coefficient.

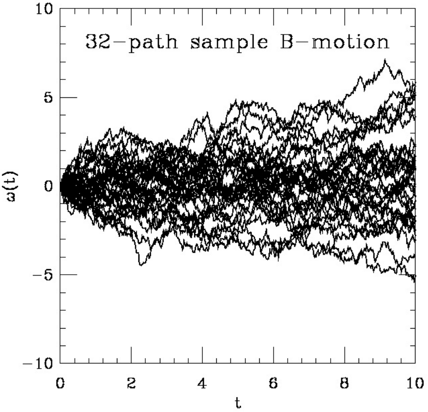


Figure: Simulation of 1-D Brownian motion

We will come back to the 2-D situation:

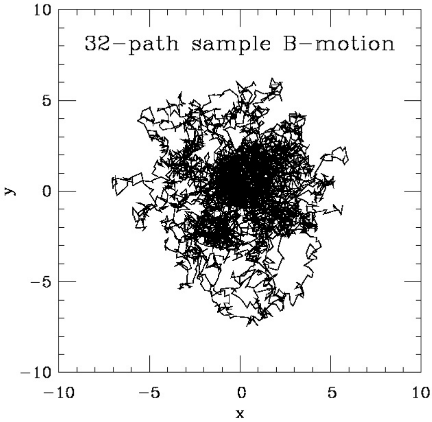


Figure: Simulation of 2-D Brownian motion

Properties of $w(t)$? (Physicists' notation is often $\langle X \rangle = \mathbf{E}X$)

$$\begin{aligned} w(0) &= 0 \\ \mathbf{E}w(t) &= 0 \\ \mathbf{E}(w(t))^2 &= t \end{aligned}$$

and p.d.f. satisfies **Heat equation**

$$\frac{\partial p(w,t)}{\partial t} = \frac{1}{2}\frac{\partial^2 p(w,t)}{\partial w^2}$$

Formal solution to LE called an **Ornstein-Uhlenbeck** process

$$v(t) = v_0 e^{-\gamma t} + \sigma e^{-\gamma t} \int_0^t e^{\gamma s} dw(s)$$

Solution to Ornstein-Uhlenbeck LE has properties

$$
\begin{aligned}
\mathbf{E}v(t) &= v_0 e^{-\gamma t} + \sigma e^{-\gamma t} \int_0^t e^{\gamma s} \mathbf{E} dw(s) \\
&= v_0 e^{-\gamma t}
\end{aligned}
$$

and

$$
\begin{aligned}
\mathbf{E}(v(t))^2 &= (v_0)^2 e^{-2\gamma t} + \sigma^2 e^{-2\gamma t} \frac{e^{2\gamma t} - 1}{2\gamma} \\
&\to \frac{\sigma^2}{2\gamma} \quad \text{as} \quad t \to \infty
\end{aligned}
$$

Anything familiar about this?

$$
\begin{aligned}
\frac{m}{2} \mathbf{E}(v)^2 &= \frac{m}{2} \frac{\sigma^2}{2\gamma} \\
&= \frac{1}{2} kT
\end{aligned}
$$

If system is non-isotropic, diffusion coefficient σ may depend on process.

$$dz = b(z)\ dt + \sigma(z)\ dw(t). \qquad \text{(SDE)}$$

Must be careful: (SDE) is shorthand for

$$z(t) = z_0 + \int_0^t b(z_s)\ ds + \int_0^t \sigma(z_s)\ dw(s).$$

The Stieltjes integral is interpreted (Itô rule)

$\int_0^t \sigma(z(s))dw(s) =$

$$\lim_{\Delta t \to 0} \sum_{i=1}^{n} \sigma(z(t_i))(w(t_{i+1}) - w(t_i))$$

and is called belated, or non-anticipating.

What's important about Itô rule:

$$\mathbf{E}\{\int_0^t \sigma(z(s))dw(s)\} = 0,$$

and

$$\mathbf{E}\{\int_0^t \sigma(z(s))dw(s)\}^2 = \int_0^t \mathbf{E}(\sigma(z(s)))^2 ds.$$

These functional integrals are called **martingales**.

Connection of B-motion to heat equation, we've seen, but there is more: Feynman-Kac formula. Solution to

$$\begin{aligned} \frac{\partial u(x,t)}{\partial t} &= \frac{1}{2}a(x)\frac{\partial^2}{\partial x^2}u(x,t) \\ &+b(x)\frac{\partial}{\partial x}u(x,t)+c(x)u(x,t), \end{aligned}$$

where $u(x, t = 0) = f(x)$, is

$$u(x,t) = \mathbf{E} f(z(t)) \; exp\{\int_0^t c(z(s))ds\}.$$

$z(t = 0) = x$ is initial condition for SDE.

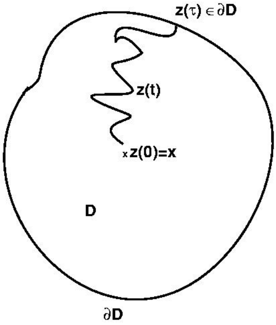
What about Dirichlet problem on domain D? $c(x) \leq 0$ here

$$\frac{1}{2} a \frac{\partial^2 u}{\partial x^2} + b \frac{\partial u}{\partial x} + cu = f(x)$$

with $u(x) = g(x)$ on boundary $x \in \partial D$. F-K solution is

$$\begin{aligned} u(x) &= \mathbf{E} g(z_\tau)\ exp\{\int_0^\tau ds\ c(z_s)\} \\ &\quad - \mathbf{E} \int_0^\tau dt\ f(z_t)\ exp\{\int_0^t ds\ c(z_s)\} \end{aligned}$$

Here $\tau =$ **first exit time**, i.e. the first time t that $z(t)$ crosses ∂D. Again, $z(t=0) = x$.


z(τ) ∈ ∂D
z(t)
x z(0)=x
D
∂D

Simulation of these things? First, to compute expectations:

$$\mathbf{E} f[z(t)] \approx \frac{1}{N} \sum_{i=1}^{N} f[z^{[i]}(t)]$$

for an N sample of paths $z(t)$, and some functional f. N paths $\{z^{[1]}, z^{[2]}, ..., z^{[N]}\}$ are integrated by some rule, e.g., simplest is via Euler (higher order in wpp '98, Milstein '95, e.g.)

$$\begin{aligned}
z_{t+h}^{[1]} &= z_t^{[1]} + b(z_t^{[1]})\; h + \sigma(z_t^{[1]})\; \Delta w^{[1]} \\
z_{t+h}^{[2]} &= z_t^{[2]} + b(z_t^{[2]})\; h + \sigma(z_t^{[2]})\; \Delta w^{[2]} \\
\cdots & \\
z_{t+h}^{[N]} &= z_t^{[N]} + b(z_t^{[N]})\; h + \sigma(z_t^{[N]})\; \Delta w^{[N]}.
\end{aligned}$$

Where, $\Delta w = \xi$ is approximately gaussian, w. variance h.

Gravitational systems - starting with Boltzmann's equation.

$$f(\mathbf{x}, \mathbf{v}, t) = \text{prob. density in 6-D } \mathbf{x}, \mathbf{v} \text{ space}$$

If phase-space is incompressible,

$$\frac{d}{dt} \int f \; d^3x \; d^3v = 0$$

or

$$\begin{aligned} \frac{\partial f}{\partial t} + \dot{\mathbf{v}} \cdot \nabla_v f + \dot{\mathbf{x}} \cdot \nabla_x f &= 0 \\ \frac{\partial f}{\partial t} - \nabla_x \Phi \cdot \nabla_v f + \mathbf{v} \cdot \nabla_x f &= 0 \quad \text{(B-T)} \end{aligned}$$

this is the collisionless Boltzmann eq.

Now include probability conservation

$$\frac{\partial f}{\partial t} + \nabla_x \cdot (\mathbf{v} f) + \nabla_v \cdot (\dot{\mathbf{v}} f) = 0 \quad \text{(P-C)}$$

and the mass density

$$\rho(\mathbf{x}) = \int f \; d^3 v$$

Multiplying (B-T) by vector $\mathbf{v}$ and integrating over $d^3 v$, we get the last Jeans' equation

$$\frac{\partial \rho \bar{\mathbf{v}}}{\partial t} + \nabla_x (\rho \overline{\mathbf{v}\mathbf{v}}) - \nabla(\rho \Phi) = 0$$

Here,

$$\begin{aligned} \bar{\mathbf{v}} &= \rho^{-1} \int \mathbf{v} \, f \, d^3 v \\ \overline{v_i v_j} &= \rho^{-1} \int v_i v_j \, f \, d^3 v \end{aligned}$$

but what about collisions? One simple model is

$$\begin{aligned} d\mathbf{x} &= \mathbf{v} dt \\ d\mathbf{v} &= -\nabla \Phi(\mathbf{x}) dt + \sigma(\mathbf{x}) d\mathbf{w}(t) \end{aligned}$$

inserting this in (B-T), and taking fluctuation averages,

$$\frac{\partial f}{\partial t} + \dot{\mathbf{v}} \cdot \nabla_v f - \nabla \Phi \cdot \nabla_x f + \frac{1}{2} (\sigma \cdot \nabla_v)^2 f = 0.$$

Now, integrate over d^3v, notice if $\sigma(\mathbf{x})$ depends only on $\mathbf{x}$, therefore

$$\int v_i \frac{\partial^2 f}{\partial v_j \partial v_k} d^3v = -\delta_{ij} \int \frac{\partial f}{\partial v_k} d^3v = 0$$

we recover Jeans' equation, even with collisions. What do these collisions look like?

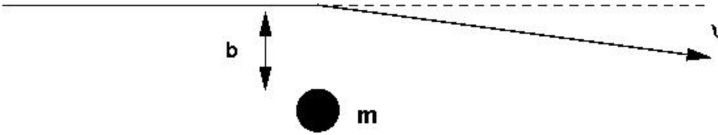


Figure: Impact parameter model

Velocity distributions are given by Fokker-Planck eq. (Spitzer and Härn, '58), and kicks ψ are typically very small:

$$\Delta v \approx \frac{2Gm}{bv}$$

and

$$\frac{\Delta v}{v} \approx \psi \sim \frac{1}{N^{2/3}}$$

where $N =$ number of stars in the system. Langevin equation is equivalent to Fokker-Planck equation. For example, Balescu's book.

Stochastic Dyer-Roeder equation: start with Sachs' equations for shear (σ), ray separation θ, in free space with scattered point-like particles:

$$\begin{aligned} \frac{d\sigma}{ds} + 2\theta\sigma &= \mathcal{F} \\ \frac{d\theta}{ds} + \theta^2 + |\sigma|^2 &= 0 \end{aligned}$$

σ is complex, $\mathcal{F}$ is the Weyl term, and s is an affine parameter - related to redshift z.

$$\theta = \frac{1}{2}\frac{d}{dz} ln(A)$$

where $A \propto D^2$ is the beam area, get two eqs.,

$$\begin{aligned} \frac{d\sigma}{ds} + 2\frac{1}{D}\frac{dD}{ds}\sigma &= \mathcal{F} \\ \frac{1}{D}\frac{d^2D}{ds^2} + |\sigma|^2 &= 0. \end{aligned}$$

In Lagrangian coordinates (contract with redshift z), the Weyl term to 1^{st} order has derivatives of the gravitational potential $\Phi(x, y)$, with $\mathbf{x} = x + i\, y$:

$$\mathcal{F} = \frac{1}{c^2}(1+z)^2 \frac{d^2\Phi}{d\mathbf{x}^2}.$$

Light "sees" shearing forces orthogonal to congruence and problem is essentially 2-D.

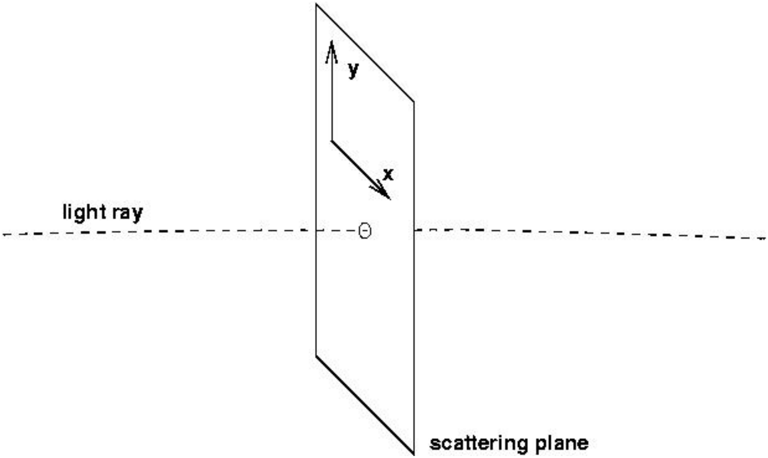


Figure: 2-D character of light scattering

Correlation length is about 7 cells, i.e. ~ 7 Mpc at $z = 0$.
Softened (2-3 cells) shears are normal in < 128 Mpc.

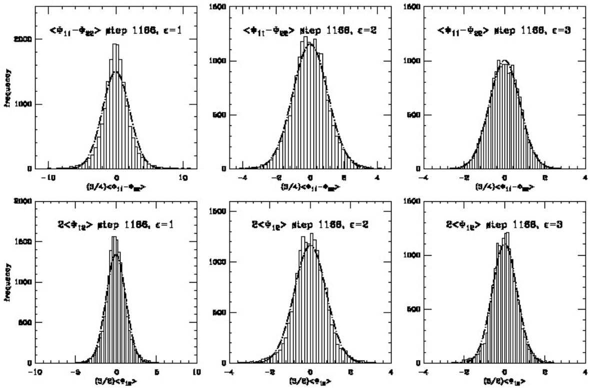


Figure: Shearing forces, from H. Couchman's code

More useful form for 1st:

$$D^2\sigma = \int_0^s D^2(s')\mathcal{F}(s')ds'.$$

Expressing the affine parameter in terms of the redshift

$$s = \int_0^z \frac{d\xi}{(1+\xi)^3\sqrt{1+\Omega\xi})}$$

Yields a generalized Dyer-Roeder eq.

$$\begin{aligned} &(1+z)(1+\Omega z)\frac{d^2D}{dz^2} \\ &+(\frac{7}{2}\Omega z + \frac{\Omega}{2} + 3)\frac{dD}{dz} \\ &\qquad + \frac{|\sigma(z)|^2}{(1+z)^5}D \quad = \quad 0. \end{aligned}$$

Shear can be well approximated by

$$\sigma(z) = \gamma \frac{3\Omega}{8\pi(D(z))^2} \times \int_0^z (D(\xi))^2 (1+\xi)(1+\Omega\xi)^{-\frac{1}{2}} dw(\xi)$$

where $w(z)$ is a complex (2-D) B-motion. Constant $\gamma \approx 0.62$ was determined by N-body simulations.

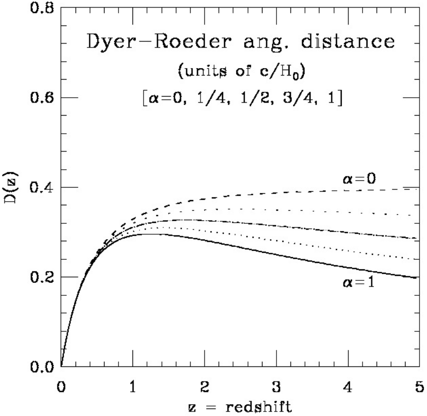


Figure: Shear free Dyer-Roeder $D(z)$

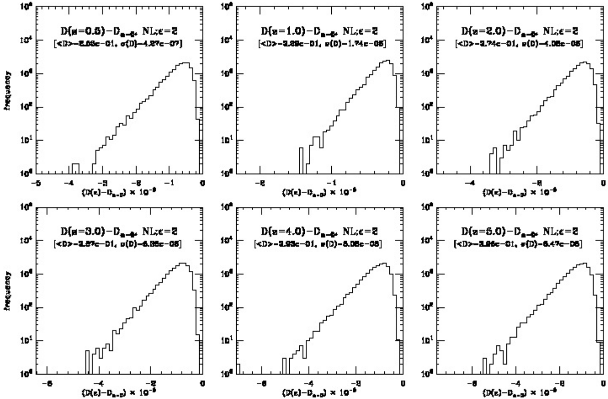


Figure: $D(z)$ histograms at $0 \leq z \leq 5$. Non-linear integration. Scales for the abscissas are: 10^{-6} for $z = 1/2$, 10^{-5} for $z = 1, 2, 3, 4, 5$.

Comments:

- Long ago, a 2-D version of Fokker-Planck eq. for $f(E, J)$ was used by BGK to get King Model (1965), Lightman and Shapiro (1977) etc. Since late 1980s, SDE (Langevin) simulation methods are much improved.
- SDE simulations will not yield details on clustering.
- However, they will be useful as initial conditions for N-body
  - power spectrum is easy to implement: $|v| \propto |k|$.
  - the local temperature $T \propto |v|^2$.
- M-C procedures will complement N-body simulations, not replace.
- SDE simulations are particularly useful in high dimensions, i.e. $D \geq 3$, particularly when there are many species.
- SDEs get distributions right, not local details.

References:

- W. C. Saslaw, *Gravitational Physics of Stellar and Galactic Systems*, Cambridge, 1987.
- R. Balescu, *Equilibrium and Nonequilibrium Stat. Mechanics*, Wiley Interscience, 1975.
- G. Milstein, *Numerical Itegration of Stochastic Differential Equations*, Kluwer, 1995.
- C.C. Dyer and R.C. Roeder, Astrophysical J., 180, pp. L31-L34, 1972.
- S. Seitz and P. Schneider, Astronomy and Astrophysics, 287, pp. 349-360, 1994.
- H.M.P. Couchman, et al, MNRAS, 308, pp. 180-201, 1998.
- W. Petersen, SINUM, 35, no. 4, pp. 1439-1451, 1998.
- W. Petersen, Stoch. Analysis and Appl., 22, no. 4, pp. 989-1008, 2004.