Monte Carlo in silico. A travel guide

Claus Beisbart

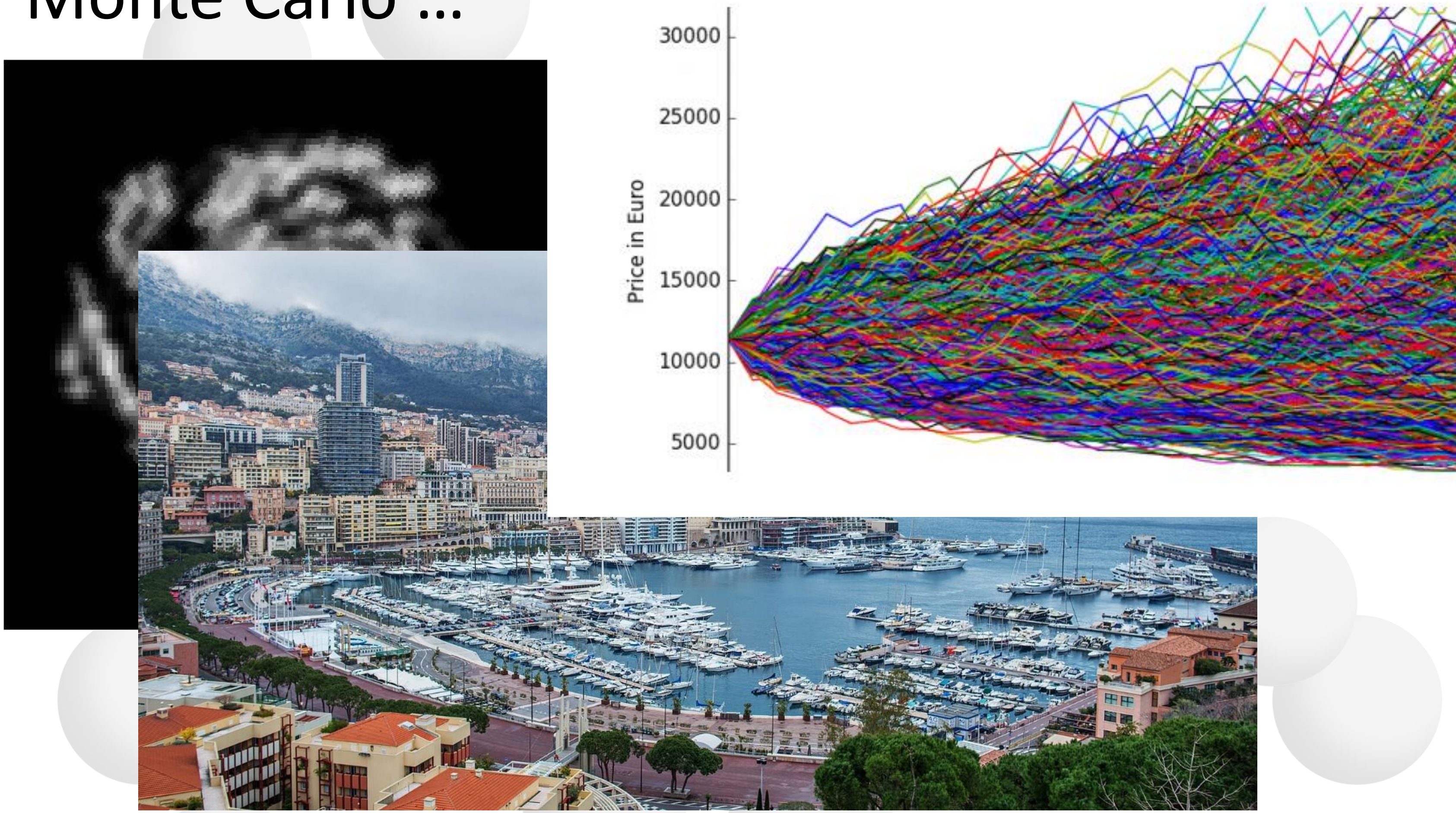
UNIVERSITÄT BERN

Workshop “From Raw Data to Measurement Results – Epistemological Problems in Data Analysis”

TU Dortmund

13.11.2025

Monte Carlo …



… is popular.

Images: B. Nyman (CC BY 2.0), R. Dahlke (spiral galaxy), datascience.eu

Broad aim of this talk:

Philosophical appraisal of Monte Carlo (MC) simulations and techniques

Focus: data analysis in cosmology and astrophysics

Overview

1. Why visit Monte Carlo?

   Philosophical discussions about MC simulations

2. What's up in Monte Carlo?

   Examples of MC methods

3. How large is Monte Carlo?

   A classification of MC methods

4. What's so special about Monte Carlo?

   MC simulations as simulations

5. What do to do with Monte Carlo?

   Functions of MC simulations

Travel guides so far>>>

1. In physics etc., MC methods are widely used.

2. Not much literature in philosophy of science discusses MC as such (exception: Falkenburg 2024).

3. In the early literature, MC simulations are often used as (prime) examples:

- Rohrlich (1990), Humphreys (1994), Galison (1996/1997), Hughes (1999)

4. Later, some authors deny that MC simulations are really simulations.

Grüne-Yanoff & Weirich (2010, p. 30)
“Thus, the Monte Carlo approach does not have a mimetic purpose: It imitates the deterministic system not in order to serve as a surrogate that is investigated in its stead but only in order to offer an alternative computation of the deterministic system’s properties. […] This contrasts with other uses of simulation discussed so far.”

Cf. Hartmann (1996, pp. 8-9), Winsberg (2010, p. 59)

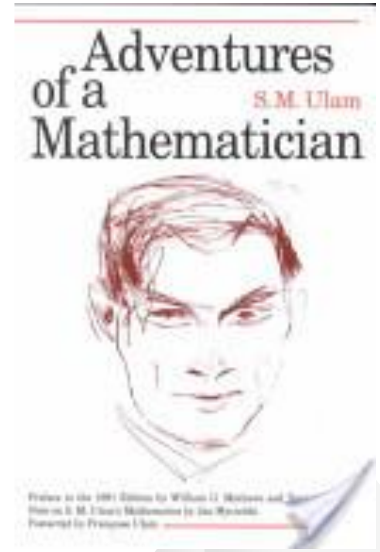
Consequence:

We need a philosophical account of MC methods and simulations!

- Classification
- Functions

2. What‘s up in Monte Carlo?

Images: B. Nyman (CC BY 2.0), R. Dahlke (spiral galaxy), datascience.eu

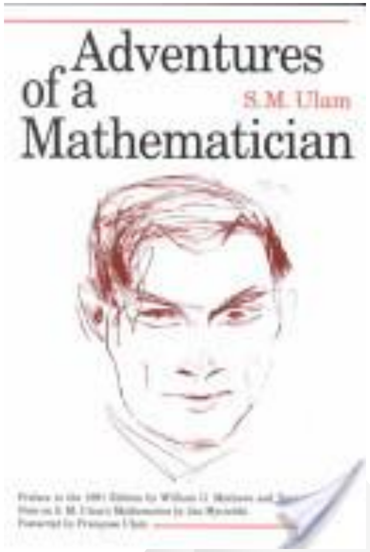


The basic idea

S. Ulam (1991, p. 197):

“[a neutron] can scatter at one angle, change its velocity, be absorbed, or produce more neutrons by a fission of the target nucleus, and so on. The elementary probabilities for each of these possibilities are individually known, to some extent […]. But the problem is to know what a branching of hundreds of thousands or millions will do. One can write down differential equations or integral differential equations for the “expected values”, but to *solve* them […] is an entirely different matter.”

Historical sites



S. Ulam (1991, p. 197 ct.‘d):

“The idea was to try thousands of such possibilities and, at each stage, to select by chance, by a “random number” with suitable probability, the fate or kind of event, to follow it in a line, so to speak, instead of considering all branches. After examining the histories of only a few thousand, one will have a good sample and an approximate answer to the problem.”

Monte Carlo today

SOPHIA (Simulations Of Photo Hadronic Interactions in Astrophysics)

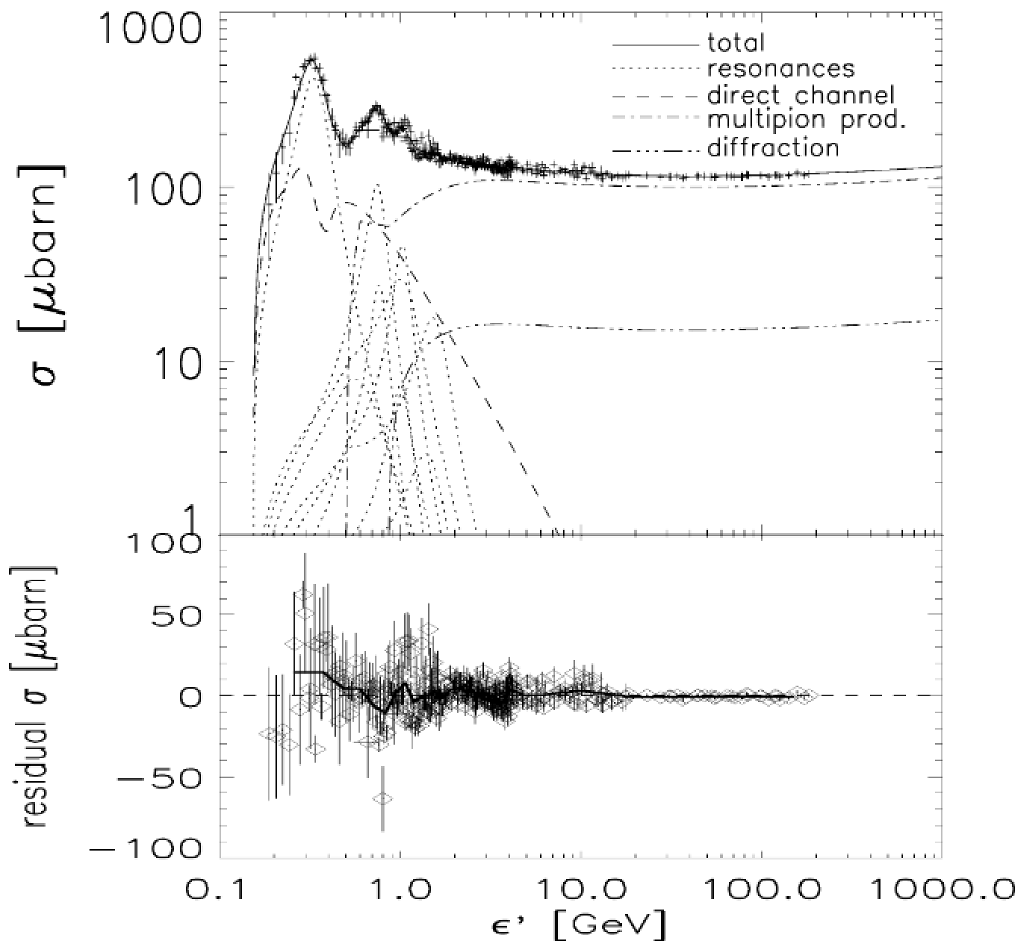
Monte

A. Mücke

[a] U

[c] P

[d] Univ



Monte Carlo today

THE ASTROPHYSICAL JOURNAL, 467:L69–L72, 1996 August 20

THE EFFECT OF LIGHT SCATTERING BY DUST IN GALACTIC HALOS ON EMISSION-LINE RATIOS

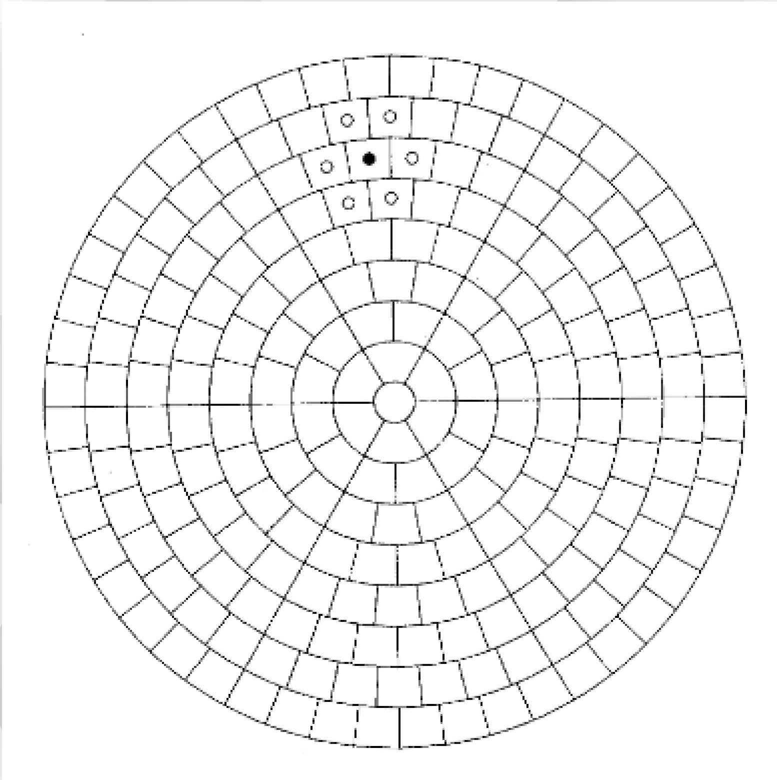
ANDREA FERRARA
Osservatorio Astrofisico di Arcetri, Largo Enrico Fermi 5, I-50125 Firenze, Italy
SIMONE BIANCHI
Dipartimento di Astronomia e Scienza dello Spazio, Università di Firenze, Largo Enrico Fermi 5, I-50125 Firenze, Italy
RALF-JÜRGEN DETTMAR
Astronomisches Institut, Ruhr-Universität Bochum, D-44780 Bochum, Germany
AND
CARLO GIOVANARDI
Osservatorio Astrofisico di Arcetri, Largo Enrico Fermi 5, I-50125 Firenze, Italy
Received 1996 May 8; accepted 1996 June 5

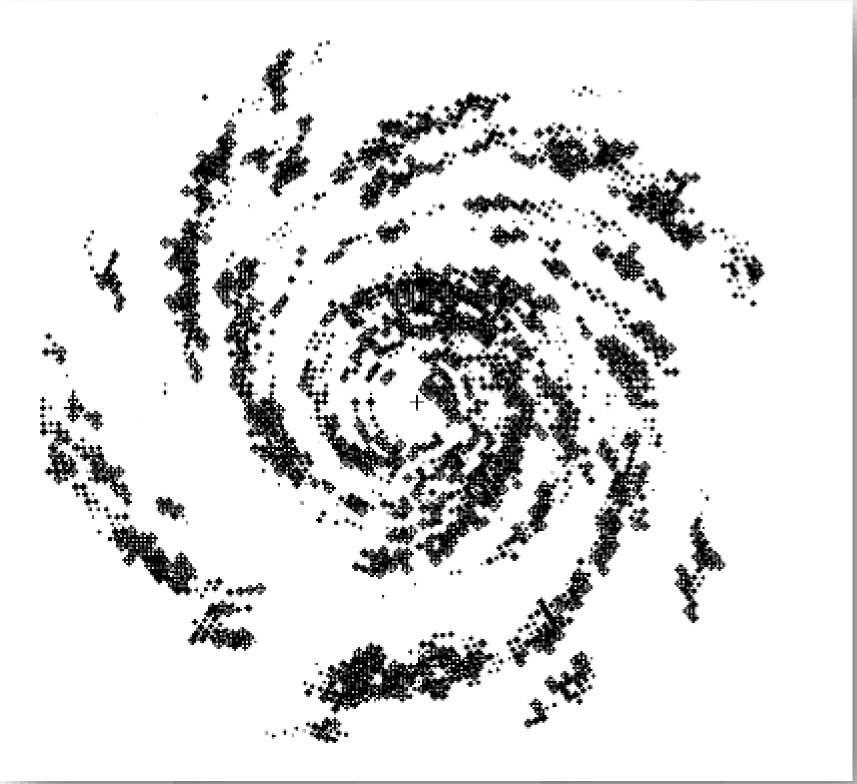
ABSTRACT

We present results from Monte Carlo simulations describing the radiative transfer of Hα line emission, produced both by H II regions in the disk and in the diffuse ionized gas (DIG), through the dust layer of the galaxy NGC 891. This allows us to calculate the amount of light originating in the H II regions of the disk and scattered by dust at high z and compare it with the emission produced by recombinations in the DIG. The cuts of photometric and polarimetric maps along the z-axis show that scattered light from H II regions is still 10% of that of the DIG at $z \sim 600$ pc whereas the degree of linear polarization is small (<1%). The importance of these results for the determination of intrinsic emission-line ratios is emphasized, and the significance and possible implications of dust at high z are discussed.

Subject headings: dust, extinction — ISM: abundances — galaxies: spiral — polarization — radiative transfer — scattering

A Monte Carlo model of galaxy structure





Seiden & Schulman (1986, Fig. 4)

Monte Carlo today

Classical and Quantum
Gravity

Bayesian methods for cosmological parameter estimation from cosmic microwave background measurements

To cite this article: Nelson Christensen *et al* 2001 *Class. Quantum Grav.* **18** 2677

View the article online for updates and enhancements.

Cosmological p

DA

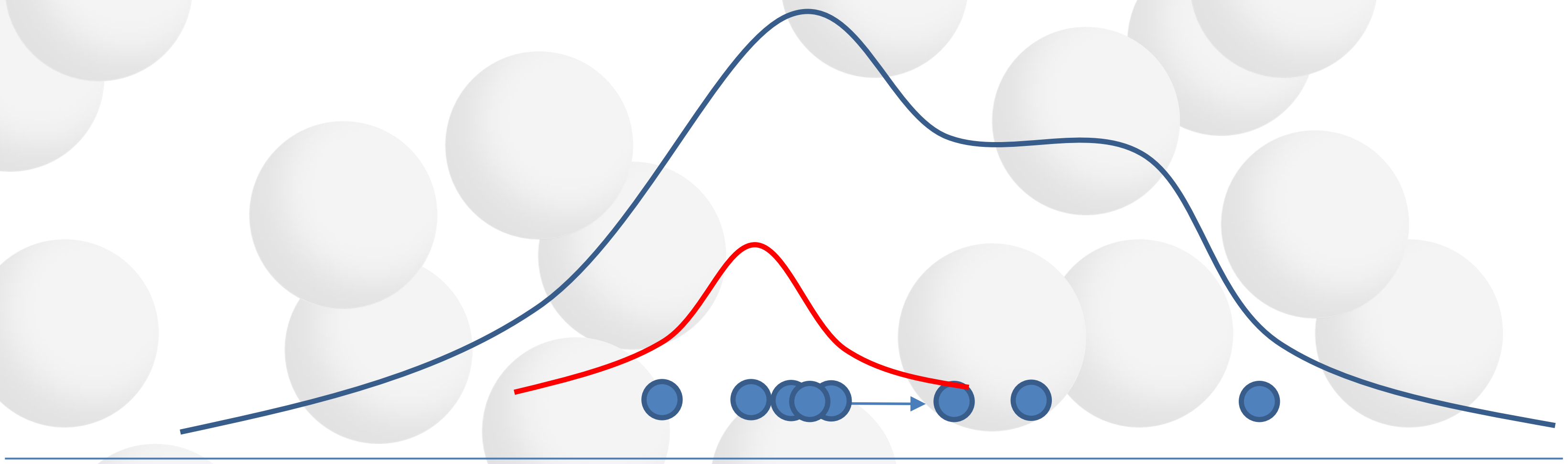
Institu

We present a fast
joint analysis of resu
constraints, including
HST Key Project, 2
Carlo method allows
9 parameter analyse
constraints on the ne
as well as demonstra
appendixes we describe
accuracy correction of results generated from an approximate method. We also discuss the different ways of converting parameter samples to parameter constraints, the effect of the prior, assess the goodness of fit and consistency, and describe the use of analytic marginalization over normalization parameters.

DOI: 10.1103/PhysRevD.66.103511 PACS number(s): 98.80.Es, 02.70.Uu, 14.60.Pq

Metropolis-Hastings: MCMC

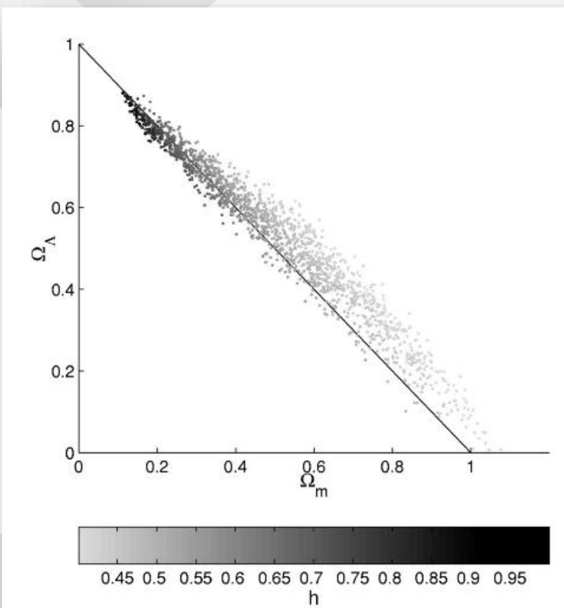
Goal: calculate moments of a probability distribution p $\sim f(x)$ by sampling points from p.
Normalization need not be known.

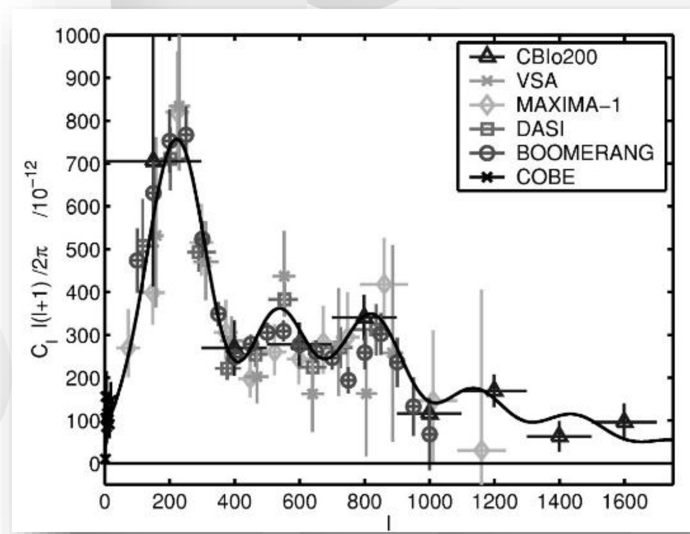


In Bayesian analysis

Calculate (marginalized) posterior probability

$$p(\theta|data)$$





Lewis & Bridle (2002)

3. How large is Monte Carlo?

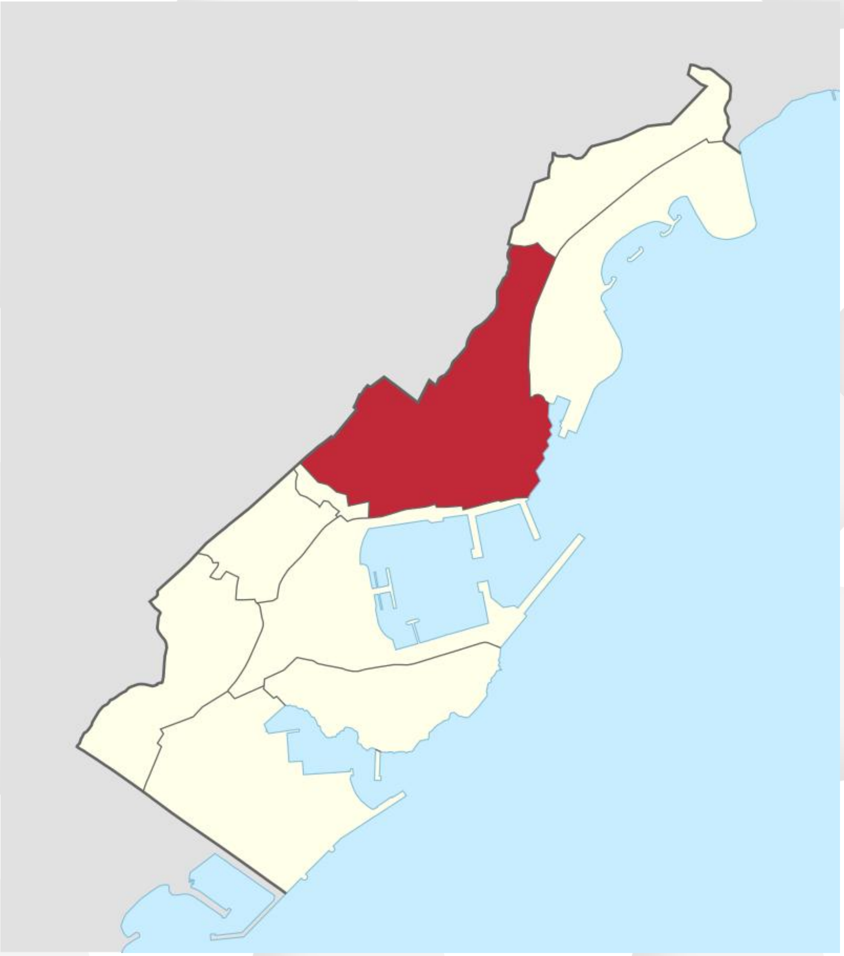
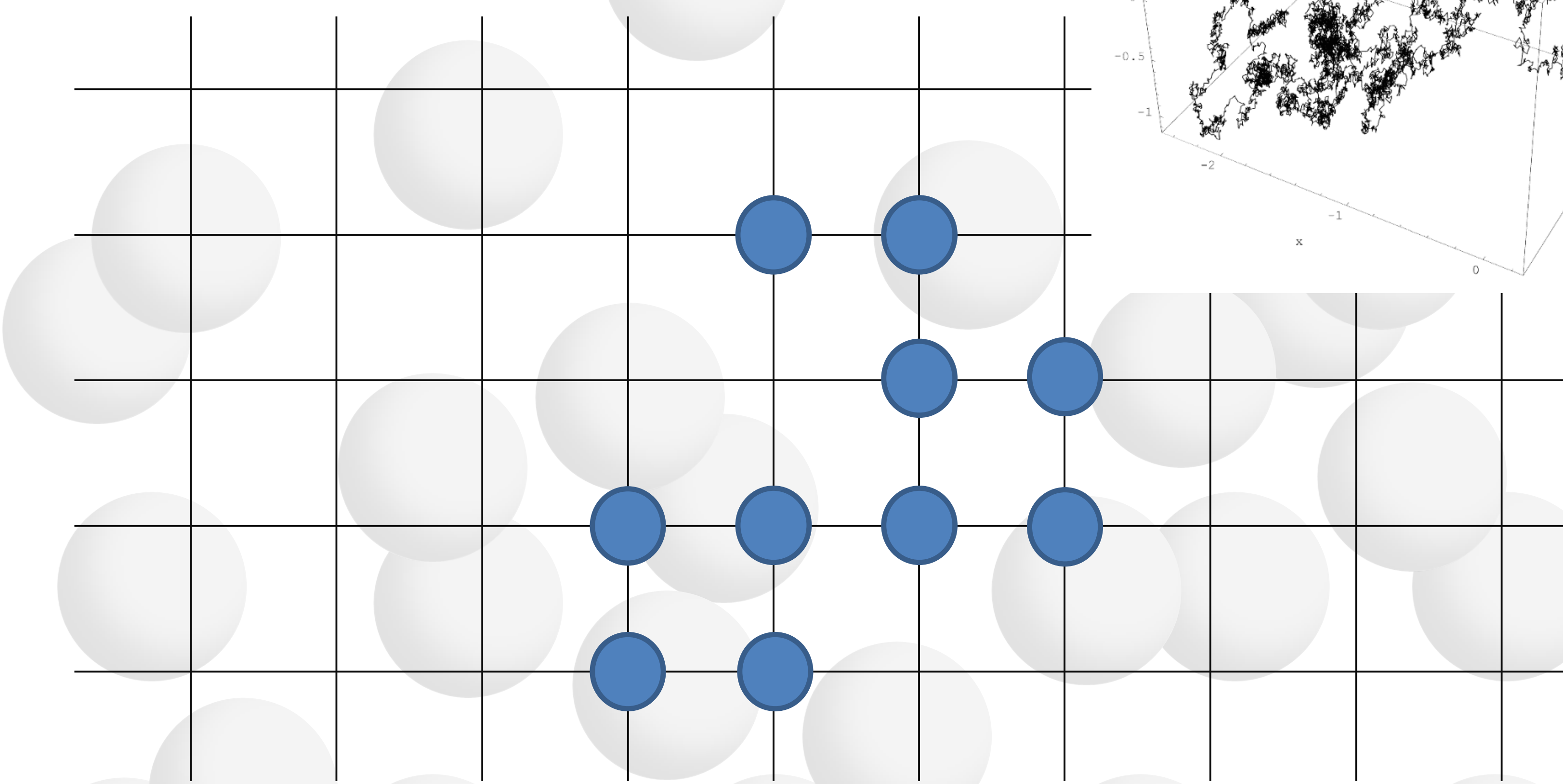


Image: User [NordNordWest](#) ([CC BY-SA 3.0 de](#))

Stochastic dynamics



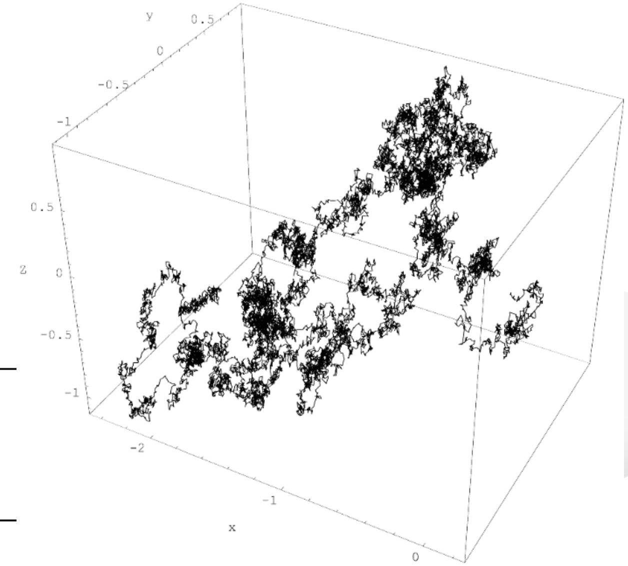


Image: T. J. Sullivan, en.wikipedia.org

Values of empirical characteristics at times i
$\rightarrow$ values of random variables X_i

X_1	X_2	X_3	X_4	X_5
$x_1^{\ 1}$	$x_2^{\ 1}$	$x_3^{\ 1}$	$x_4^{\ 1}$	$x_5^{\ 1}$
$x_1^{\ 2}$	$x_2^{\ 2}$	$x_3^{\ 2}$	$x_4^{\ 2}$	$x_5^{\ 2}$
…	…	…	…	…

sample trajectories

$E[X_1]$

estimate expectation value etc.

(direct) Monte Carlo Simulation

A generalization

Stochastic process: Family of random variables X_i

$\rightarrow$ Use random numbers to evaluate features (expectation values, ...) of stochastic processes.

Name: Stochastic simulation

Mathematical description

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

x_i Random numbers

Another generalization:

$$\mathrm{E}[f] \approx \frac{1}{N}\sum_{i=1}^{N} f(x_i)$$

$$\int_a^b f(x)dx = (b-a)\mathrm{E}_P[f] \approx \frac{b-a}{N}\sum_{i=1}^{N} f(x_i)$$

Monte Carlo integration

x_i Random numbers

Another aspect:

$$\mathrm{E}[f] \approx \frac{1}{N}\sum_{i=1}^{N} p(x_i) f(x_i)$$

$$\int_a^b f(x)p(x)dx = (b-a)\mathrm{E}_P[f] \approx \frac{b-a}{N}\sum_{i=1}^{N} f(x_i)$$

Monte Carlo sampling

x_i Random numbers

Further generalization:

MC methods:

Methods that use random or pseudo-random numbers.

James (1980, p. 1147)

NB. The (pseudo-)random numbers are often defined using a probabilistic description.

How large is Monte Carlo?

Classification>>>

MC methods

…

MC integration

…

MC simulations

Narrow sense

4. What's so special about Monte Carlo?

How does MC simulation qua stochastic simulation work?

Compare to deterministic computer simulations.

Analyzing MC simulations

computer

Computer states display numerical values of solution to model equations

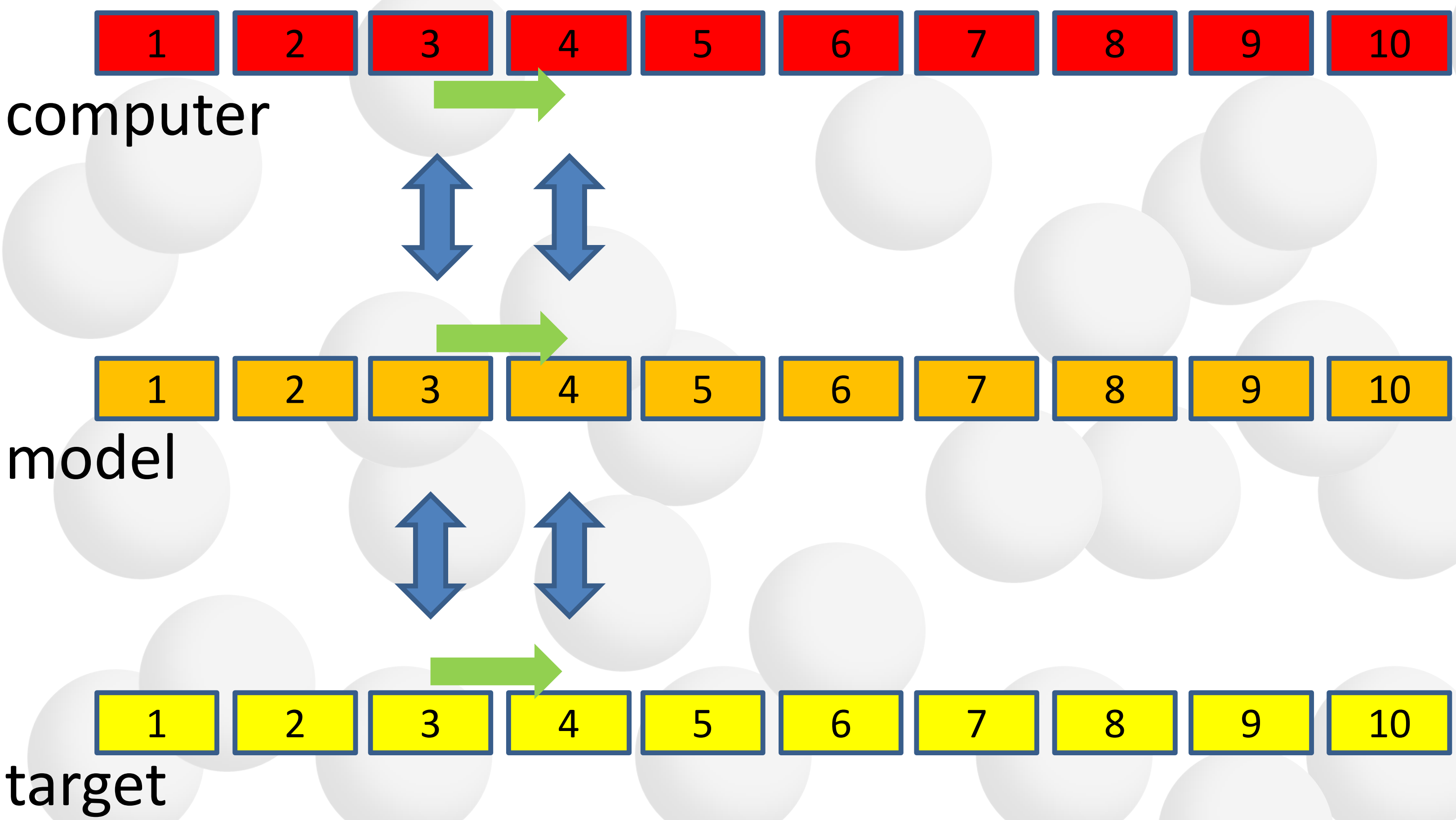
mathematical model

model states trace values of empirical characteristics

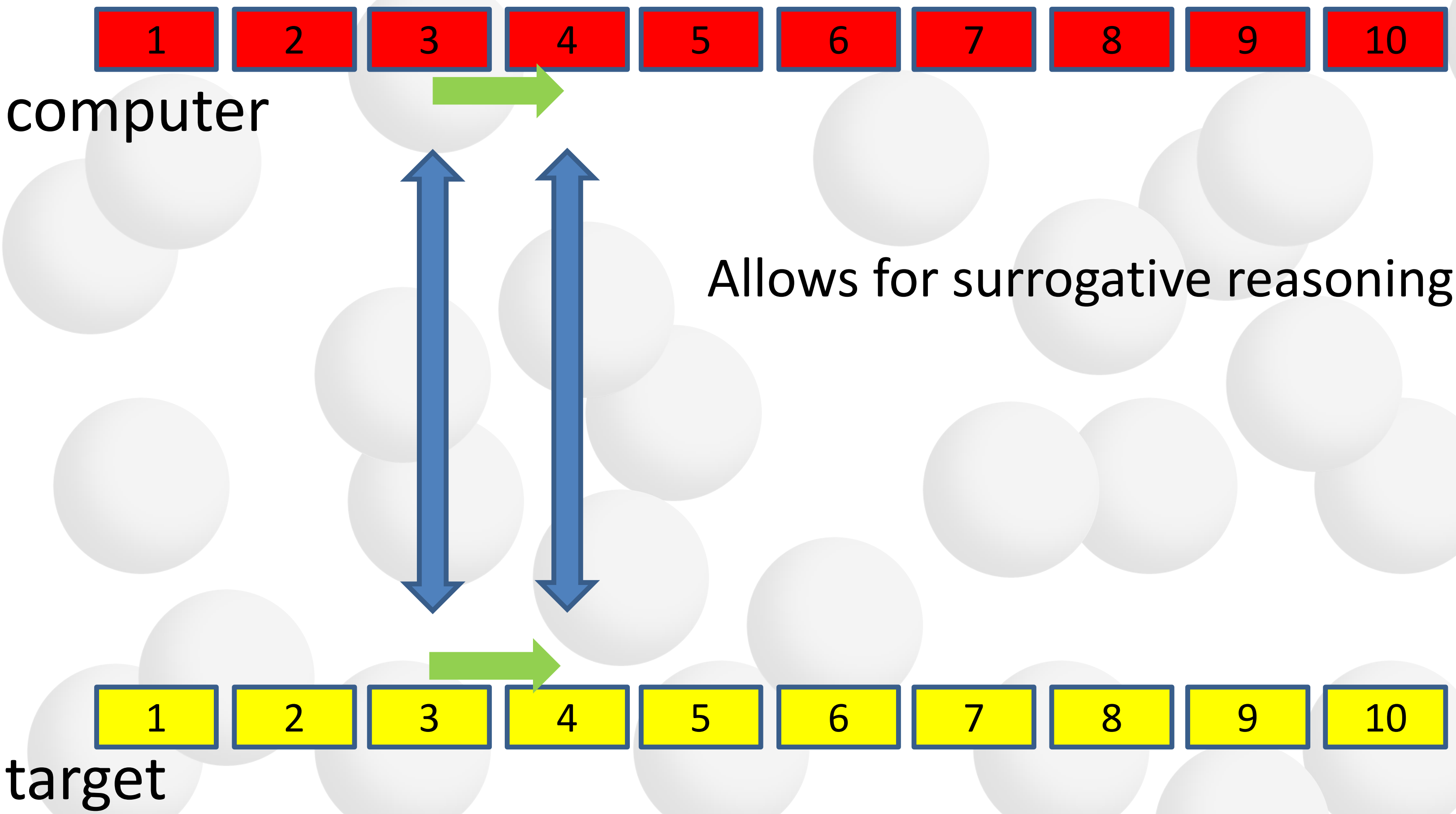
target

Cf. Barberousse et al. (2009), Burks (1975), Zeigler (1976), Norton & Suppe (2001)

Analyzing MC simulations



Analyzing MC simulations



Allows for surrogative reasoning

The story matches well-known definitions of computer simulations:

a. Hartmann (1996, Sec. 2.2): „a simulation imitates one process by another process”.

b. Humphreys (2004, p. 110): Core simulation provide solutions to computational models.

But: determism presumed!

What is different with MC simulations?

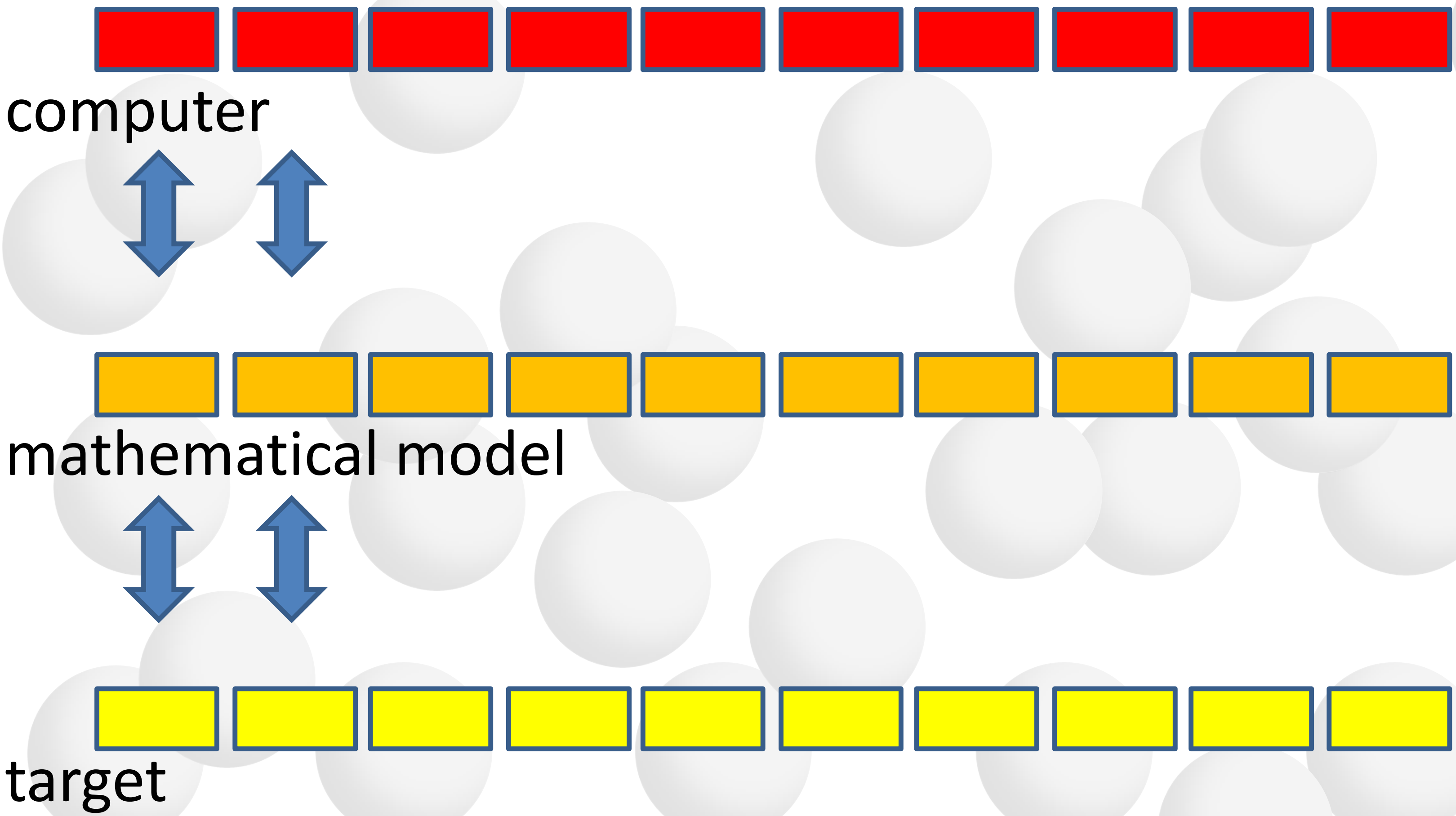
Issue 1>>> Order of computational states

X_1	X_2	X_3	X_4	X_5
$x_1{}^1$	$x_2{}^1$	$x_3{}^1$	$x_4{}^1$	$x_5{}^1$
$x_1{}^2$	$x_2{}^2$	$x_3{}^2$	$x_4{}^2$	$x_5{}^2$
…	…	…	…	…

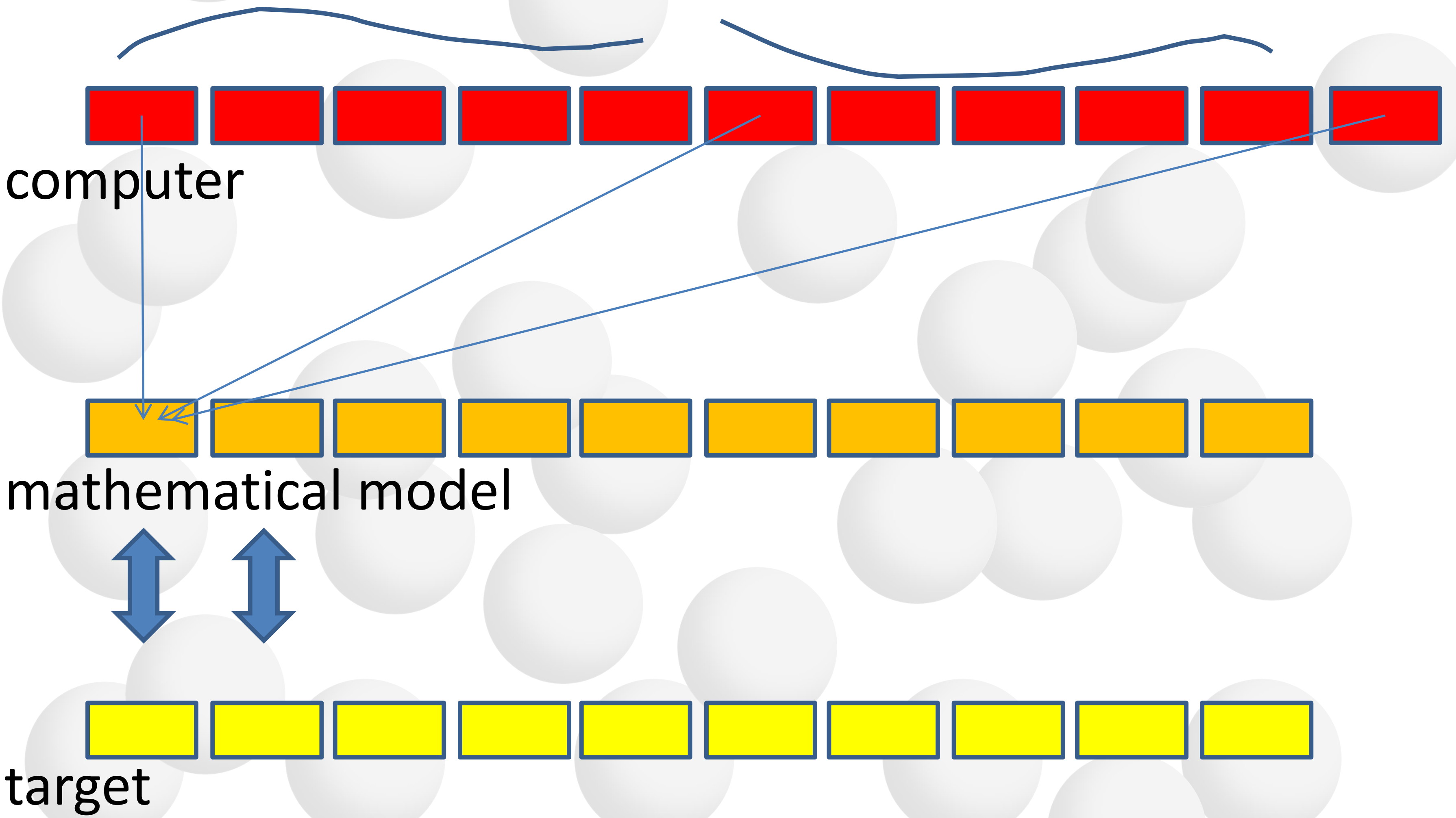
Commonly, one sample trajectory is simulated after the other.

But only averages over sample trajectories characterize the solution.

Analyzing MC simulations



Analyzing MC simulations



Consequences:

Winsberg (2010, p. 59):
Possible argument: If you stop an MC simulation at some time, then this time has no determinate counterpart in the process that is simulated. Thus, an MC simulation does not represent a process in the target and is not a real simulation.

This argument fits well with Hartmann’s view of simulations.

Under the definition by Humphreys (2004, p. 110),

MC simulations *are* simulations.

Thus, the definitions part company at this point.

>>>Which definition should we prefer?

Analyzing MC simulations

The argument from epistemological irrelevance:

X_1	X_2	X_3	X_4	X_5
$x_1^{\,1}$	x_2			
$x_1^{\,2}$	x_2			
…	…			

X_1	X_2	X_3	X_4	X_5
$x_1^{\,1}$	$x_2^{\,1}$	$x_3^{\,1}$	$x_4^{\,1}$	$x_5^{\,1}$
$x_1^{\,2}$	$x_2^{\,2}$	$x_3^{\,2}$	$x_4^{\,2}$	$x_5^{\,2}$
…	…	…	…	…

No epistemological difference!

The order of computational states cannot be a problem for the classification.

Caveat

But there are other differences.

Issue 2: MC simulations output probabilities and expectation values rather than values of empirical characteristics.

Deterministic simulations:

$$f_i \rightarrow \text{empirical characteristics}$$

Monte Carlo simulations:

$$x_i \rightarrow \textit{probabilities}\ (\ \text{empirical characteristics}\ )$$

Questions>>>

a. How can probabilities be used to describe a target?

b. How can we understand the way the probabilities are produced?

A moot point

Are MC integrations and indirect MC simulations also computer simulations?

- Buffon’s needle experiment
- A time series producing the distribution

But not essential for function of experiments.

Functions

Falkenburg (2024) stresses:

- Complex dynamics: infer consequences from models
- Instrumental use: contribute to analysis of experiments (in particular error analysis, today often synthetic data for training ML tools).

Cosmology:

- No experiments proper (but see Boge's talk)
- But some simulations conceptually very close to MC simulations of particle processes.
- Error estimation an important issue in astrophysics, MC methods important here.
- The Seiden-Schulman model has different functions: toy model, unification with statistical physics

Supershort travel guide

- MC methods are underexplored.
- MC methods perform many functions.
- Some MC methods are stochastic simulations. They differ from deterministic ones in interesting ways. Still, there is a case to treat them analogously with other simulations.
- Other MC methods can be illustrated as simulations, but this illustration doesn’t have epistemic value.

References

Barberousse, A., Franceschelli, S., & Imbert, C., 2009, Computer Simulations as Experiments, Synthese 169, 557–574

Beisbart, C. ,2011, A Transformation of Normal Science. A Philosophical Account of Computer Simulations. Habilitation Thesis, TU Dortmund, available upon request.

Beisbart, C., 2012, How Can Computer Simulations Produce New Knowledge, European Journal for Philosophy of Science 2, 395–434

Burks, A. W., 1975, Models of Deterministic Systems, Mathematical Systems Theory 8, 295–308

Dietrich, M. R., 1996, Monte Carlo Experiments and the Defense of Diffusion Models in Molecular Population Genetics, Biology and Philosophy 11, 339–356.

Falkenburg, Brigitte (2024). Computer simulation in data analysis: A case study from particle physics. Studies in History and Philosophy of Science Part A 105 (C):99-108.

Ferrara, A., Bianchi, S., Dettmar, R. J., & Giovanardi, C. (1996). The effect of light scattering by dust in galactic halos on emission-line ratios. *The Astrophysical Journal*, *467*(2), L69.

References

Galison, P., 1996 Computer Simulations and the Trading Zone, in: The Disunity of Science. Boundaries, Contexts, and Power (Galison, P. & Stump, D. J., eds.), Stanford University Press, Stanford, 118–157

Galison, P., 1997, Image and Logic. A Material Culture of Microphysics, University of Chicago Press, Chicago

Hartmann, S., 1996, The World as a Process: Simulations in the Natural and Social Sciences, in: Modelling and Simulation in the Social Sciences from the Philosophy of Science Point of View (Hegselmann, R., Troitzsch, K. G., & Mueller, U., eds.), Kluwer, Dordrecht, quoted from the revised version at http://philsci-archive.pitt.edu/archive/00002412/, 77–100

Grüne-Yanoff, T. & Weirich, P., 2010, The Philosophy and Epistemology of Simulation: A Review, Simulation & Gaming 41, 20–50

Hughes, R. I. G., 1997, Models and Representation, Philosophy of Science (Proceedings) 64, S325–S336

References

Hughes, R. I. G., 1999, The Ising Model, Computer Simulation, and Universal Physics, in: Models as Mediators. Perspectives on Natural and Social Sciences (Morgan, M. S. & Morrison, M., eds.), Cambridge University Press, Cambridge, 97–145

Humphreys, P., 1994, Numerical Experimentation, in: Patrick Suppes. Scientific Philosopher. Volume 2 (Humphreys, P., ed.), Kluwer, Dordrecht, 103–118

Humphreys, P., 2004, Extending Ourselves: Computational Science, Empiricism, and Scientific Method, Oxford University Press, New York

James, F., 1980, Monte Carlo Theory and Practice, Rep. Prog. Phys. 43, 1145–1187

O'Hagan, A., 1987, Monte Carlo is Fundamentally Unsound, Journal of the Royal Statistical Society. Series D (The Statistician) 36, no. 2/3, 24–249

Lewis, A., & Bridle, S. (2002). Cosmological parameters from CMB and other data: A Monte Carlo approach. *Physical Review D*, *66*(10), 103511.

Mücke, A., Rachen, J. P., Stanev, T., Protheroe, R. J., & Engel, R. (1999). Photohadronic processes in astrophysical environments. *Publications of the Astronomical Society of Australia*, *16*(2), 160-166.

References

Mücke, A., Engel, R., Rachen, J. P., Protheroe, R. J., & Stanev, T. (2000). Monte Carlo simulations of photohadronic processes in astrophysics. *Computer Physics Communications*, *124*(2-3), 290-314.

Norton, S. D. & Suppe, F., 2001, Why Atmospheric Modeling is Good Science, in: Changing the Atmosphere (Edwards, P. & Miller, C., eds.), MIT Press, Cambridge, MA, 67–106

Rohrlich, F., 1990, Computer Simulation in the Physical Sciences, PSA: Proceedings of the Biennial Meeting of the Philosophy of Science Association 1990, 507–518

Schulman, L. S., & Seiden, P. E. (1986). Percolation and galaxies. *Science*, *233*(4762), 425-431.

Ulam, S. (1991). Adventures of a Mathematician, University of California Press, Berkeley (first ed. 1976).

Winsberg, E., Science in the Age of Computer Simulations, University of Chicago Press, Chicago, 2010

Zeigler, B. P., 1976, Theory of Modelling and Simulation., J. Wiley, New York