Reproducibility, Computability and the Scientific Method

Peter V. Coveney

Centre for Computational Science,
Department of Chemistry
University College London

Computational Science Laboratory
Institute for Informatics
Faculty of Science
University of Amsterdam

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SEVENTH FRAMEWORK PROGRAMME

Technology Strategy Board

European Commission
HORIZON 2020

CompBioMed

ECMA

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PRACE

Distributed European Infrastructure for Supercomputing Applications

JÜLICH FORSCHUNGSZENTRUM

XSEDE Extreme Science and Engineering Discovery Environment

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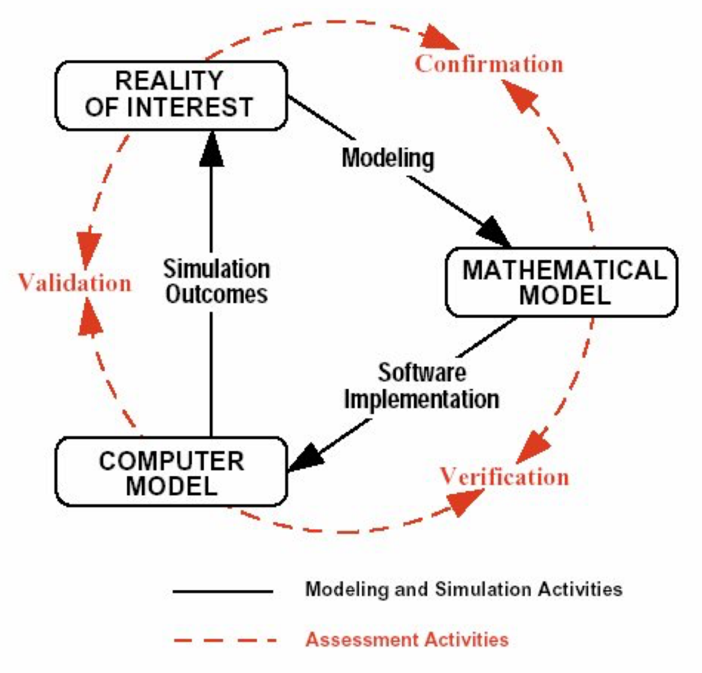
Contents

- What is VVUQ?
- Systematic vs random errors in computer simulation
- Examples in single scale and multiscale modelling and simulation
- VECMA VVUQ Toolkit: http://www.vecma-toolkit.eu/
- **A new pathology of IEEE floating point numbers**

What is VVUQ?



B.H.Thacker, et al., "Concepts of Model Verification and Validation." 2004. DOI: 10.2172/835920.

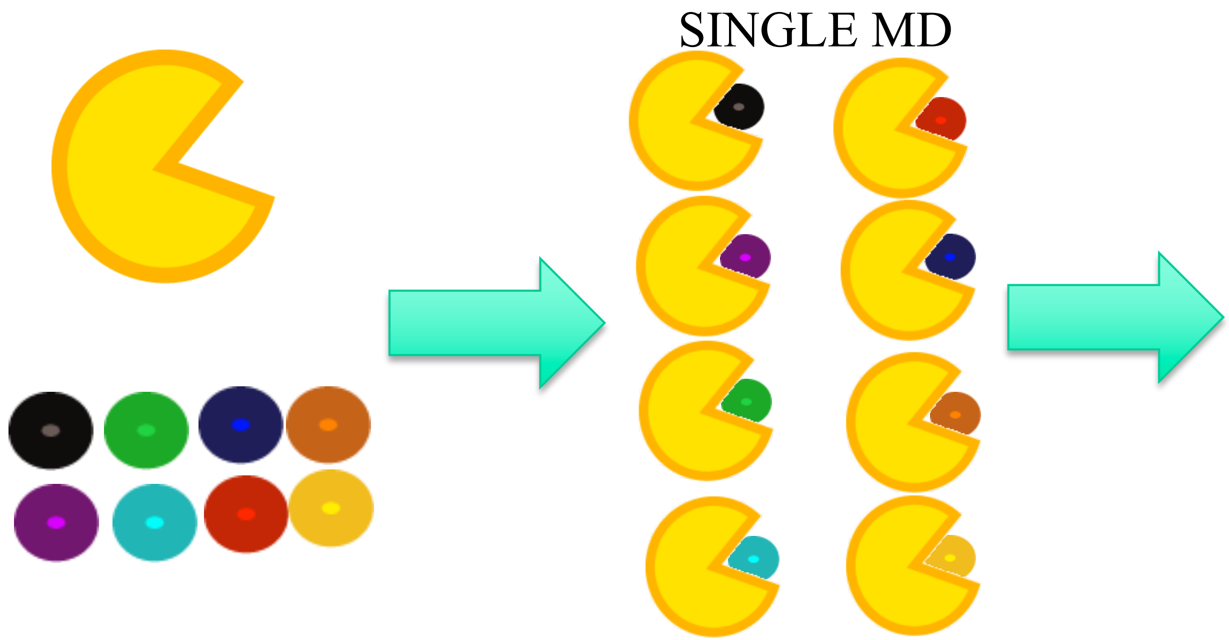
- Verification
  - Does the computational model fit the mathematical description?
- Validation
  - Is the model an accurate representation of the real world?
- **U**ncertainty **Q**uantification
  - How do variations in the numerical and physical parameters affect simulation outcomes?

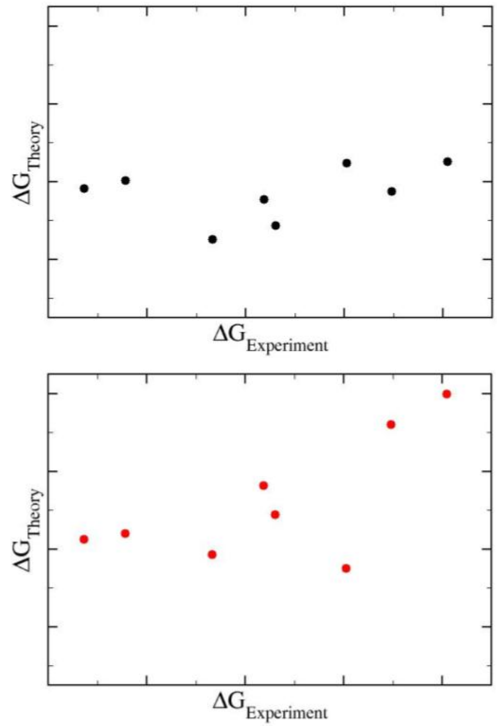
Errors in Computer Simulation
Molecular Dynamics (MD)

Systematic (epsitemic) errors

Preference/bias of different structures from some force fields, which requires extensive studies to identify:

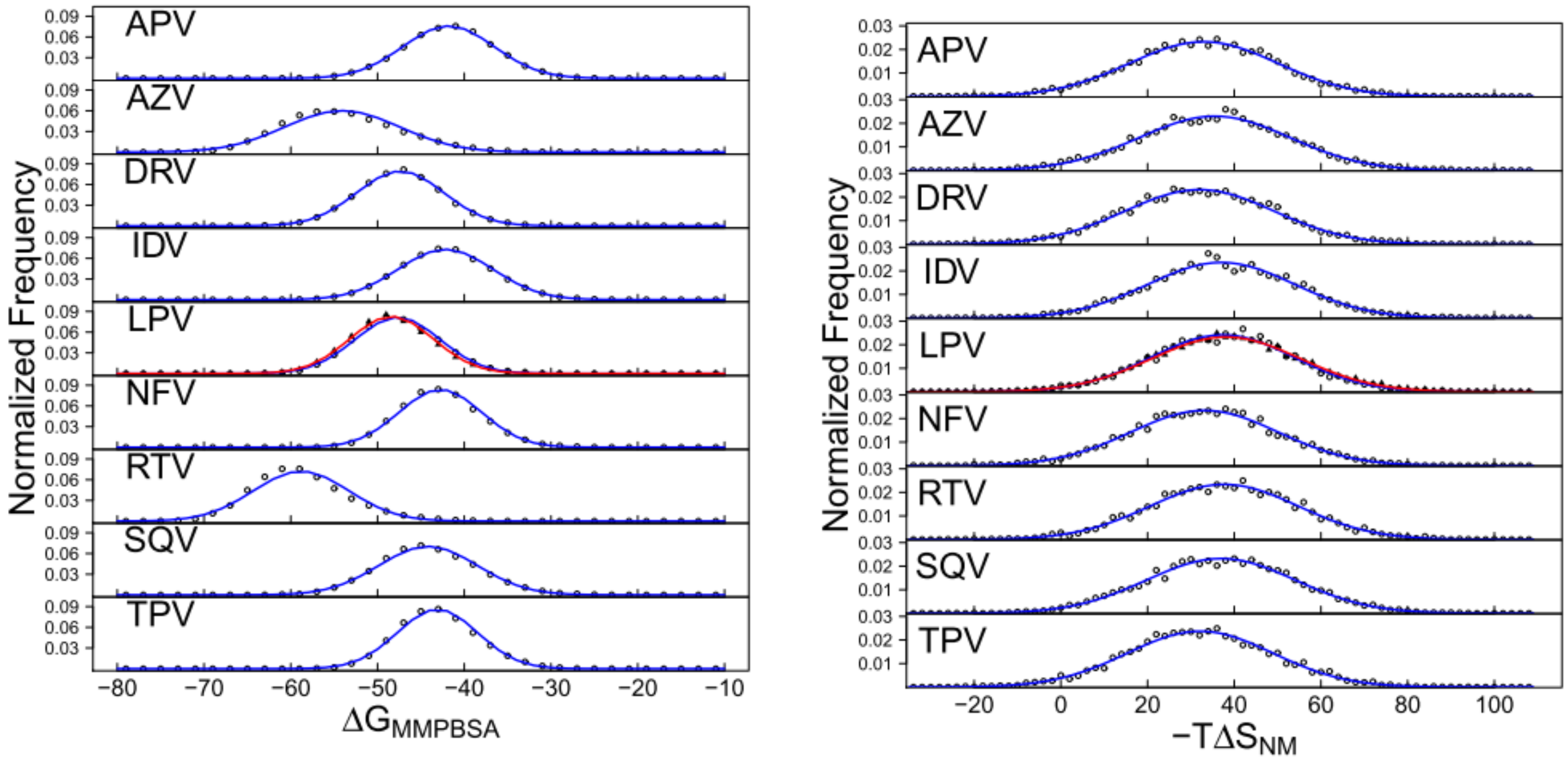
Stochastic (aleatory) errors





- The MM/PBSA results follow well defined Gaussian distributions.
- Configurational entropies, obtained from normal mode estimates, closely resemble normal distributions.

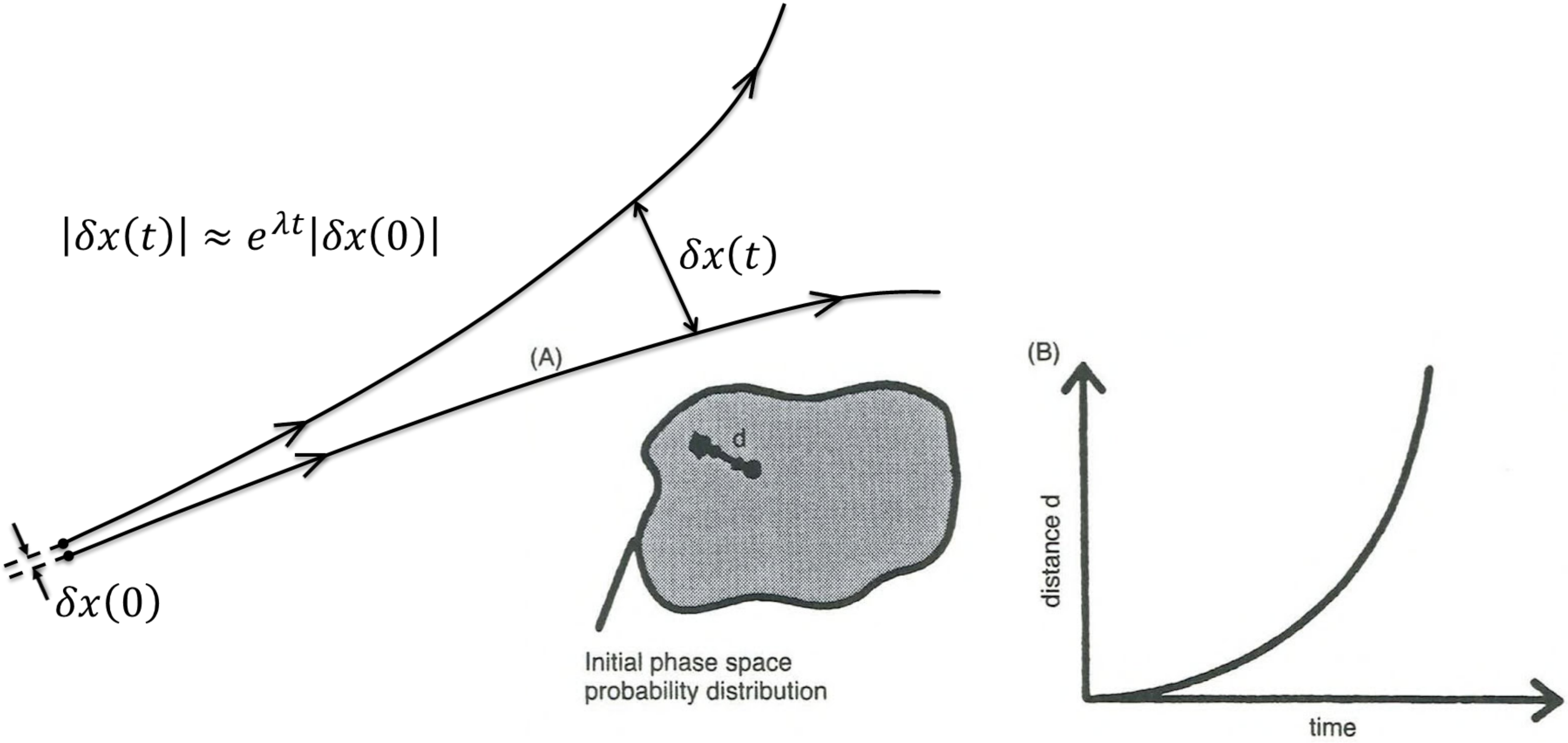
Drug – HIV-1 protease



Wright, Hall, Kenway, Jha & Coveney, JCTC, (2014), DOI: 10.1021/ct4007037.

Stochastic errors & chaotic systems

- Stochastic errors arise due to the chaotic nature of dynamics in
  - eg. classical MD and turbulence
- Such chaotic systems exhibit extreme sensitivity to initial conditions
- Long-time trajectories have low accuracy



P. V. Coveney and R. Highfield, "The arrow of time: a voyage through science to solve time's greatest mystery", W. H. Allen, London, 1990.
P.V. Coveney, S. Wan, *Phys. Chem. Chem. Phys.* 2016, 18, 30236−30240.

Dealing with stochastic errors

- Ideal goal is to find out the (usually) equilibrium distribution function – BUT difficult

- Sample the behavior to compute expectation values of observables – must do this well

- Use extensive ensemble and time averaging

- The statistical theory of turbulence is based on such an approach

Sampling of chaotic systems

A new pathology in the simulation of chaotic dynamical systems on digital computers

Bruce M. Boghosian (Tufts University)
Peter V. Coveney (UCL)
Hongyan Wang (Tufts University)

Boghosian, Bruce M., Peter V. Coveney, and Hongyan Wang. "A New Pathology in the Simulation of Chaotic Dynamical Systems on Digital Computers" *Advanced Theory and Simulations* (2019): 1900125.

The generalised Bernoulli map (1)

Bernoulli map: a simple dynamical system which exhibits chaotic behavior

$x_{t+1} = 2\, x_t \, mod \; 1 \qquad x \in [0,1)$

The generalised Bernoulli map is also known as the β shift:

$x_{t+1} = \beta\, x_t \, mod \; 1 \qquad x \in [0,1),$

- a one-parameter map where β is either an integer or a rational non-integer (> 1).

Many things are known about the behaviour of this map using continuum mathematics. For one thing, all β shifts are ergodic and have a unique invariant measure of maximum entropy.

The late time dynamical properties of the β shift can be obtained from the unstable periodic orbit (UPO) structure underlying the map.

From the set of countable UPOs, one can compute ensemble averages of observables using Ruelle's dynamical zeta function.

Ruelle, David. *Thermodynamic formalism: the mathematical structure of equilibrium statistical mechanics*. Cambridge University Press, 2nd edn, 2004

The generalised Bernoulli map (2)

- A simple, yet prototypical driven, dissipative dynamical chaotic system with a single free parameter β
- Many of its exact properties are known
- Its state space is in correspondence with the real numbers in the interval $[0,1)$.
- The initial condition is denoted by x_0.
- The state of the system at time $j + 1$, denoted by x_{j+1}, is given by

$$x_{j+1} = f\beta(x_j) := \beta x_j \bmod 1$$

- We consider values of $\beta > 1$

Mathematical properties of the map (1)

- Has a dense, complex attracting set
- An exact expression for its invariant measure is known
- Topologically conjugate to many engineering, biological, chemical and mathematical systems
- Can calculate exact expectation values of observables $O(x) = O_{\mathrm{ex}}$ using term-by-term integration over the known invariant measure

Mathematical properties of the map (2)

- For any integer value of $\beta \geq 2$, the Perron–Frobenius equation can be used to demonstrate that the invariant measure of the dynamics is uniform on $[0,1)$

- For non-integer β, the invariant measure is much more complicated, but an exact expression for it is given by the following series due to Hofbauer

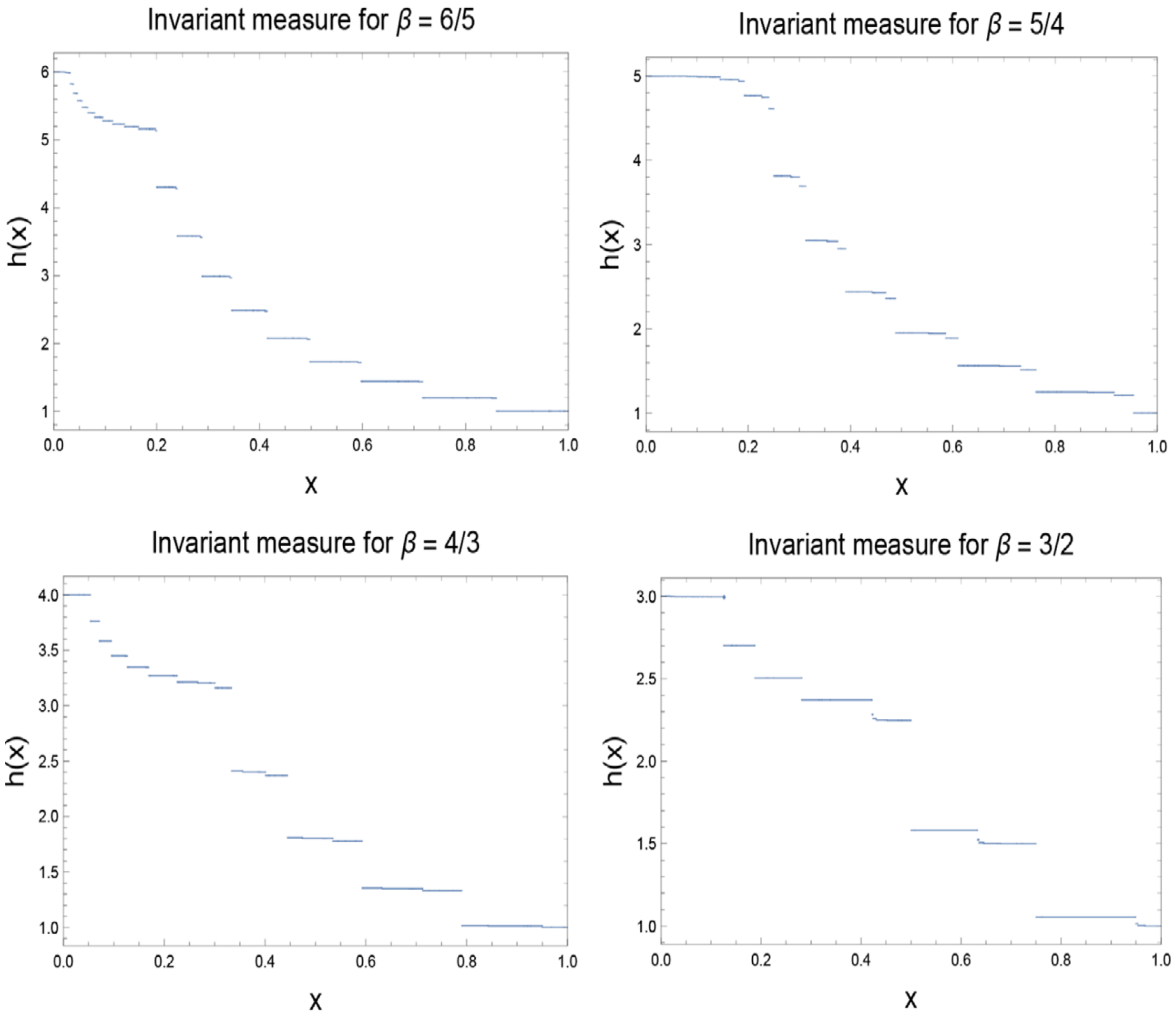
$$h_\beta(x) := C \sum_{j=0}^{\infty} \beta^{-j}\, \theta(1_j - x)$$

where $x_j := f_\beta^j(x)$ (so that, in particular, 1_j denotes $f_\beta^j(1)$), θ is the Heaviside function and C is a normalization constant.

Hofbauer, Franz. "*β-shifts have unique maximal measure*." Monatshefte für Mathematik **85.3** (1978): 189-198.

Mathematical properties of the map (3)

- The Hofbauer series makes manifest that the invariant measure has discontinuities at a dense set of points in [0,1)
- Examples for four non-integer values shown
- Caution: Graphs are less smooth than they appear



Invariant measures of the generalized Bernoulli map f_β for $\beta = \frac{6}{5}, \frac{5}{3}, \frac{4}{3}, \frac{3}{2}$. These are normalized so that $h_\beta(1) = 1$, which corresponds to $C = 1$ in the Hofbauer series

The β shift – floating point representation (1)

- The map can be represented & simulated on digital computers using standard IEEE floating-point numbers

- Single-precision IEEE floating-point numbers consist of 32 bits, of the form $\sigma, e_1, e_2, \ldots, e_8, m_1, m_2, \ldots m_{23}$ where σ is the sign bit, e_j are the exponent bits & m_j the mantissa bits.

- Similar construction for double-precision numbers, but using 52 mantissa bits and 11 exponent bits.

- **Floating point numbers are dyadic** (numbers whose denominators are powers of two)

- Dyadic numbers are a poor representation of the rational numbers

The β shift – floating point representation (2)

Floating point calculations:

- For the β shift in single precision, we can perform the numerical analysis using all the available 4 billion single precision floating point numbers.

- Calculation proceeds by enumerating the Unstable Periodic Orbits (UPOs)

- We compute averages over the limit cycles, then weight those averages by the fractional sizes of the corresponding basins of attraction in [0, 1)

- Equivalent to an ideal floating-point simulation of the system, for an infinite period of time and using an infinite number of ensemble elements.

- We are able to compute this result because there are just about a billion single-precision floating-point numbers in [0, 1).

Floating point pathology: β even integer

- Floating-point arithmetic causes highest damage to the dynamics for even values of β
- Consider $\beta = 2$
- The binary digits shift one place to the left with each iteration
- 1 iteration → left shift bits by 1 place → loss of 1 bit of precision with each application of the map
- Result will be zero
  - after 23 iterations for single-precision arithmetic
  - after 52 iterations for double-precision arithmetic
- The invariant measure will be a Kronecker delta at $x = 0$
- In the hypothetical limiting case of number of mantissa bits approaching ∞, the Kronecker delta would effectively approach a **delta distribution** at $x = 0$
- f.p. arithmetic's predicted exact time-asymptotic result will *never* be a uniform measure, the correct answer for the real-valued dynamics
- This pathology is fundamental to f.p. arithmetic & independent of choice of radix

F.P. representation: loss of UPO structure

- All rational numbers lie on periodic or eventually periodic orbits, since their base-β digit representations will (eventually) repeat
- All irrational numbers lie on chaotic trajectories
- The state space therefore consists of a dense set of unstable periodic orbits

- Table shows that the periodic orbit spectrum for single precision floating-point numbers for odd integer β is very different from that of the real continuum dynamical system

- **Only orbits consisting of dyadic fractions can be represented precisely**, and these have periods that are restricted to powers of two

Equivalence class			Periods					Orbit characteristics	
β	$S_i^{\pm}$	k	2^0	2^1	2^2	2^3	…	$T_{\max}$	N_{orb}
3	S_2^-	0	2	3	2	2	2	2^{22}	47
5	S_2^+	0	4	2	2	2	2	2^{22}	48
7	S_3^-	0	2	7	4	4	4	2^{21}	89
9	S_3^+	0	8	4	4	4	4	2^{21}	92
11	S_2^-	1	2	3	2	2	2	2^{22}	47
13	S_2^+	1	4	2	2	2	2	2^{22}	48
15	S_4^-	0	2	15	8	8	8	2^{20}	169
17	S_4^+	0	16	8	8	8	8	2^{20}	176

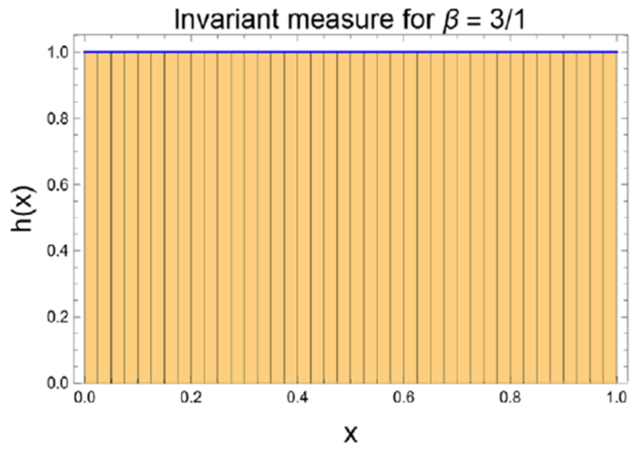
Orbit statistics for odd values of β from 3 to 17, including the class $S_i^{\pm} \in C$ to which it belongs, the value of k within that set, the number of orbits of various periods, the length $T_{\max}$ of the longest orbit, and the total number of orbits N_{orb}

Floating point pathology: β odd integer

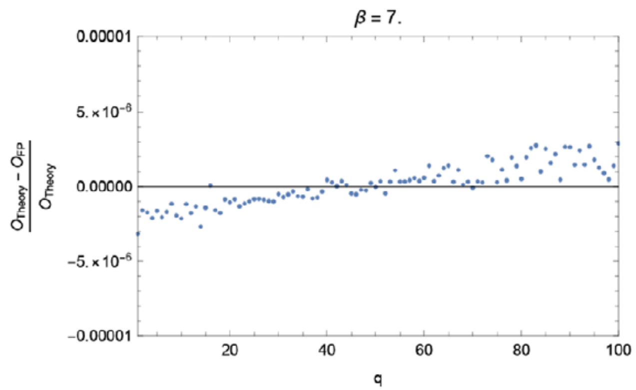
- We compare O_{ex} with the ideal floating-point simulation results O_{fp}

- The initial conditions comprise an infinite ensemble randomly sampled from $[0,1)$, each of which is allowed to run for an infinite length of time.

- Relative error between the expectation values is due to the newfound pathology

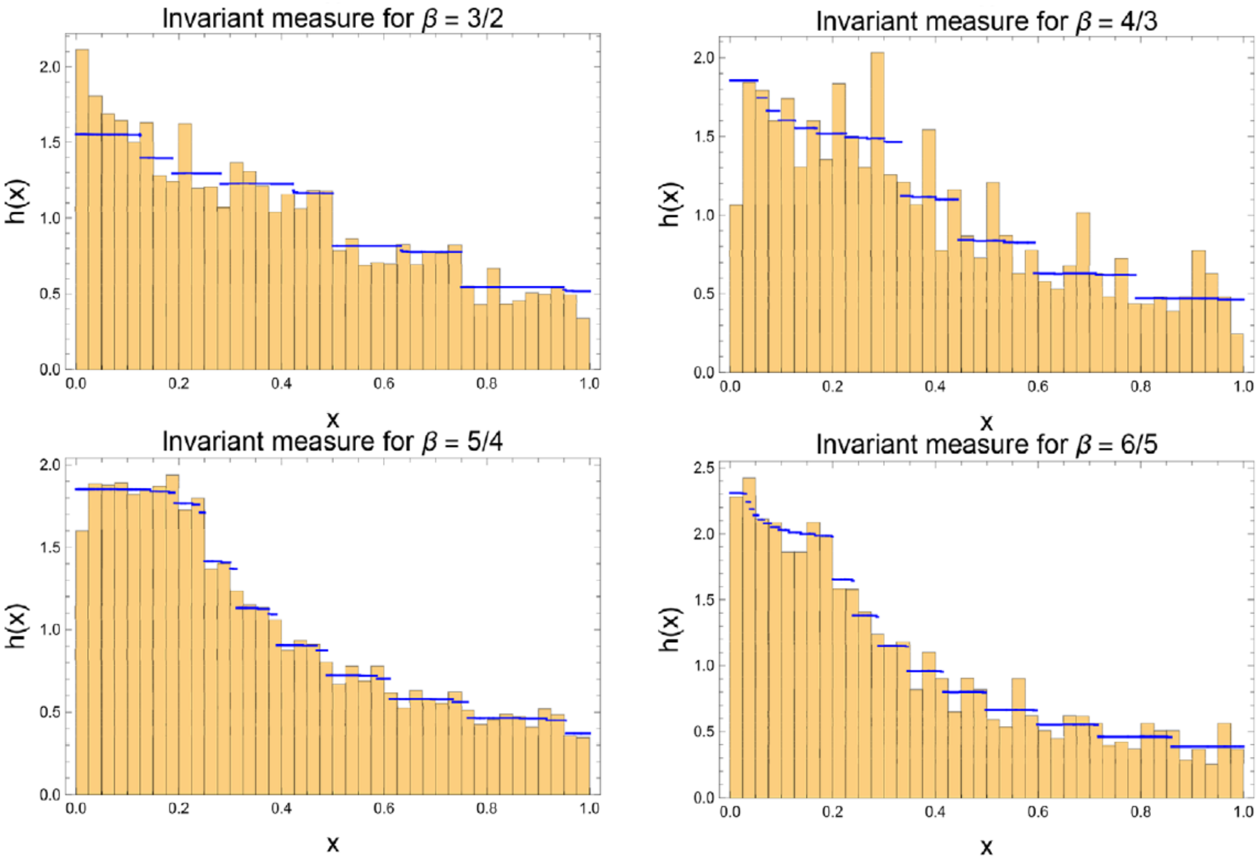


This also holds true for $\beta = 5,7,9$



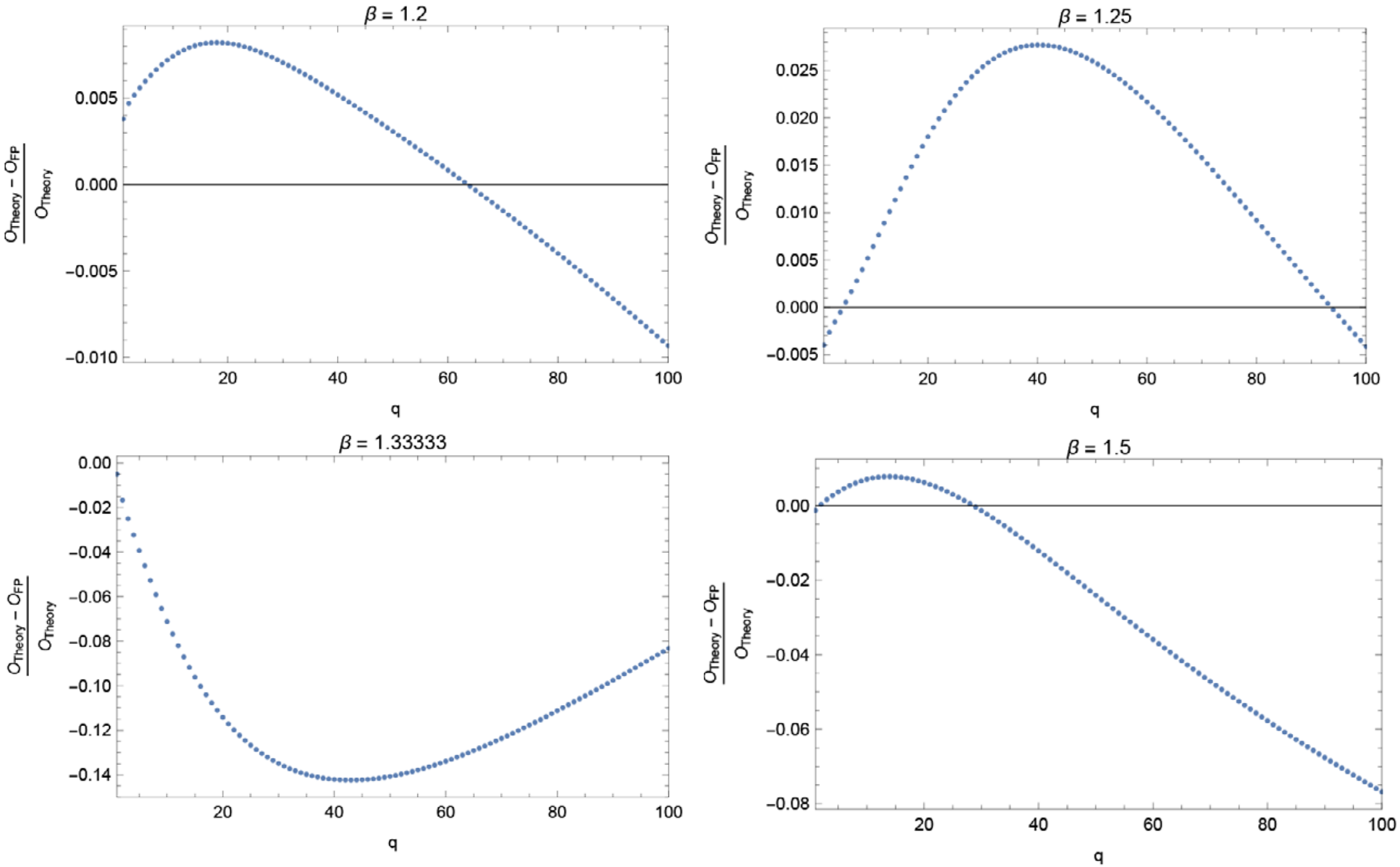
Relative error and invariant measure for β odd integer ($\beta = 7$)

Floating point pathology: non-integer β



- Discrepancy between the exact (blue) and numerical (histogram) invariant measures for the generalized Bernoulli map f_β for $\beta = 3,5,7,9$ and for $\beta = \frac{3}{2}, \frac{4}{3}, \frac{5}{4}, \frac{6}{5}$
- This simulates the average we would obtain if we could run over both an infinite length of time and an infinite ensemble size.
- While the agreement is good for odd integer β (though still greater than round off), it is seen to be very poor for non-integer β

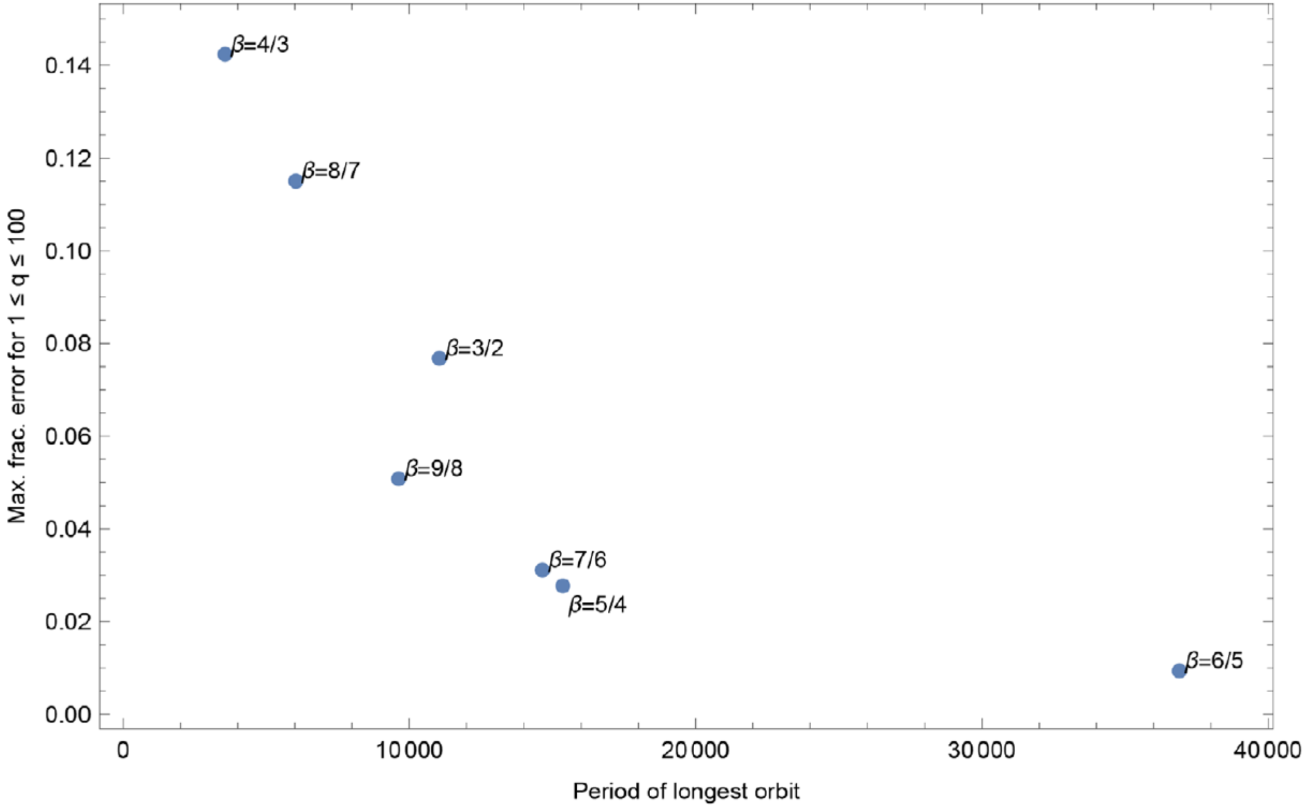
Floating point representation (non-integer β)



Relative error of the floating-point calculation of the expectation value of x^q for the generalized Bernoulli map $f_\beta$for $\beta = \frac{6}{5}, \frac{5}{4}, \frac{4}{3}, \frac{3}{2}$ simulating the average we would obtain if we could run over both an infinite length of time and an infinite ensemble size

The f.p. error is related to longest period UPO

- This egregious discrepancy in the invariant measure is the origin of the order unity differences observed between the theoretical and numerical expectation values of x^q



Maximum relative error of the floating-point calculation of the expectation value of x^q for $1 \leq q \leq 100$ for various values of β, versus the period of the longest orbit present in the floating point dynamics

Summary of floating point analysis (1)

- Floating point numbers have a strong detrimental influence on the map due to
    - their discrete and finite nature, and
    - the delicate structure of the attracting set of chaotic dynamical systems

- For even integer values of β, the long time behaviour is completely wrong, subsuming the known anomalous behaviour for $\beta = 2$

- For non-integer β, relative errors in observables can reach 14%

- For odd integer β values, floating-point results are more accurate, yet possess relative errors two orders of magnitude larger than those attributable to round-off.

Mitigation

- Alternative representations of real (rational) numbers
  - next generation arithmetic
- Investigating unums and posits ~ Gustafson (*)
- Consider analogue computation

* J. L. Gustafson, *The End of Error: Unum Computing*, Chapman and Hall/CRC Press, Boca Raton, FL, USA 2015.