UN5390: Scientific Computing I

Michigan Technological University
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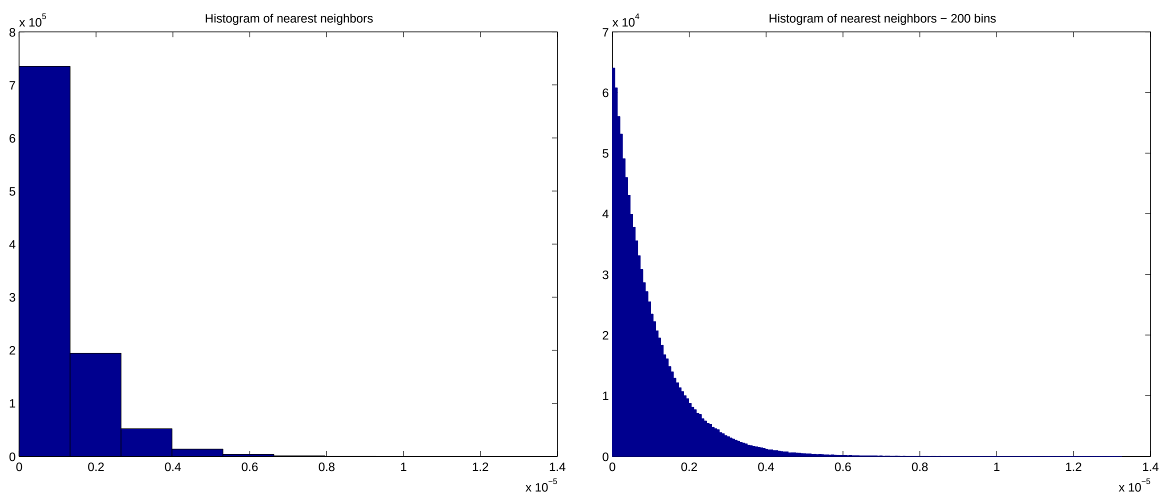
Assignment # 01
John Sanderson(`john@mtu.edu`) · Dr. Jane Jameson(`jane@mtu.edu`)

Problem 1

Eqn. 39.3 in our textbook [1] gives the number of collisions of molecules per unit time (and per unit area of wall surface) [2, 3] in spherical polar co-ordinates and it reads

$$d\nu \;=\; \frac{N}{V}\,\left(\frac{m}{2\pi\,kT}\right)^{3/2}\; e^{-mv^2/2kT}\; v^3\;\sin\theta\;\cos\theta\; d\theta\; d\phi\; dv \tag{1.1}$$



(a) Generic

(b) 200 bins

Figure 1: Histogram of nearest neighbors

In order to find the number of impacts of gas molecules on unit area of the wall per unit time for which the angle between the direction of velocity of the molecule and the normal to the surface lies between θ and $\theta\,+\,d\theta$, we need to integrate the above expression with respect to. ϕ and v. [4]

$$d\nu_\theta \;=\; \frac{N}{V}\,\left(\frac{m}{2\pi\,kT}\right)^{3/2}\;\left[\int_0^{2\pi}\;\int_0^{\infty}\; v^3\; e^{-mv^2/2kT}\; dv\; d\phi\right]\;\sin\theta\;\cos\theta\; d\theta$$

$$d\nu_\theta \;=\; 2\,\pi\,\frac{N}{V}\,\left(\frac{m}{2\pi\,kT}\right)^{3/2}\,\left[\int_0^\infty\,v^3\,e^{-mv^2/2kT}\,dv\,\right]\,\sin\theta\;\cos\theta\;d\theta$$

Using the integral

$$\int_0^\infty\,x^m\,e^{-ax^2}\,dx \;=\; \frac{\Gamma[(m+1)/2]}{2\,a^{(m+1)/2}} \tag{1.2}$$

and the relation, $\Gamma(n+1) \;=\; n!$ (for integral values of n), we obtain

$$d\nu_\theta \;=\; 2\,\pi\,\frac{N}{V}\,\left(\frac{m}{2\pi\,kT}\right)^{3/2}\,\left[\frac{1}{2\left(\frac{m}{2kT}\right)^2}\right]\,\sin\theta\;\cos\theta\;d\theta$$

Simplifying, we have

$$d\nu_\theta \;=\; \frac{N}{V}\,\left(\frac{2\,k\,T}{m\,\pi}\right)^{1/2}\,\sin\theta\;\cos\theta\;d\theta \tag{1.3}$$

Problem 2

Integrating Eqn. (1.1) with respect to θ and ϕ, we get the number of impacts of gas molecules on unit area of the wall per unit time for which the absolute magnitude of the velocity lies between v and $v + dv$ as [4]

$$d\nu_v = \frac{N}{V} \left(\frac{m}{2\pi\, kT}\right)^{3/2} \left[\int_0^{2\pi} \int_0^{\pi/2} \sin\theta\ \cos\theta\ d\theta\ d\phi\right] v^3\, e^{-mv^2/2kT}\, dv$$

$$d\nu_v = 2\,\pi\, \frac{N}{V} \left(\frac{m}{2\pi\, kT}\right)^{3/2} \left[\int_0^{\pi/2} \sin\theta\ \cos\theta\ d\theta\right] v^3\, e^{-mv^2/2kT}\, dv \tag{2.1}$$

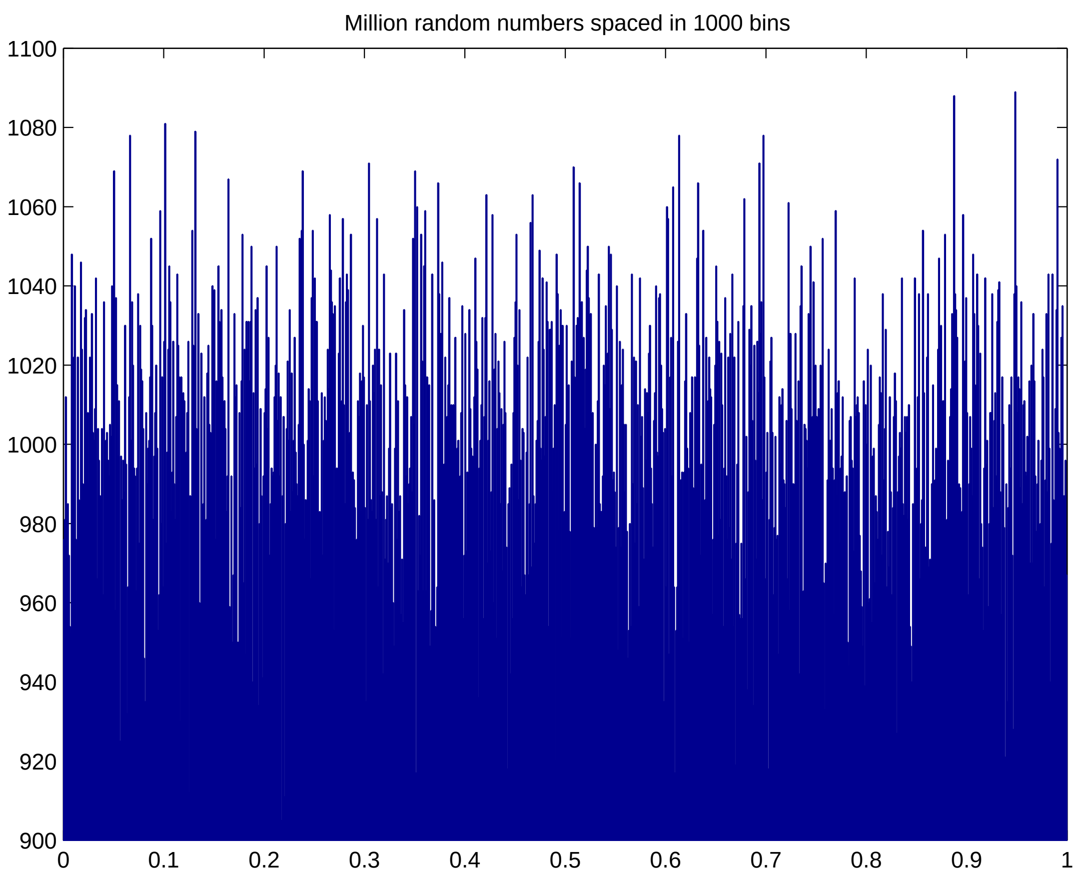


Figure 2: Million random numbers spaced in 1000 bins

Let us consider

$$I \;=\; \int_0^{\pi/2} \sin\theta\; \cos\theta\; d\theta$$

Taking $\cos\theta \;=\; \mu$, we get $d\mu \;=\; -\sin\theta\; d\theta$. When, $\theta \;=\; 0$, $\mu \;=\; 1$ and when $\theta \;=\; \pi/2$, $\mu \;=\; 0$. Thus,

$$I \;=\; -\int_1^0 \mu\; d\mu \;=\; \frac{1}{2} \tag{2.2}$$

Using Eqn. (2.2) in (2.1), we get

$$d\nu_v \;=\; 2\,\pi\, \frac{N}{V}\; \left(\frac{m}{2\pi\, kT}\right)^{3/2}\; \left(\frac{1}{2}\right)\; v^3\; e^{-mv^2/2kT}\; dv$$

Simplifying, we get

$$d\nu_v \;=\; \frac{N}{V}\; \pi\; \left(\frac{m}{2\pi\, kT}\right)^{3/2}\; v^3\; e^{-mv^2/2kT}\; dv \tag{2.3}$$

Problem 3

Cross-section of a molecule of radius r is given by [5]

$$\sigma = 4\,\pi\,r^2 \tag{3.1}$$

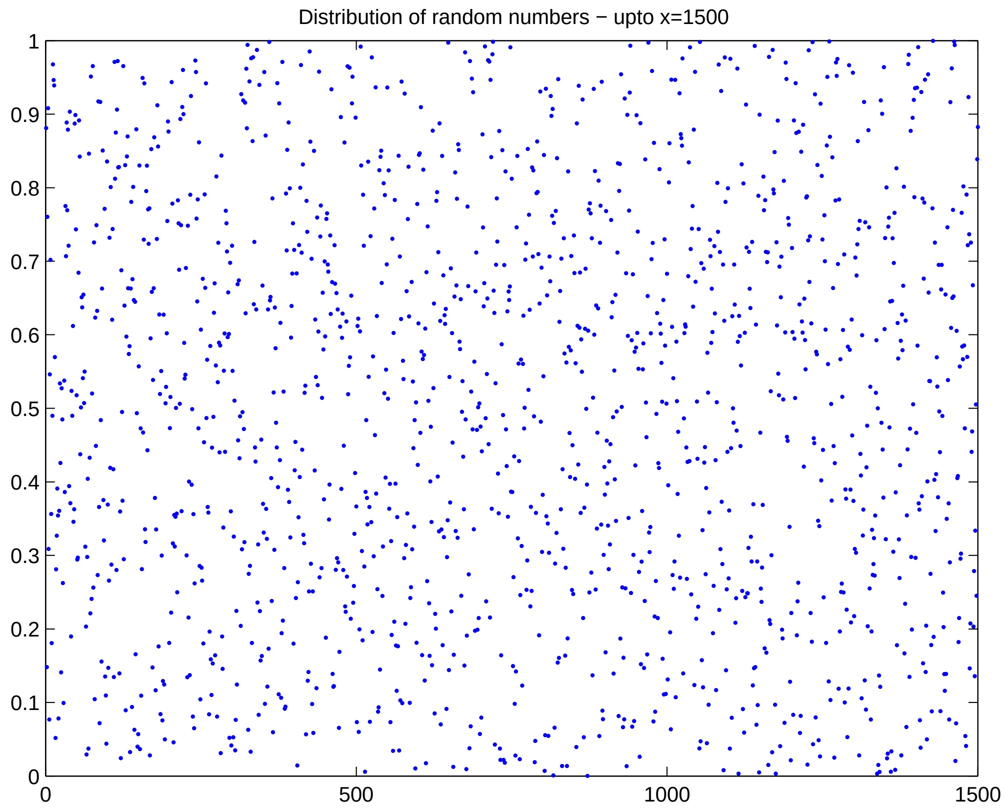


Figure 3: Distribution of random numbers

Eqn. 39.5 in our textbook gives the number of collisions per unit time between one molecule and the rest as

$$\nu' = \frac{N}{V}\,\frac{\pi}{2}\,\left(\frac{m}{\pi\,kT}\right)^{3/2}\,\int_0^\infty e^{-m\tilde{v}^2/4kT}\,\sigma\,\tilde{v}^3\,d\tilde{v} \tag{3.2}$$

Substituting for σ in this, we get

$$\nu' = \frac{N}{V}\,\frac{\pi}{2}\,\left(\frac{m}{\pi\,kT}\right)^{3/2}\,4\,\pi\,r^2\,\int_0^\infty e^{-m\tilde{v}^2/4kT}\,\tilde{v}^3\,d\tilde{v}$$

This integral can be evaluated using Eqn. (1.2). We obtain

$$\nu' = \frac{N}{V}\,\frac{\pi}{2}\,\left(\frac{m}{\pi\,kT}\right)^{3/2}\,4\,\pi\,r^2\,\frac{1}{2\left(\frac{m}{4kT}\right)^2}$$

$$\nu' = \frac{N}{V}\,\frac{\pi}{2}\,\left(\frac{m}{\pi\,kT}\right)^{3/2}\,4\,\pi\,r^2\,\frac{16}{2}\,\left(\frac{kT}{m}\right)^2$$

$$\nu' = 16\,r^2\,\frac{N}{V}\,\sqrt{\pi}\,\left(\frac{kT}{m}\right)^{-3/2}\,\left(\frac{kT}{m}\right)^2$$

Simplifying, we get [1]

$$\nu' = 16\,r^2\,\sqrt{\frac{\pi\,k\,T}{m}}\,\frac{N}{V}$$

$$\nu' = 16\,r^2\,\sqrt{\frac{\pi\,k\,T}{m}}\,P \tag{3.3}$$

Problem 4

The mindmap, created using TikZ/PGF [6], describing the state of the universe is schematically represented in Fig. 4.

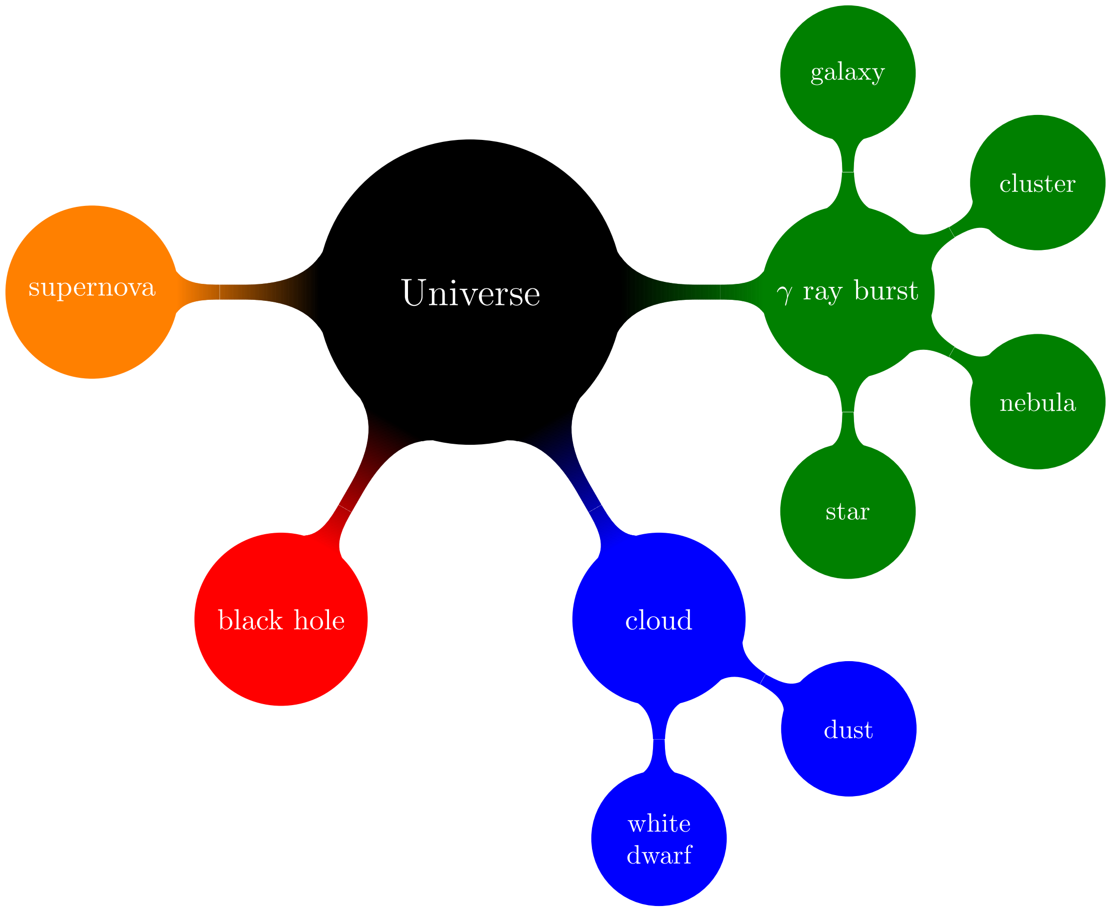


Figure 4: Mind map schematically representing the state of the universe

Most massive stars explode in a supernova when they exhaust their fuel, leaving behind a neutron star or a black hole. But the first stars were much larger than their modern-day counterparts, about 55,000 times the mass of the sun, and may have had a different fate. These very large stars could actually be totally obliterated, seeding their entire host galaxy and even some nearby galaxies with elements ranging from carbon to silicon and leaving nothing at all behind. This image shows the helium core of a star just one day into such an explosive finish. Nuclear reactions are converting helium into oxygen, powering the swirling instabilities that ripple through the star, as shown in Fig. 5.

A single molecule can serve as a nanometer-sized detector of acoustic strain. Such a nanomicrophone has the great advantage that it can be placed very close to acoustic signal

$$\begin{tikzcd}
 & f^*E_V \arrow[rr] \arrow[dl] \arrow[dd, dotted] & & E_V \arrow[dl] \arrow[dd] \\
f^*E \arrow[rr] \arrow[dd] & & E \arrow[dd] & \\
 & U \arrow[rr, dotted] \arrow[dl, dotted] & & V \arrow[dl] \\
M \arrow[rr] & & N &
\end{tikzcd}$$

Figure 5: Boxed representation of the future of our universe

sources and high sensitivities can be achieved. We demonstrate this scheme by monitoring the fluorescence intensity of a single dibenzoterrylene molecule in an anthracene crystal attached to an oscillating tuning fork. The characterization of the vibration amplitude and of the detection sensitivity is a first step towards detection and control of nanomechanical oscillators through optical detection and feedback.

References

[1] N. Giordano and H. Nakanishi. *Computational Physics*. Pearson Prentice Hall, Upper Saddle River, NJ, USA, 2006.

[2] Unknown author. *The Planet Math*. `http://planetmath.org/encyclopedia/Sphere.html`, 2009.

[3] Department of Mathematics and Statistics. *McMaster University*. `http://www.math.mcmaster.ca/~spiro/teaching/hypersphere.pdf`, 2008.

[4] J. D. Watson and F. H. C. Crick. Molecular structure of nucleic acids: A structure for deoxyribose nucleic acid. *Nature*, 171:737, 1953.

[5] A. Einstein, B. Podolsky, and N. Rosen. Can quantum-mechanical description of physical reality be considered complete? *Phys. Rev. B*, 47:777, 1935.

[6] General public. *TEXamples*. `http://www.texample.net/tikz/examples/`, 2014.