2008

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Blais, J. A. Rod; Grebenitcharsky, R.; Zhang, Z.

Blais, J.A.R., R. Grebenitcharsky and Z. Zhang [2008]: Exploring Monte Carlo Simulation Strategies for Geoscience Applications. Poster presentation at the Fall Meeting of the American Geophysical Union in San Francisco, CA.

http://hdl.handle.net/1880/49759

conference proceedings

Exploring Monte Carlo Simulation Strategies for Geoscience Applications

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Introduction

- Stochastic simulations are widely used in geoscience!
- Monte Carlo estimates are often needed for definite integrals
- Pseudorandom sequences imply quadrature computations
- Quasirandom sequences can optimize the pseudorandom results
- Chaotic random sequences offer challenging new strategies
- Numerical experimentation generally required for analysis
- Expected error bounds need confirmation and clarification
- Geodetic and other potential applications abound
- Investigations are continuing …

Randomness

- **In mathematics, only processes can be random!**
- **In simple terms, random most often means nondeterministic**
- **In physics, random usually means noncomputable or unpredictable**
- **In practice, there are various ways to simulate random sequences**
- **Pseudorandom sequences are commonly generated using some linear congruential model applied recursively, such as**

  $$x_n \equiv c \odot x_{n-1} \quad \text{modulo } \pi \qquad \text{(for large prime } \pi \text{ and constant c)}$$

  or lagged Fibonacci congruential sequence, such as

  $$x_n \equiv x_{n-p} \odot x_{n-q} \quad \text{modulo } \pi \quad \text{(for large primes } \pi \text{ and p, q)}$$

  in which $\odot$ usually stands for ordinary multiplication
- **Quasirandom sequences are regularized pseudorandom sequences**

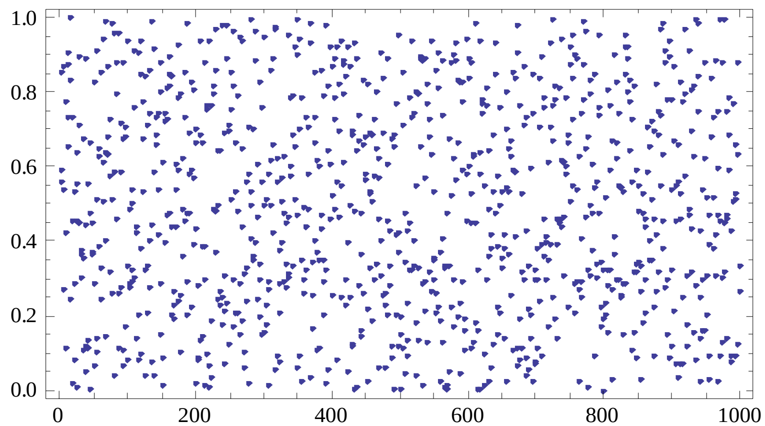
Chaos & Chaotic Randomness

- **Chaos refers to unstable dynamical nonlinear systems which are especially sensitive to their initial conditions**
- **Chaotic maps can be erratic, mixing / ergodic and thus ‘random’**
- **Several families of chaotic processes may be used to simulate random processes using specific choices of parameters**
- **The logistic map generated by $x_n = 4\ x_{n-1}\ (1-x_{n-1})$, $n = 1, 2, \ldots,$ for some seed x_0, over the interval (0, 1), exhibits randomness with an approximate density**

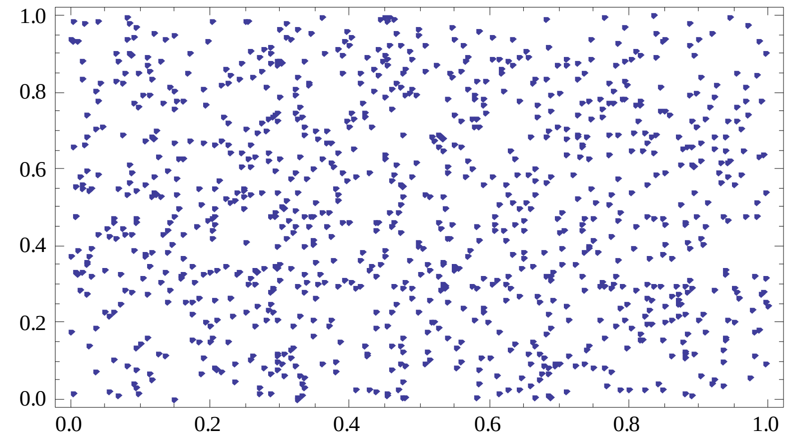
  $$\rho(x) = 1 / \pi\ [x\ (1 - x)]^{1/2}$$

  which needs to be taken into account in Monte Carlo applications
- **Other strategies using higher-order Chebychev polynomials are sometimes used in practice [Umeno, 2000]**

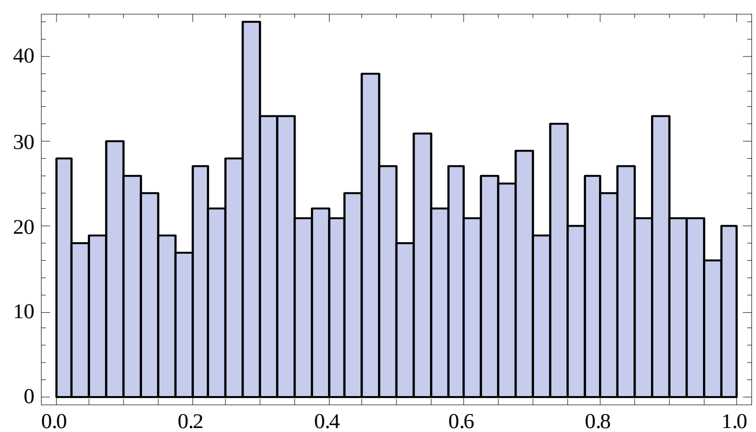
Pseudorandom Sequences



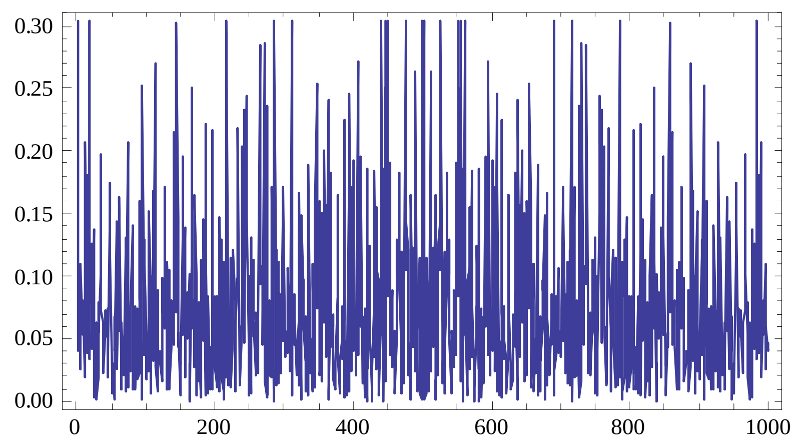
Spatial Plot of Pseudorandom Sequence



Phase Plot of Pseudorandom Sequence

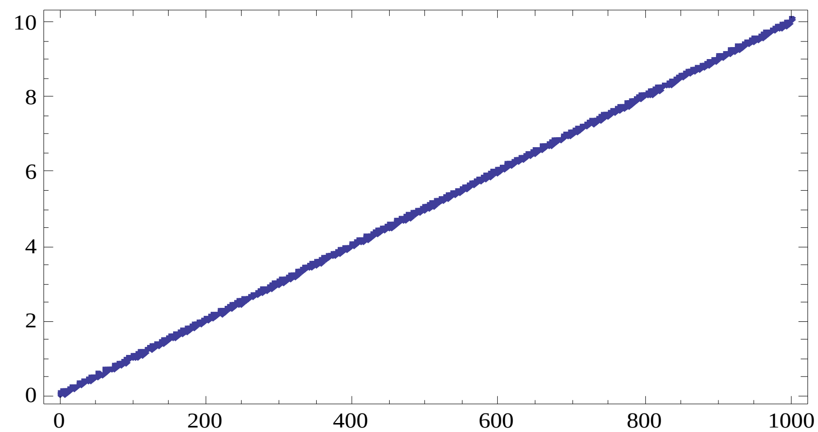


Histogram of Pseudorandom Sequence

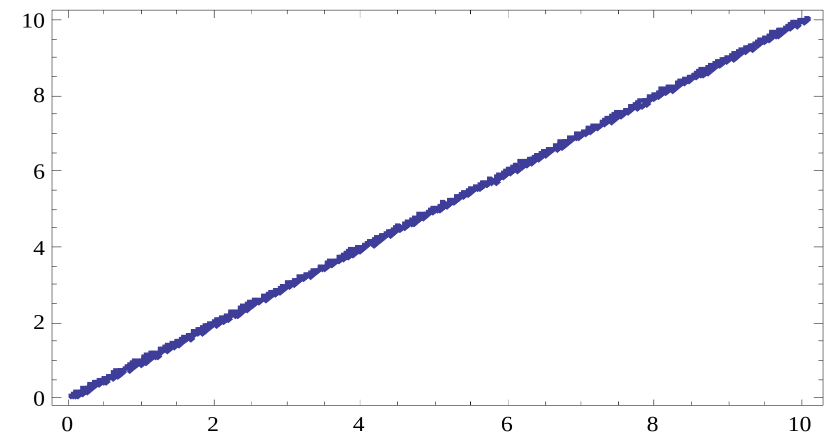


Periodogram of Pseudorandom Sequence

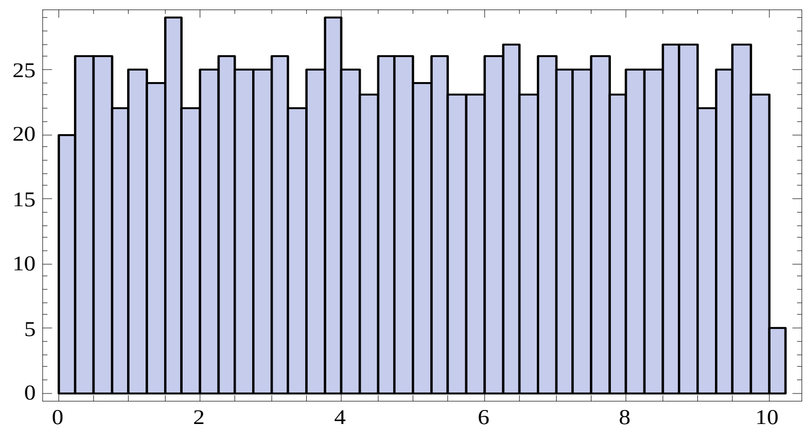
Quasirandom Sequences



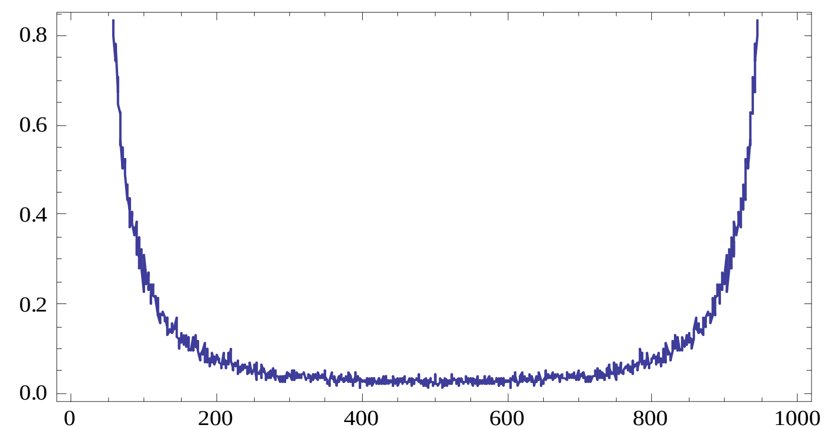
Spatial Plot of Quasirandom Sequence



Phase Plot of Quasirandom Sequence

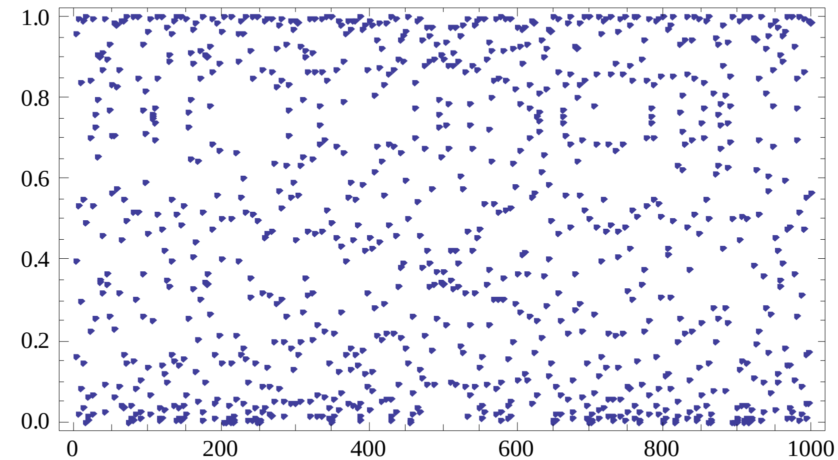


Histogram of Quasirandom Sequence

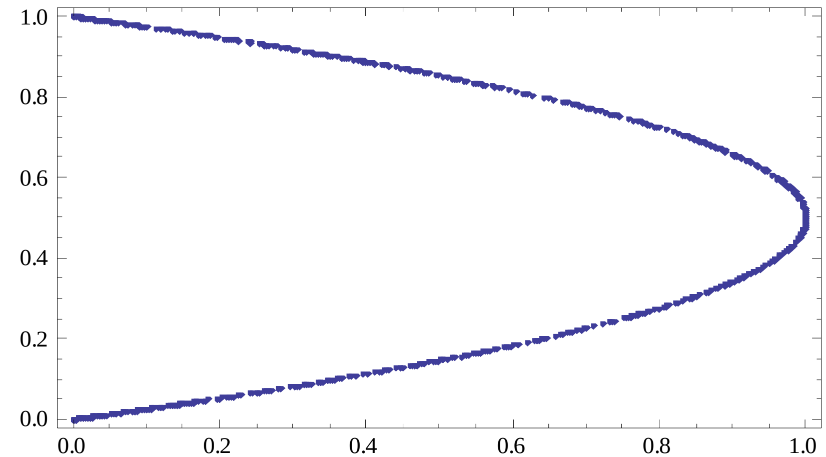


Periodogram of Quasirandom Sequence

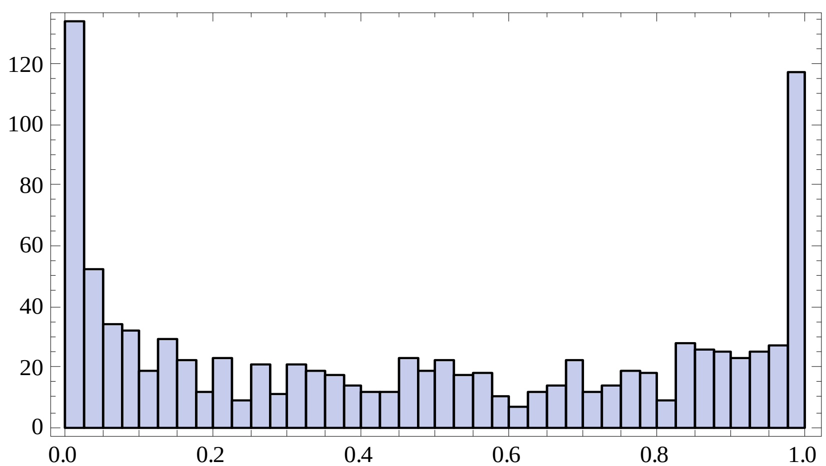
Chaotic Random Sequences



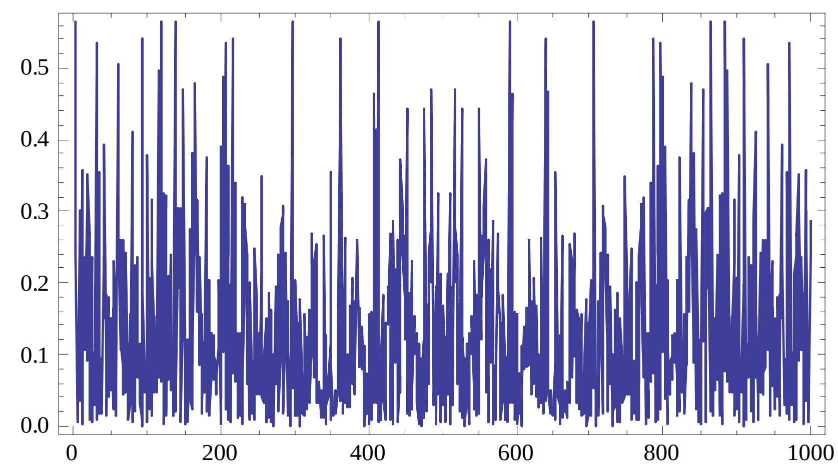
Spatial Plot of Chaotic Random Sequence



Phase Plot of Chaotic Random Sequence



Histogram of Chaotic Random Sequence



Periodogram of Chaotic Random Sequence

Monte Carlo Simulations

Numerical Recipes state:

$$\int_V \mathbf{f}\, \mathbf{dV} \approx \mathbf{V} \langle \mathbf{f} \rangle \pm \sqrt{\left(\langle \mathbf{f}^2 \rangle - \langle \mathbf{f} \rangle^2\right) / \mathbf{N}}$$ **implying a variance O(1/N)**

However, more recently,

Random Number Generators	**Variance of Error**
Standard Arithmetical Pseudorandom Numbers	$V(N) = O(1/N)$
Quasirandom Numbers (General, spatial dim. s)	$V(N) = O((\ln N)^{2s}/N^2)$
Superefficient Chaotic Monte Carlo*	$V(N) = O(1/N^2)$
Chaotic Monte Carlo (General)	$V(N) = O(1/N)$

* Under the 'superefficiency condition' implied by the dynamical correlation for large N, see e.g. [Umeno, 2000, 1999, 1998]

Numerical Experimentation

PMC / QMC / CMC	N = 10	N = 10^2	N = 10^3	N = 10^4
$\int_0^1 e^x dx$	1.56693421	1.63679860	1.70388586	1.71894429
	1.56693421	1.71939163	1.71994453	1.71812988
$\cong$ **1.718281828459045**	1.67154678	1.73855363	1.76401394	1.72791977
$\int_0^1 \int_0^1 e^{xy} dxdy$	1.23409990	1.31809139	1.31787793	1.31790578
	1.23409990	1.31785979	1.31789668	1.31790120
$\cong$ **1.317902151454404**	1.21656321	1.27903348	1.34063983	1.31179521
$\int_0^1 \int_0^1 \int_0^1 e^{xyz} dxdydz$	1.14046759	1.14625944	1.14650287	
	1.14046759	1.14649963	1.14649879	
$\cong$ **1.146499072528643**	0.99503764	1.14428655		

Analysis of Simulations

Pseudorandom Approach:

- Using Mathematica 6 random number generator
- Very good results in general

Quasirandom Approach:

- Using Mathematica 6 random number generator
- With equal partition into 10 subintervals per dimension
- Best results in general

Chaotic Random Approach:

- Using Logistic Map with corresponding density correction
- Results generally comparable to pseudorandom results

Geodetic Application

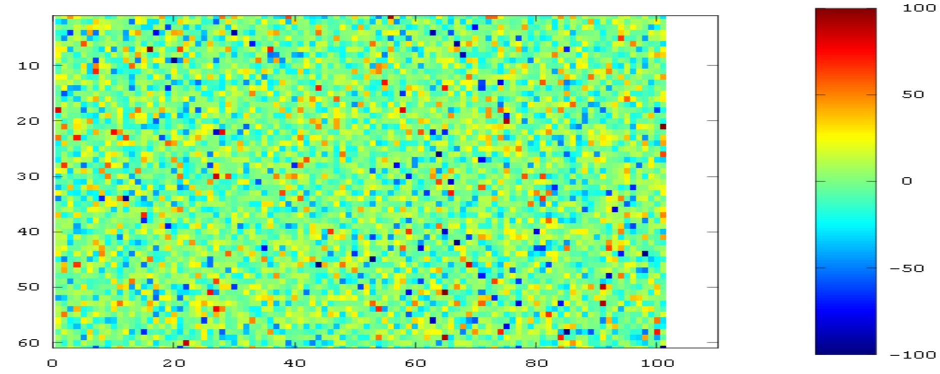
<u>Inverse Problem</u>: Recovery of ocean bathymetry from gravity data

1. **Computation of gravity disturbance at sea level using local water depth**
   Simplification: attraction of prism below grid point only.
2. **With simulated surface gravity disturbance, estimate ocean depth using Simulated Annealing (SA) with pseudorandom, quasirandom and chaotic random numbers.**
3. **Example of depth estimates vs 2221.384 ± 0.170 m & no. of iter'ns for 1 σ:**

	10 iter'ns	**10^2 iter'ns**	**10^3 iter'ns**	**10^4 iter'ns**	**Required no. of iterations for 1 σ**
PMC	2136.802	2192.537	2224.223	2222.018	1880
QMC	2138.915	2206.914	2220.626	2220.981	7450
CMC	2061.340	2181.327	2219.515	2222.320	6299

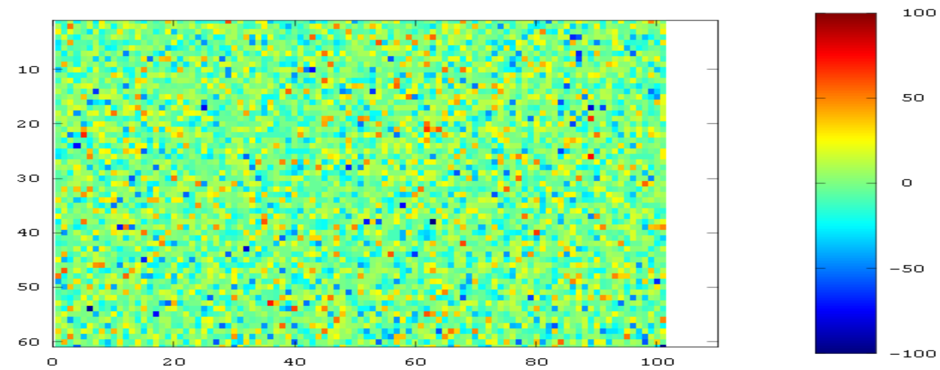
Pseudorandom – 100 iterations

Number of Samples	Min (m)	Max (m)	Mean (m)	Std (m)
6161	-121.687	106.544	-0.768	20.926



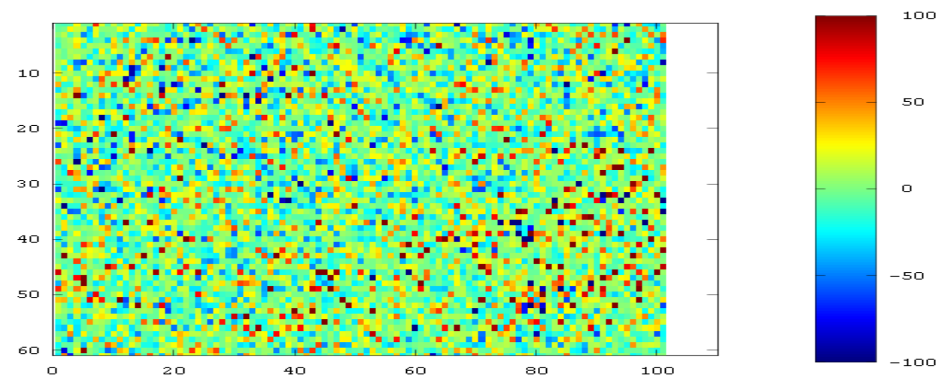
Quasirandom – 100 iterations

Number of Samples	Min (m)	Max (m)	Mean (m)	Std (m)
6161	-106.478	72.487	-0.909	18.535



Chaotic random – 100 iterations

Number of Samples	Min (m)	Max (m)	Mean (m)	Std (m)
6161	-332.100	260.758	1.675	32.295



Concluding Remarks

- **Pseudorandom numbers and Monte Carlo simulations are very useful!**
- **Quasirandom Monte Carlo approaches appear most optimal and adaptive**
- **Chaotic random numbers using Logistic Map seem somewhat deficient**
- **Chaotic Monte Carlo limited experimentation shows no better than $O(N^{-1})$**
- **More research is clearly warranted for $O(N^{-2})$ error behavior …**
- **Geodetic and other geoscience MC applications are very promising**
- **Uncertainty modeling in nonlinear and/or nonGaussian contexts require MCs**
- **Research and computational experimentation are continuing for gravity terrain corrections, geopotential downward continuation & uncertainty characterization**