

Particle Transport,
Deposition and Removal

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Brownian Motion

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Outline

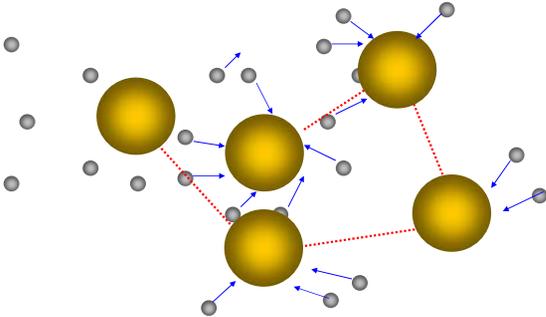
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- Introduction to Aerosols
- Drag Forces
- Cunningham Corrections
- Lift Forces
- **Brownian Motion**
- Particle Deposition Mechanisms
- Gravitational Sedimentation
- Aerosol Coagulation

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A Particle under Random Molecular Impact

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Langevin Equation $\Rightarrow \frac{du}{dt} + \beta u = n(t)$

$\beta = 3\pi\mu d / C_c m = 1/\tau$

N(t) = White Noise

Spectral Intensity $\Rightarrow S_{nn} = \frac{2kT\beta}{\pi m}$

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Brownian Motion - Solving a Stochastic Equation

Autocorrelation Function

$R(\tau) = \overline{u(t+\tau)u(t)}$

Fourier Transform

$$R_{uu}(\tau) = \frac{1}{2} \int_{-\infty}^{+\infty} e^{i\omega\tau} S_{uu}(\omega) d\omega$$

Fourier Transform

$$S_{uu}(\omega) = \frac{1}{\pi} \int_{-\infty}^{+\infty} e^{-i\omega\tau} R_{uu}(\tau) d\tau$$

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Brownian Motion - Solving a Stochastic Equation

System Function

$$S_{uu}(\omega) = |H(\omega)|^2 S_{mm}(\omega)$$

System Function

$$H(\omega) = \frac{1}{i\omega + \beta}$$

Response Power Spectrum

$$S_{uu}(\omega) = \frac{2kT\beta / \pi m}{\omega^2 + \beta^2}$$

Autocorrelation

$$R_{uu}(\tau) = \frac{kT}{m} e^{-\beta|\tau|}$$

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Brownian Motion

Mass Diffusivity

$$D = \frac{1}{2} \frac{d}{dt} \overline{x^2(t)}$$

Position

$$x(t) = \int_0^t u(t_1) dt_1$$

Variance

$$\overline{x^2(t)} = \int_0^t \int_0^t R_{uu}(\tau_1 - \tau_2) d\tau_1 d\tau_2$$

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Variance

$$\overline{x^2(t)} = 2 \int_0^t (t-\tau) R_{uu}(\tau) d\tau$$

Diffusivity

$$D = \int_0^\infty R_{uu}(\tau) d\tau$$

Diffusivity

$$D = \frac{kT}{\beta m} = \frac{kTC_c}{3\pi\mu d}$$

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Brownian Motion -Markov Process Fokker-Planck Approach

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Fokker-Planck Equation

$$\frac{\partial f}{\partial t} - \frac{\partial}{\partial u} (\beta u f) = \frac{kT\beta}{m} \frac{\partial^2 f}{\partial u^2}$$

Probability Density

$$f = \frac{1}{\sqrt{2\pi kT/m}} e^{-\frac{mu^2}{2kT}}$$

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Brownian Motion in a Force Field

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Langevin Equation

$$\ddot{x} + \beta \dot{x} - \frac{F(x)}{m} = n(t)$$

$$F(x) = -\frac{\partial V(x)}{\partial x}$$

Fokker-Planck Equation

$$\frac{\partial f}{\partial t} = -\frac{\partial(\dot{x}f)}{\partial x} + \frac{\partial}{\partial \dot{x}} \left[\left(\beta \dot{x} - \frac{1}{m} F(x) \right) f \right] + \frac{kT\beta}{m} \frac{\partial^2 f}{\partial \dot{x}^2}$$

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Brownian Motion in a Force Field

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Probability Density

$$f = C_0 \exp \left\{ -\frac{m}{kT} \left[\frac{\dot{x}^2}{2} - \int_0^x \frac{F(x_1) dx_1}{m} \right] \right\}$$

$$f = C_0 \exp \left\{ -\frac{1}{kT} \left[\frac{m\dot{x}^2}{2} + V(x) \right] \right\}$$

Gravitational Field

$$f = C_0 e^{-\frac{m\dot{x}^2}{2kT}} e^{-\frac{mg(x-x_0)}{kT}}$$

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Computer Simulation Procedure

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White Noise

$$\overline{n(t)} = 0$$

$$\overline{n(t_1)n(t_2)} = 2\pi S_{nn} \delta(t_1 - t_2)$$

- Choose a time step ($\Delta t \ll \tau$)
- Generate a sequence of uniform random numbers ($0 < U < 1$)
- Transform to Gaussian random numbers.

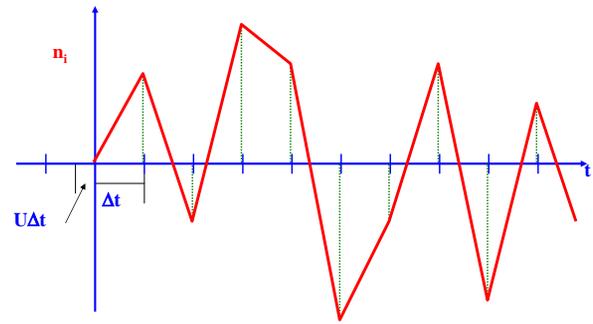
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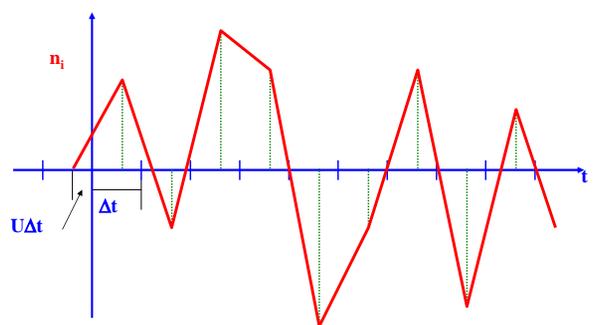
Computer Simulation Procedure Clarkson University

- $G_1 = \sqrt{-2 \ln U_1} \cos 2\pi U_2$
- $G_2 = \sqrt{-2 \ln U_1} \sin 2\pi U_2$
- Amplitude of the Brownian force is given by $n(t_i) = G_i \sqrt{\frac{\pi S_{nn}}{\Delta t}}$
- The generated sample of Brownian force need to be shifted by $U\Delta t$

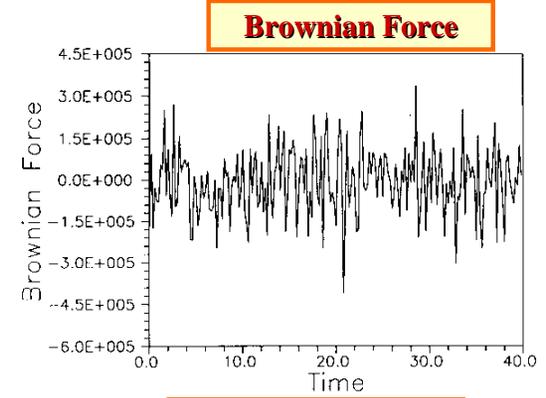
Sample Simulated White Noise Process Clarkson University



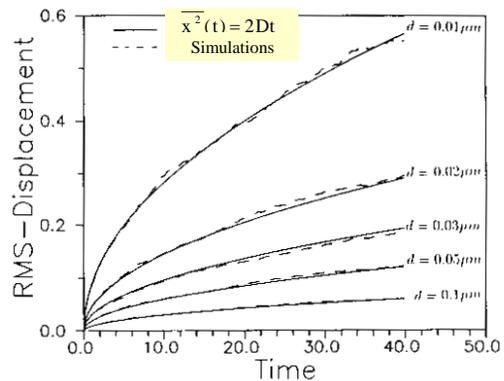
Sample Simulated White Noise Process Clarkson University



Particle Dispersion and Deposition in Viscous Sublayer Clarkson University



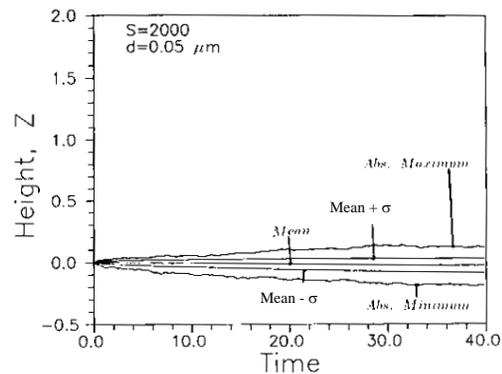
Particle Dispersion in Viscous Sublayer



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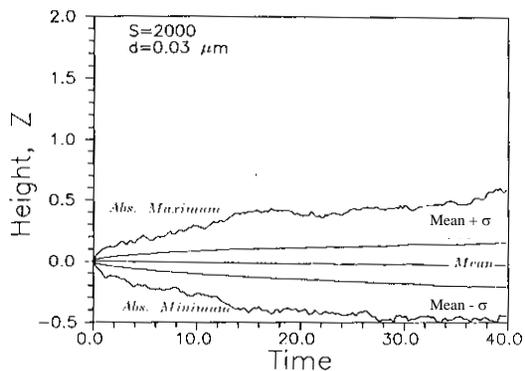
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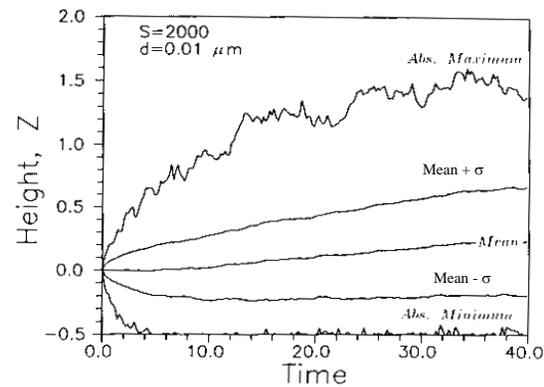
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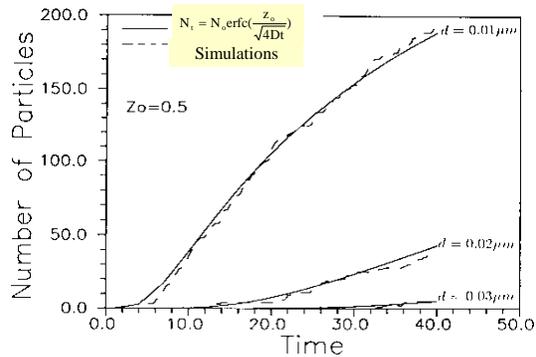
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Particle Dispersion in Viscous Sublayer



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Java Applet for Brownian Motion

Equation of Motion

$$\frac{d\mathbf{u}^p}{dt} = \frac{1}{\tau} (\mathbf{u}^f - \mathbf{u}^p) + \mathbf{g} + \mathbf{n}(t)$$

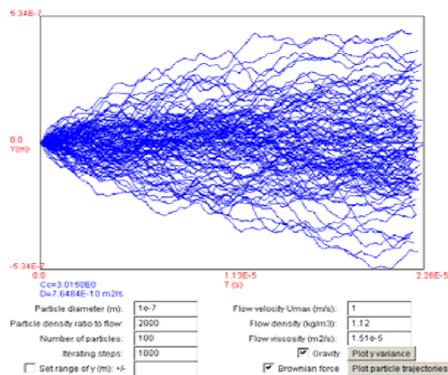
Variance

$$\sigma_y^2(t) = 2Dt$$

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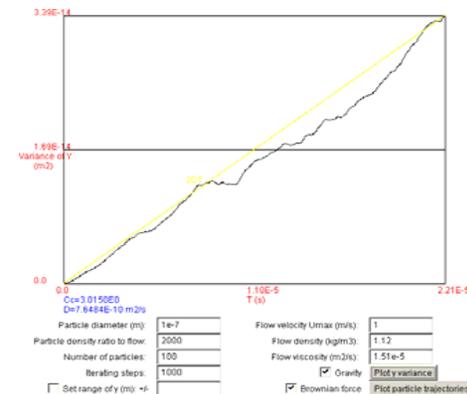
Particle Dispersion -Java Applet for particle trajectory analysis



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