# Computational Astrophysics I: Introduction and basic concepts 

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## Random numbers and Monte-Carlo methods

Many physical process can be described in two pictures:

- microscopic, individual, e.g., particle-particle interactions are considered realization usually with help of $\rightarrow$ Monte-Carlo (MC) methods
- macroscopic, only the effective coaction is described $\rightarrow$ usually analytical equations


## Example: Thermodynamics

microscopic: motion of particles, e.g., $\overline{v^{2}}=\frac{1}{N} \sum_{i=1}^{N} v_{i}^{2}$
effective theory: thermodynamics (via statistical physics) averages particle quantities, e.g.,
$\frac{1}{2} m \overline{v^{2}}=\frac{3}{2} k_{\mathrm{B}} T$, so $\overline{v^{2}} \rightarrow T$

## Monte-Carlo simulation

Computer algorithm based on a large number of repeated random experiments to obtain a representative sample of the possible configurations.

## Example: Radiative transfer

- microscopic: interaction of photons with atoms/ions/molecules
$\rightarrow$ MOCASSIN for Monte-Carlo simulation of photon propagation in gaseous nebulae
$\rightarrow$ MCRH (Noebauer 2015) MC radiation hydrodynamics for stellar winds
advantage: arbitrary geometries (e.g., torus) and density distributions (inhomgeneities) and processes; good for scattering (special non-LTE case)
disadvantage: feedback on matter (often iteratively calculated) hard to implement because of MC noise
- macroscopic: radiative transfer equation $($ RTE $)=$ effective theory, i.e. light (intensity $I_{\nu}$ ) instead of single photons
$\rightarrow$ Cloudy spectral synthesis code for astrophysical plasmas
$\rightarrow$ PoWR for emergent spectra of stellar atmospheres
advantage: feedback on matter (non-LTE) via iteration (boundary conditions, e.g., conservation of energy) $\rightarrow$ non-LTE population numbers
disadvantage: hard to program (numerical stability); consistent only for some geometries, usally 1d, e.g., spherical symmetry

For MC methods we need good and many random numbers. Usual base are uniformly distributed random numbers (=same probability for every event). Humans are not a good source for random numbers:


Figure: random numbers, created by colleagues $\rightarrow$ not uniformly distributed, too few $\rightarrow$ direct, severe consequence: don't make up your own passwords!

## Random numbers II

Other sources: rolling dices, tossing coins $\rightarrow$ low rate
most programming languages have a builtin random function, which gives pseudo-random numbers, e.g., in C/C++ integers (!) from [0,RAND_MAX]

```
#include <cstdlib>
    int i = rand () ;
```

- output of next random number of a sequence
- restart by srand(i) ;

To get uniformly distributed random numbers $\in[0 ; 1]$ :
r = rand()/double(RAND_MAX) ;

## Definition

A result (a state) is random, if it was not predictable.
Quality tests for random numbers:

- uniform distribution: random numbers should be fair
- sequential tests: for ntuple repetitions (usually only for $n=2$ und $n=3$ )
- run tests: for monotonically increasing/decreasing sequences, and duration of stay in a certain interval
- and more...
$\rightarrow$ there is no sufficient criterion for randomness tests


## Non-uniform distributions

- random number generators give uniform (pseudo) random numbers $\in[0$, RAND_MAX] $\rightarrow r \in[0,1]$ (from now on)
- we need often different distributions, e.g., normal (Gaussian) distributions or uniform distributions on an interval $x \in[a, b]$
- i.e., we need a transformation that maps $r$ to $x$, so


## Inverse transformation

$$
\begin{equation*}
x=P^{-1}(r) \tag{1}
\end{equation*}
$$

## Non-uniform random numbers II

First, for the case of discrete numbers

- e.g., two events $(1,2)$ with probabilities $p_{1}$ and $p_{2}$, such that

$$
\begin{equation*}
p_{1}+p_{2}=1 \tag{2}
\end{equation*}
$$

How can we choose with help of $r$ ?

- obvious choice: for $r<p_{1}$ event 1 , otherwise event 2

- for the case of 3 possible events with $p_{1}, p_{2}, p_{3}: r<p_{1} \rightarrow$ event 1 , $p_{1}<r<p_{1}+p_{2} \rightarrow$ event 2 , else event 3

- in general for $n$ events, event $i$ is selected if for $r$ :

$$
\begin{equation*}
\sum_{j=0}^{i-1} p_{j} \leq r \leq \sum_{j=0}^{i} p_{j} \quad \text { where } p_{0} \equiv 0 \tag{3}
\end{equation*}
$$

## Non-uniform random numbers III

For continuous distributions:

- need the probability density function $p(x)$, where $p(x) \cdot d x$ is probability that $x$ is in the interval $[x, x+d x]$
- moreover, $p(x)$ is normalized:

$$
\begin{equation*}
\int_{-\infty}^{+\infty} d x p(x)=1 \tag{4}
\end{equation*}
$$

## Example: uniform distribution

$$
p_{\mathrm{u}}(r)= \begin{cases}1, & \text { if } 0 \leq r \leq 1  \tag{5}\\ 0, & \text { else }\end{cases}
$$



## Non-uniform random numbers IV

- for the continuous case (continuum limit $i \rightarrow x$ ) in the Eqn. (3)

$$
\sum_{j=0}^{i-1} p_{j} \leq r \leq \sum_{j=0}^{i} p_{j} \quad \text { where } p_{0} \equiv 0
$$

both sums are equal and become the integral:

$$
\begin{equation*}
P(x)=\int_{-\infty}^{x} p\left(x^{\prime}\right) d x^{\prime}=r \tag{6}
\end{equation*}
$$



This corresponds to the cumulated distribution function

$$
\begin{equation*}
P(x)=\int_{-\infty}^{x} p\left(x^{\prime}\right) d x^{\prime} \tag{7}
\end{equation*}
$$

i.e. the probability to get a random number smaller or equal $x$. Geometrically: fraction of the area left of (smaller than) $x$. We state:

$$
\begin{align*}
P(x) & =r  \tag{8}\\
\Rightarrow x & =P^{-1}(r) \tag{9}
\end{align*}
$$

i.e. exactly as $r$ also $P(x)$ is uniformly distributed.

Therefore, the probability to find $P(x)$ in the interval $[P(x), P(x)+d P(x)]$ is $d P(x)=d r$ (Eq. 8).

The relation between $d P(x)$ and $d x$ is obtained by derivating Eq. (7) $\rightarrow$ Fundamental theorem of calculus:

$$
\begin{equation*}
\frac{d P(x)}{d x}=p(x) \tag{10}
\end{equation*}
$$

for $0 \leq r \leq 1$ it is also:

$$
\begin{equation*}
d P(x)=p(x) d x=p_{\mathrm{u}}(r) d r \tag{11}
\end{equation*}
$$

I.e., because of Eq. (8) is $x$ distributed according to $p(x)$

To obtain such $p(x)$ distributed random numbers, one has to solve Eq. (9)

## Inverse transformation

(1) Insert the required distribution $p(x)$ into:

$$
\begin{equation*}
r=P(x)=\int_{-\infty}^{x} p\left(x^{\prime}\right) d x^{\prime} \tag{12}
\end{equation*}
$$

(2) solve for $x$, i.e. find

$$
\begin{equation*}
P^{-1}(r)=x \tag{13}
\end{equation*}
$$

Not for all $p(x)$ are the corresponding conditions fulfilled (solvable integral and invertibility)

## Non-uniform random numbers VIII

## Example for inverse transformation

Let

$$
\begin{align*}
& p(x)= \begin{cases}a e^{-a x}, & \text { if } 0 \leq x \leq \infty \\
0, & x<0\end{cases}  \tag{14}\\
& P(x)=\int_{0}^{x} a e^{-a x^{\prime}} d x^{\prime}=1-e^{-a x}=r  \tag{15}\\
& \Rightarrow x=-a^{-1} \ln (1-r) \tag{16}
\end{align*}
$$

and $(1-r)$ is exactly distributed as $r$, so:

$$
\begin{equation*}
x=P^{-1}(r)=-a^{-1} \ln r \tag{17}
\end{equation*}
$$

The evaluation of In on a computer is relatively time consuming $\rightarrow$ inverse transformation not always the best method

## Probability distributions in Physics I

Probability distributions are fundamental in, e.g., statistical mechanics and non-relatitivistic quantum mechanics:

- Boltzmann distribution: $p_{i} \propto \exp \left(-\frac{E_{i}}{k_{\mathrm{B}} T}\right)$ for some state $i$ usually: discrete states (statistical mechanics), hence

$$
\begin{equation*}
p_{i}=\frac{N_{i}}{N}=\frac{\exp \left(-\frac{E_{i}}{k_{\mathrm{B}} T}\right)}{\sum_{j=1}^{m} \exp \left(-\frac{E_{j}}{k_{\mathrm{B}} T}\right)} \tag{18}
\end{equation*}
$$

for $N_{i}$ particles in state $i$ and a total number of $N$ particles with $m$ states but might be also continuous, e.g., barometric formula for molecule of mass $m$, height $h$ above ground

$$
\begin{equation*}
\rho(h) \propto \exp \left(-\frac{m g h}{k_{\mathrm{B}} T}\right) \tag{19}
\end{equation*}
$$

$\rightarrow$ computer generated samples via Markov Chain Monte Carlo (MCMC), in particular $\rightarrow$ Metropolis algorithm (see below)

- Maxwell-Boltzmann distribution: continuous distribution of particle velocity in one direction (e.g., radial sightline) with $v_{\text {th }}=\sqrt{\frac{2 k_{\mathrm{B}} T}{m}}$

$$
\begin{equation*}
p\left(v_{x}\right) d v_{x}=\left(\frac{m}{2 \pi k_{\mathrm{B}} T}\right)^{1 / 2} \exp \left(-\frac{m v_{x}^{2}}{2 k_{\mathrm{B}} T}\right) d v_{x}=\frac{1}{v_{\mathrm{th}} \sqrt{\pi}} \exp \left(-\frac{v_{x}^{2}}{v_{\mathrm{th}}^{2}}\right) \tag{20}
\end{equation*}
$$

Application: thermal Doppler broadening of spectral lines where $\Delta \nu_{\text {th }}=\nu_{0} \cdot v_{\text {th }} / c$ Mean value $\left\langle v_{x}^{2}\right\rangle=2 \int_{0}^{\infty} v_{x}^{2} p\left(v_{x}\right) d v_{x}=\frac{1}{2} v_{\mathrm{th}}^{2}=\frac{k_{\mathrm{B}} T}{m}=v_{\mathrm{s}}^{2} \rightarrow$ isothermal sound speed $\rightarrow$ example for a "moment" of a distribution
For 3D, absolute value, speed $v: d^{3} v=d v_{x} d v_{y} d v_{z}=v^{2} d v d \Omega$ integration $\rightarrow 4 \pi v^{2} d v$ and $v^{2}=v_{x}^{2}+v_{y}^{2}+v_{z}^{2}$ :

$$
\begin{equation*}
p(v) d v=4 \pi\left(\frac{m}{2 \pi k_{\mathrm{B}} T}\right)^{3 / 2} v^{2} \exp \left(-\frac{m v^{2}}{2 k_{\mathrm{B}} T}\right) d v \tag{21}
\end{equation*}
$$

Hence, mean $\left\langle v^{2}\right\rangle=\int_{0}^{\infty} v^{2} p(v) d v=\frac{3 k_{\mathrm{B}} T}{m}$
$\rightarrow$ compare definition of $T$ as measure of mean kinetic energy

- in non-relativistic QM (1d):
the squared modulus of the wave function $|\psi(x, t)|^{2}$ gives probability of particle in "volume" $d x$ around $x$ at time $t \rightarrow p(x, t) d x=|\psi(x, t)|^{2} d x$
Physical quantities (observables), have corresponding operators, e.g., momentum $p_{\text {op }} \rightarrow-\imath \hbar \partial / \partial x$; expectation or average value of observable $A$ :

$$
\begin{equation*}
\langle A\rangle=\int \psi^{*}(x, t) A_{\mathrm{op}} \psi(x, t) d x \tag{22}
\end{equation*}
$$

And $\psi$ evolves according to Schrödinger equation

$$
\begin{equation*}
\imath \hbar \frac{\partial \psi(x, t)}{\partial t}=-\frac{\hbar^{2}}{2 m} \frac{\partial^{2} \psi(x, t)}{\partial x^{2}}+V(x, t) \psi(x, t) \tag{23}
\end{equation*}
$$

$\rightarrow$ because of similarity to diffusion equation (with imaginary time), solutions to Eq. (23) can be found by random walk (see below)

- the specific intensity $I_{\nu}(\vec{x}, t, \vec{n}, \nu)=\frac{d E}{d \vec{A} \cdot \vec{n} d \Omega d \nu d t}$ is a 7-dim distribution function on a 4-dim spacetime manifold ( $\vec{x}, t$ ), describing unpolarized radiation. Note: $I_{\nu}=n_{\text {phot }} c h \nu \geq 0$ (where $n_{\text {phot }}$ is photons / volume / solid angle / frequency interval) Moments of the specific intensity (radiation field) $=$ integrals over all directions, in 1 d (plane parallel, spherical symmetry) over $\mu=\cos \theta, n$-th moment: $\frac{1}{2} \int_{-1}^{+1} \mu^{n} I_{\nu}(\mu) d \mu$

| $n$ | symbol | integral | type |
| :--- | :--- | :--- | :--- |
| 0. | $J_{\nu}$ | $=\frac{1}{2} \int_{-1}^{+1} I_{\nu}(\mu) d \mu$ | mean intensity, energy density $E_{\nu}=\frac{4 \pi}{c} J_{\nu}, J_{\nu} \geq 0$ |
| 1. | $H_{\nu}$ | $=\frac{1}{2} \int_{-1}^{+1} \mu I_{\nu}(\mu) d \mu$ | (Eddington-) flux, can be neg. (e.g. "inward" flux) |
| 2. | $K_{\nu}$ | $=\frac{1}{2} \int_{-1}^{+1} \mu^{2} I_{\nu}(\mu) d \mu$ | radiation pressure $K_{\nu}=\frac{c}{4 \pi} P_{\nu}$ |
| 3. | $N_{\nu}$ | $=\frac{1}{2} \int_{-1}^{+1} \mu^{3} I_{\nu}(\mu) d \mu$ | flux-like, i.e., can be negative |

$\rightarrow$ usually: MC simulations of radiation field require large number of runs for individual photons to recover macroscopic quantities $I, J$, etc. correctly

Non-uniform distributions II

## Box-Muller method I

non-uniform distribution:

- with help of the inversion method we can get non-uniform random numbers from uniform random numbers $\rightarrow$ condition: $P(x)$ invertable
- for the Gaussian normal distribution:

$$
\begin{equation*}
p(x)=\frac{1}{\sqrt{2 \pi \sigma^{2}}} \exp \left(-\frac{x^{2}}{2 \sigma^{2}}\right) \tag{24}
\end{equation*}
$$

$P(x)$ is not analytical representable (error function)

- idea: 2d-transformation where:

$$
\begin{equation*}
p(x, y) d x d y=\frac{1}{2 \pi \sigma^{2}} e^{-\left(x^{2}+y^{2}\right) / 2 \sigma^{2}} d x d y \tag{25}
\end{equation*}
$$

- change to polar coordinates:

$$
\begin{equation*}
r=\sqrt{x^{2}+y^{2}} \quad \theta=\tan ^{-1} \frac{y}{x} \tag{26}
\end{equation*}
$$

- let $\rho=r^{2} / 2$ and set $\sigma=1$ :

$$
\begin{equation*}
p(x, y) d x d y=p(\rho, \theta) d \rho d \theta=\frac{1}{2 \pi} e^{-\rho} d \rho d \theta \tag{27}
\end{equation*}
$$

- now generate random numbers $\rho$ according to exponential distribution, so $\rho=-\ln u$ (u standard uniform distributed) and $\theta$ uniform distributed on $[0,2 \pi)$, than

$$
\begin{equation*}
x=\sqrt{-2 \ln u} \cos \theta \quad \text { und } \quad y=\sqrt{-2 \ln u} \sin \theta \tag{28}
\end{equation*}
$$

are each according to Eq. (24) with $\sigma=1$ and $\mu=0$ distributed
Alternative: Rejection method (see below)

Example: Neutron transport

Application for non-uniform random numbers!
Transport of neutrons through matter - one of the first MC applications!

- consider a plate of thickness $t$
- plate is infinite in $z$ and $y$ direction, $x$-axis perpendicular to the plate
- at each point within the plate: probability $p_{\mathrm{c}}$, that neutron gets absorbed (captured) and probability $p_{\mathrm{s}}$ that neutron is scattered
- after each scattering: find scattering angle $\theta$ in xy plane


Determine scattering angle \& scattering path length

1. Isotropic scattering:

$$
\begin{align*}
p(\theta, \phi) d \theta d \phi & =d \Omega / 4 \pi  \tag{29}\\
\text { because of } d \Omega=\sin \theta d \theta d \phi: &  \tag{30}\\
p(\theta, \phi) & =\frac{\sin \theta}{4 \pi} \tag{31}
\end{align*}
$$

obtain $p(\theta)$ and $p(\phi)$ by integration over the complementary angle:

$$
\begin{align*}
& p(\theta)=\int_{0}^{2 \pi} p(\theta, \phi) d \phi=2 \pi \frac{\sin \theta}{4 \pi}=\frac{1}{2} \sin \theta  \tag{32}\\
& p(\phi)=\int_{0}^{\pi} p(\theta, \phi) d \theta=\frac{1}{4 \pi}(-\cos \pi+\cos 0)=\frac{1}{2 \pi} \tag{33}
\end{align*}
$$

I.e. $p(\theta, \phi)=p(\theta) p(\phi) \rightarrow$ independent variables

## Neutron transport III

If random variable $\phi$ is wanted $(p(\phi) \equiv$ const.):

$$
\begin{equation*}
\phi=2 \pi r \tag{34}
\end{equation*}
$$

To get random $\theta$ according to Eq. (32) $\rightarrow$ inversion method:

$$
\begin{align*}
r & =P(\theta)=\int_{0}^{\theta} \frac{1}{2} \sin x d x=-\frac{1}{2}(\cos \theta-\cos 0)  \tag{35}\\
\cos \theta & =1-2 r \tag{36}
\end{align*}
$$

I.e. $\cos \theta$ is uniformly distributed on $[-1 ; 1]$ and $\phi$ on $[0 ; 2 \pi]$. Solve for $\theta$ possible, but unnecessary, as required for $x$ component of the path $\rightarrow$
2. scattering path length:

$$
\begin{equation*}
x=\ell \cos \theta \tag{37}
\end{equation*}
$$

where $\ell$ from $p(\ell) \sim e^{-\ell / \lambda}$ (see example for inversion method):

$$
\begin{equation*}
\ell=-\lambda \ln r \tag{38}
\end{equation*}
$$

$\lambda \rightarrow$ mean free path (e.g., $\lambda=(\sigma n)^{-1}$ )

Algorithm, start at $x=0$ :
(1) determine, if neutron is scattered or captured. If captured: increment number of absorbed neutrons, go to 5 step
(2) scattering: "dice" $\cos \theta$ and $\ell$, move to $x$ position by $\ell \cos \theta$
(3) if $x<0$ : increment number of reflected neutrons, if $x>t$ : increment number of transmitted neutrones; go to 5
(4) repeat step $1-3$ until final result is achieved for all neutrons
(5) repeat step 1-4 with more incident neutrons


