Review of the Merits of the Stochastic Dynamic Equations and the Monte Carlo Approach in Modeling and Understanding Systems

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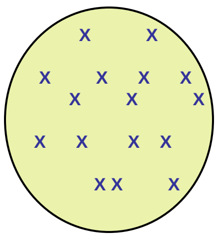
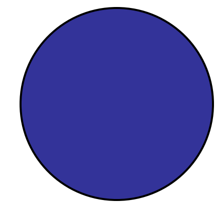
In today's world we want to know the future and the uncertainty of the forecast of that future – how good is that forecast. Mathematically, in a numerical model, one must deal with the uncertainty in the initial conditions and physics of the model. This can be done in two ways:



Monte Carlo (MC)



SDE

The Monte Carlo approach: draw upon a finite number of random deviates – Usually from a normal distribution with a pre-defined variance or from a set of stochastic dynamic equations (SDE) which begin with an infinite ensemble of initial states – with that same predefined variance

The MC approach is just an approximation to the SDE method; however the SDE method involves many equations and a serious closure issue!

Time derivative for the mean (μ_i) of X_i involve 2^{nd} moments ($\sigma_{i,j}$); time derivative of 2^{nd} moments involve 3^{rd} moments ($T_{i,j,k}$); time derivative of n-th moment involve moments of n+1 -- where the subscripts are indices of the variables

The MC approach is the only practical way to deal with large scale grid models; future multi-processor computers will allow ever larger sample sizes

Look at Lorenz eq. for his famous strange attractor, a simple model of convection – where P = 10 and B = 8/3 to show the merits of both the MC and SDE

$$\dot{X} = P(Y - X) \qquad \dot{Y} = -XZ + RX - Y \qquad \dot{Z} = XY - BZ$$

Fixed point (FP) solutions occur for R < 24.74 and chaos occurs for R ≥ 24.74

Use R = 14 for FP and R = 28 for chaos; express [X, Y, Z] as [X(1), X(2), X(3)]

In 4th order scheme: rhs of these eq. are evaluated 4 times / time step; in each the current X's are put in XT and predicted values put in XP. For MC in FORTRAN:

```
      DO  100   J = 1, K    [ where K may be 100, 1000 or 40,000 = MC sample size]

      XP(J,1) = P * (XT(J,2)  - XT(J,1))

      XP(J,2) =  – XT(J,1) * XT(J,3) + R * XT(J,1) - XT(J,2)

      XP(J,3) = XT(J,1) * XT(J,2) -  B * XT(J,3)

100   continue
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Full SDE equations found in Epstein (Tellus, 1969) for the 2nd moments; and 3rd moments In Fleming (MWR,1971) A few Lorenz equations are shown below

$\mu(1)^{\cdot} = X(1)^{\cdot} = P * (X(2) - X(1))$

$\mu(2)^{\cdot} = X(2)^{\cdot} = - X(1) * X(3) - X(6) + R * X(1) - X(2)$

$\mu(3)^{\cdot} = X(3)^{\cdot} = X(1) * X(2) + X(5) - B * X(3)$

$\sigma(1,1)^{\cdot} = X(4)^{\cdot} = 2.0 * P * \{ X(5) - X(4) \}$

$\sigma(2,2)^{\cdot} = X(7)^{\cdot} = - 2.0 * \{ X(1) * X(8) + X(3) * X(5) + X(14) \} + 2 R * X(5) - 2 * X(7)$

$\sigma(3,3)^{\cdot} = X(9)^{\cdot} = 2.0 * \{ X(1) * X(8) + X(2) * X(6) + X(14) - B * X(9) \}$

Covariance terms: $\sigma(1,2) = X(5) = \dots$ $\sigma(1,3) = X(6) = \dots$ $\sigma(2,3) = X(8) = \dots$

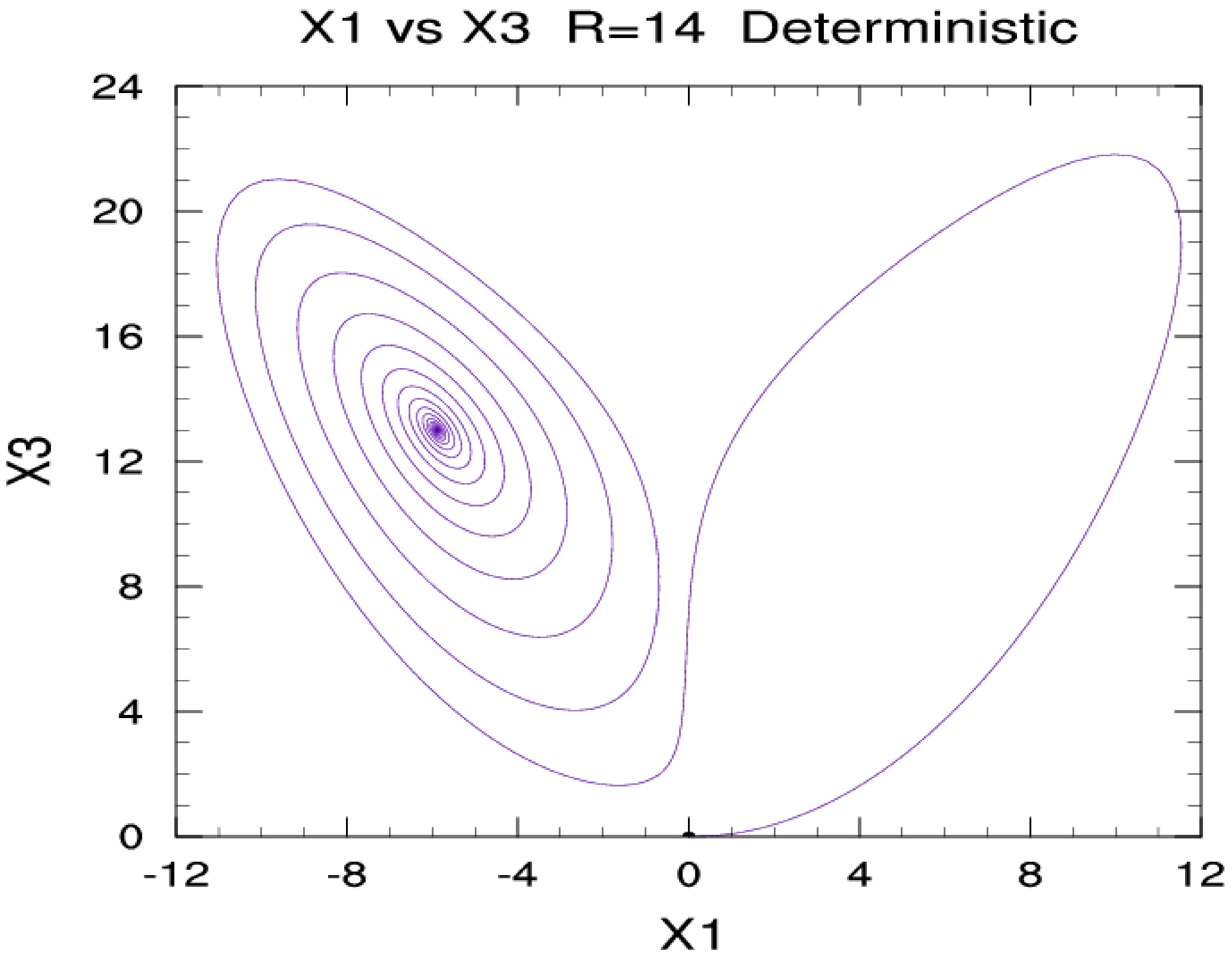
The 3rd moment terms: $X(10) = T(1,1,1)$, $X(11) = T(1,1,2)$ … $X(19) = T(3,3,3)$

$X(19)^{\cdot} = T(3,3,3)^{\cdot} = 3 [\mu(1) T(2,3,3) + \mu(2) T(1,3,3) - \sigma(1,2) \sigma(3,3) + \lambda(1,2,3,3) - B T(3,3,3)$

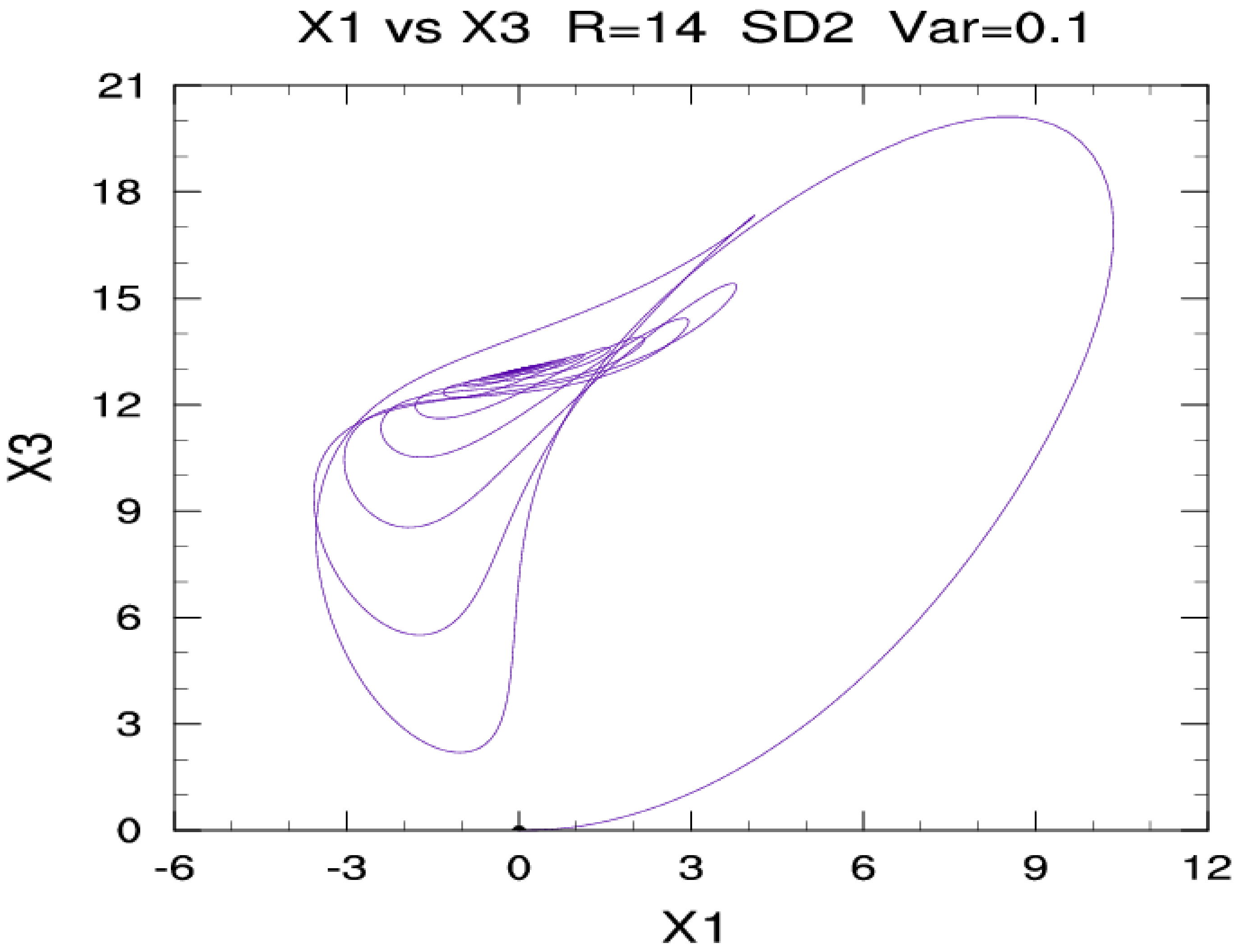
We will show deterministic solution for R = 14; SD2 solution (3rd moments = 0);

SD3 solution (3rd moments included and a proper closure on the 4th);

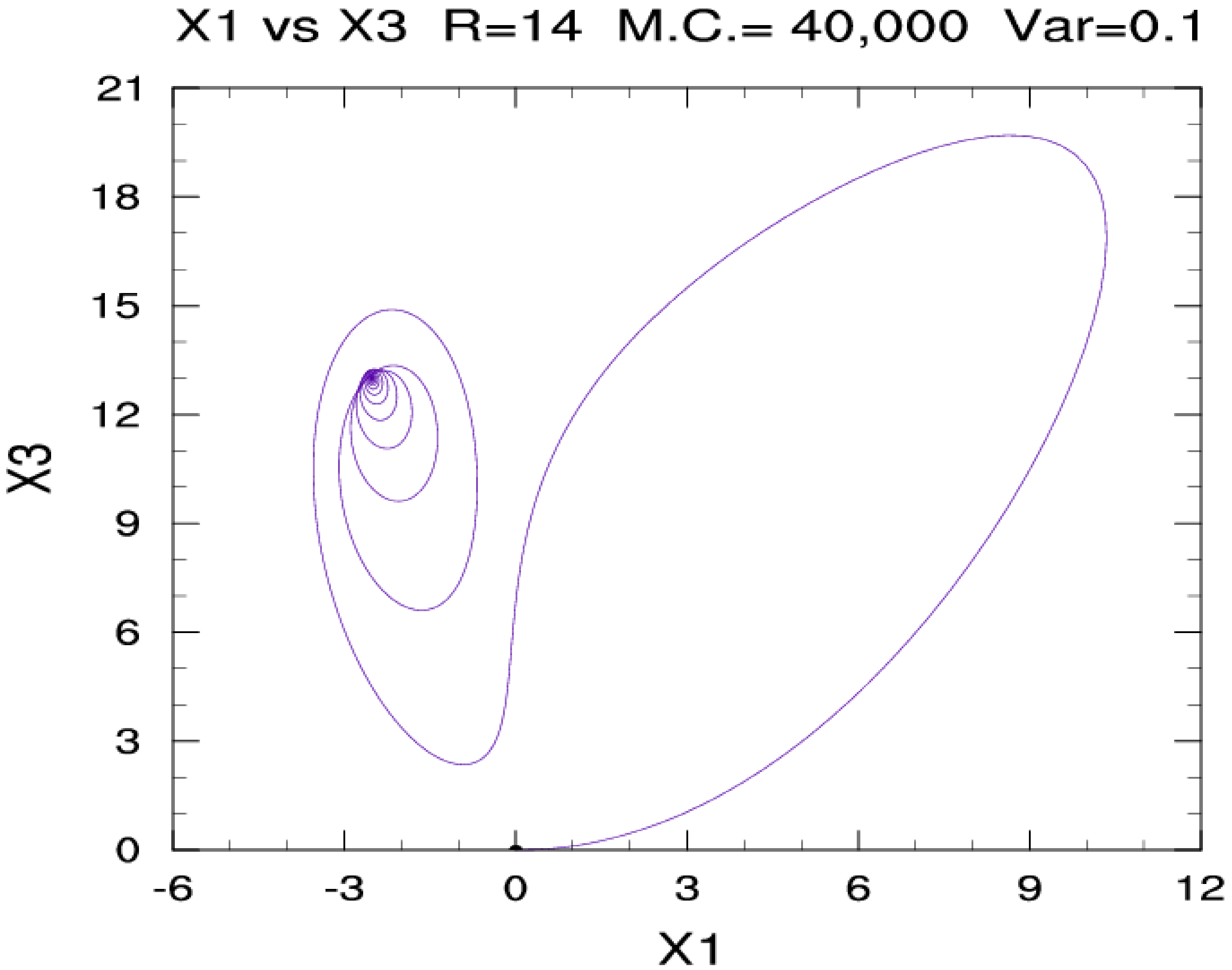
Monte Carlo solution (with a sample size of 40,000);



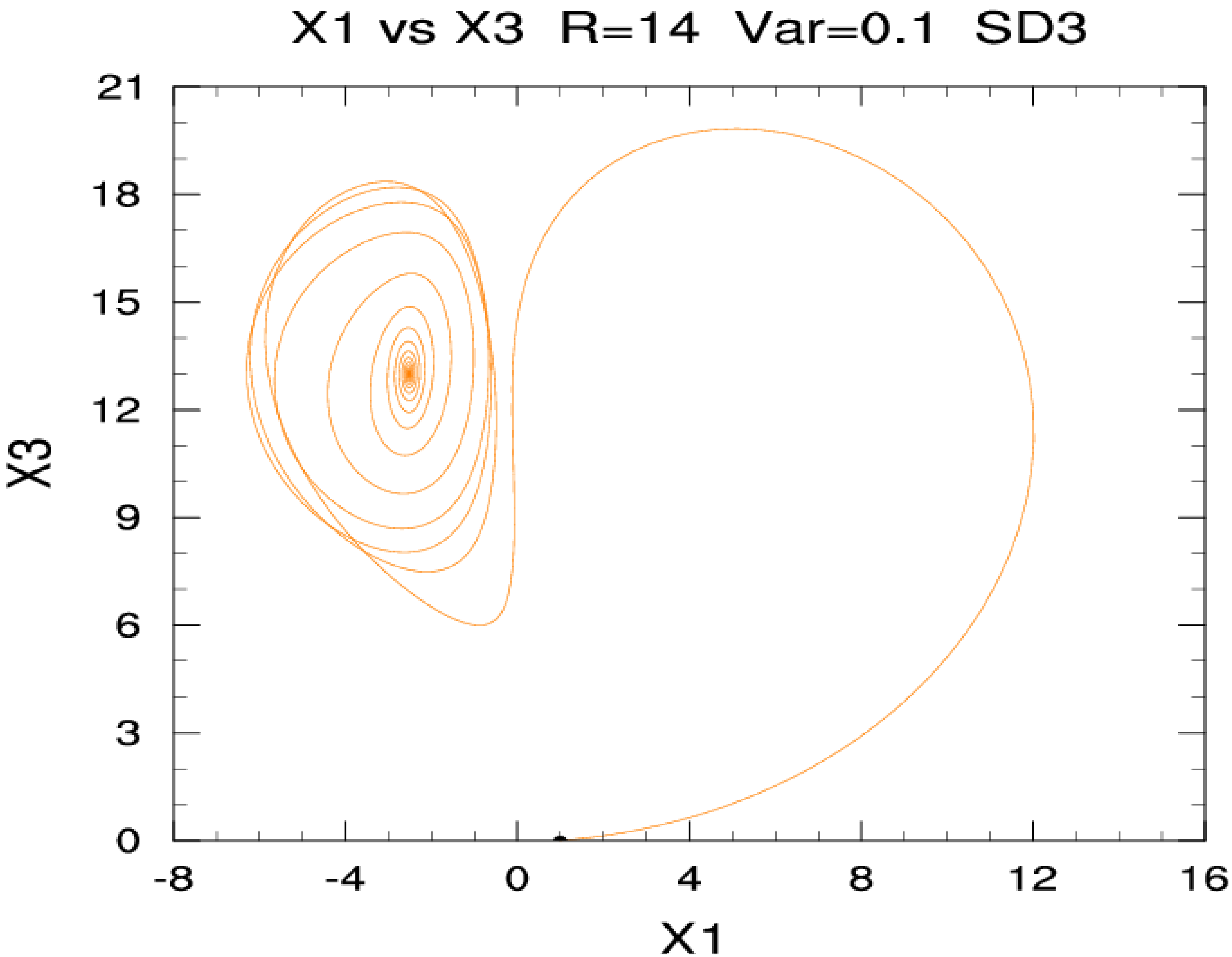
I. C. are [0,1,0] for [X1, X2, X3] R = 14 gives FP solution; theory gives:
X3 = R-1 = 13 and X1=X2 = $\pm [\, B\,(R-1)\,]^{1/2} = \pm [\, 8/3\,(13)]^{1/2} = \pm 5.888$
Here, the negative solution is the result (- 5.888)



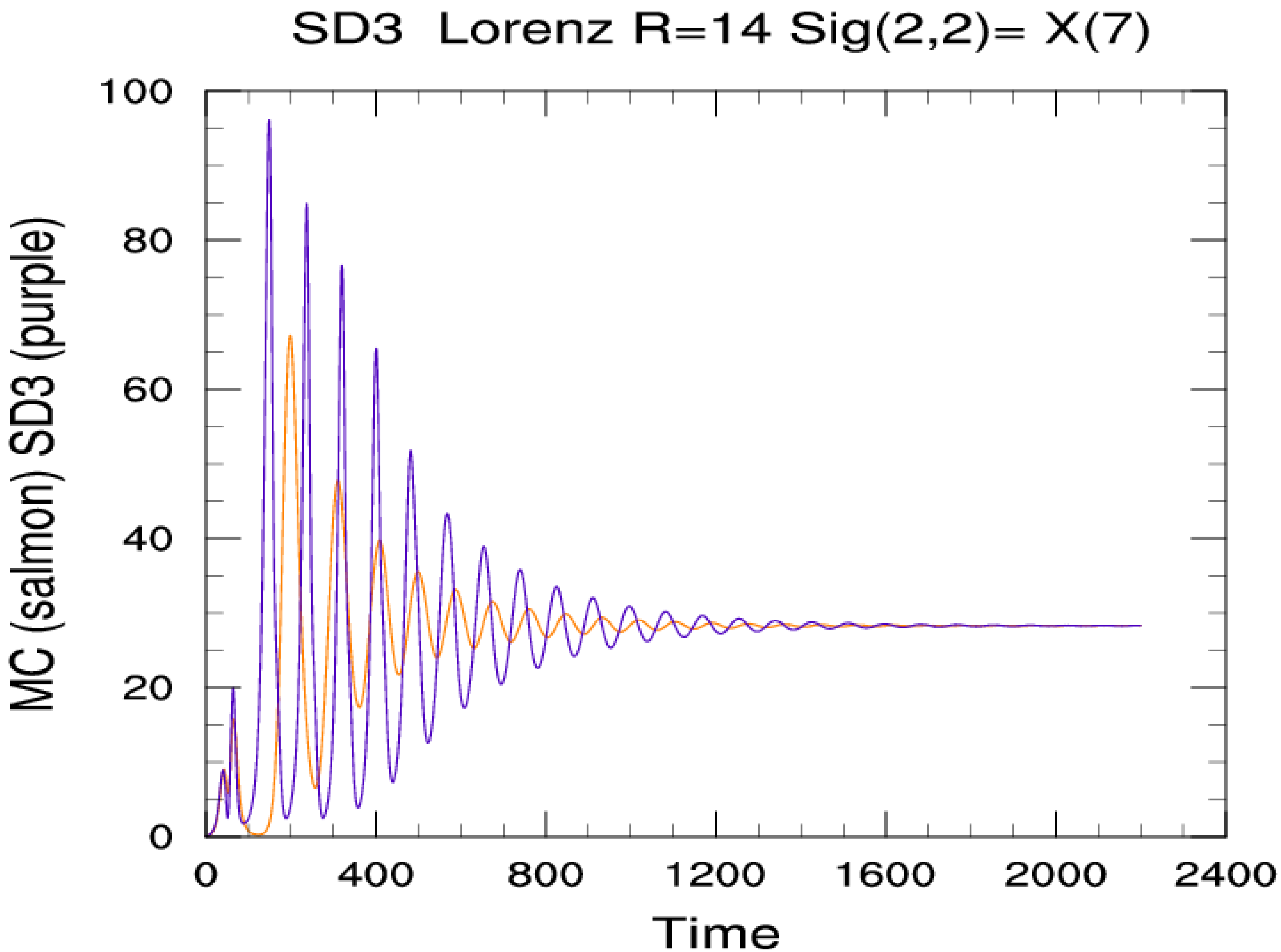
SD2 result: A small variance has been added to each variable = 0.1 X3 = R-1 = 13 is correct; but X1 = X2 = 0, (both ± 5.888 are possible solutions, but is this SD2 answer correct?



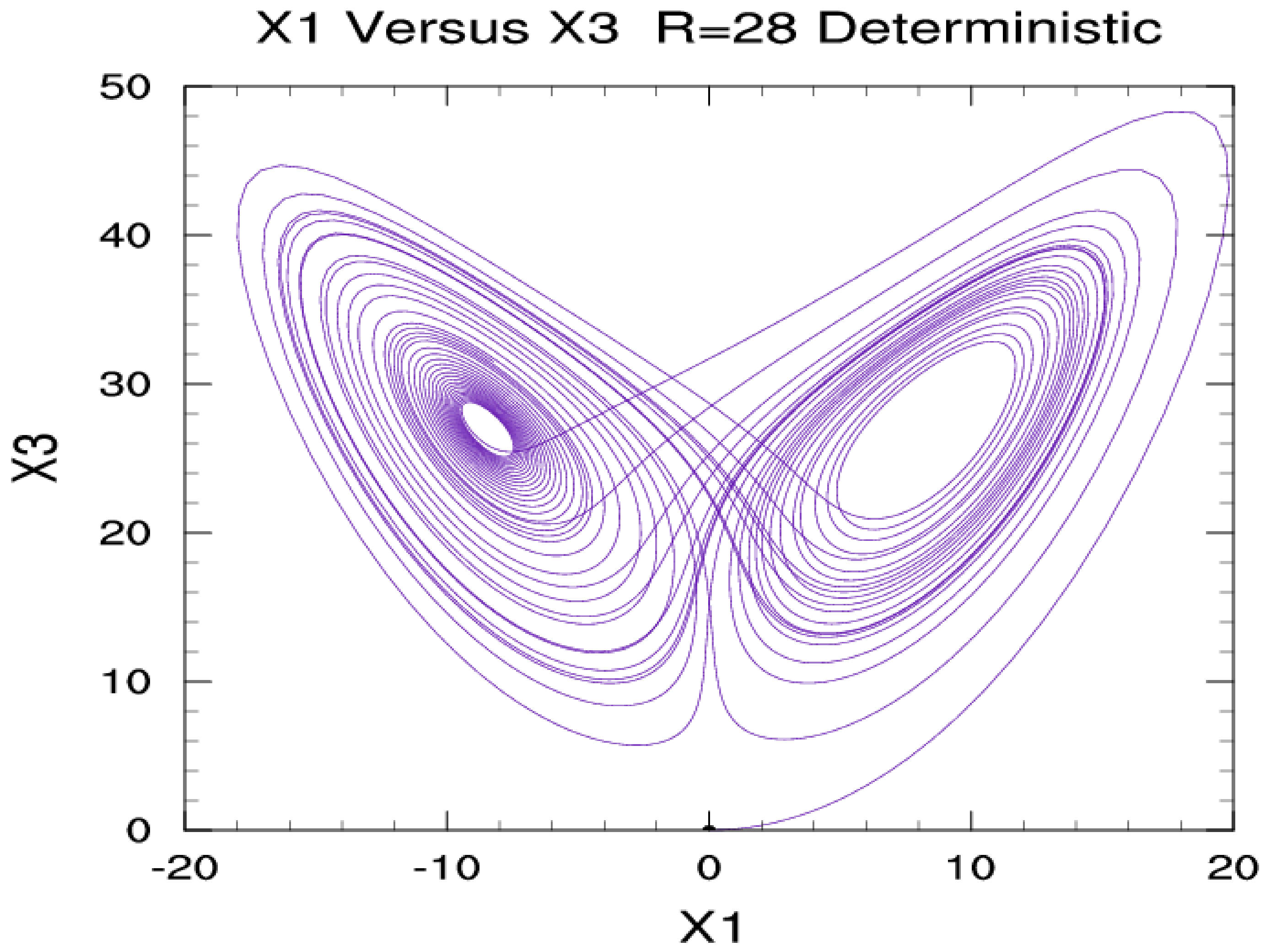
Here is M. C. run with 40,000 samples – thus this is the proper statistical answer X(3) = 13 and X1 = X2 = - 2.52; SD2 failed to capture the negative shift.



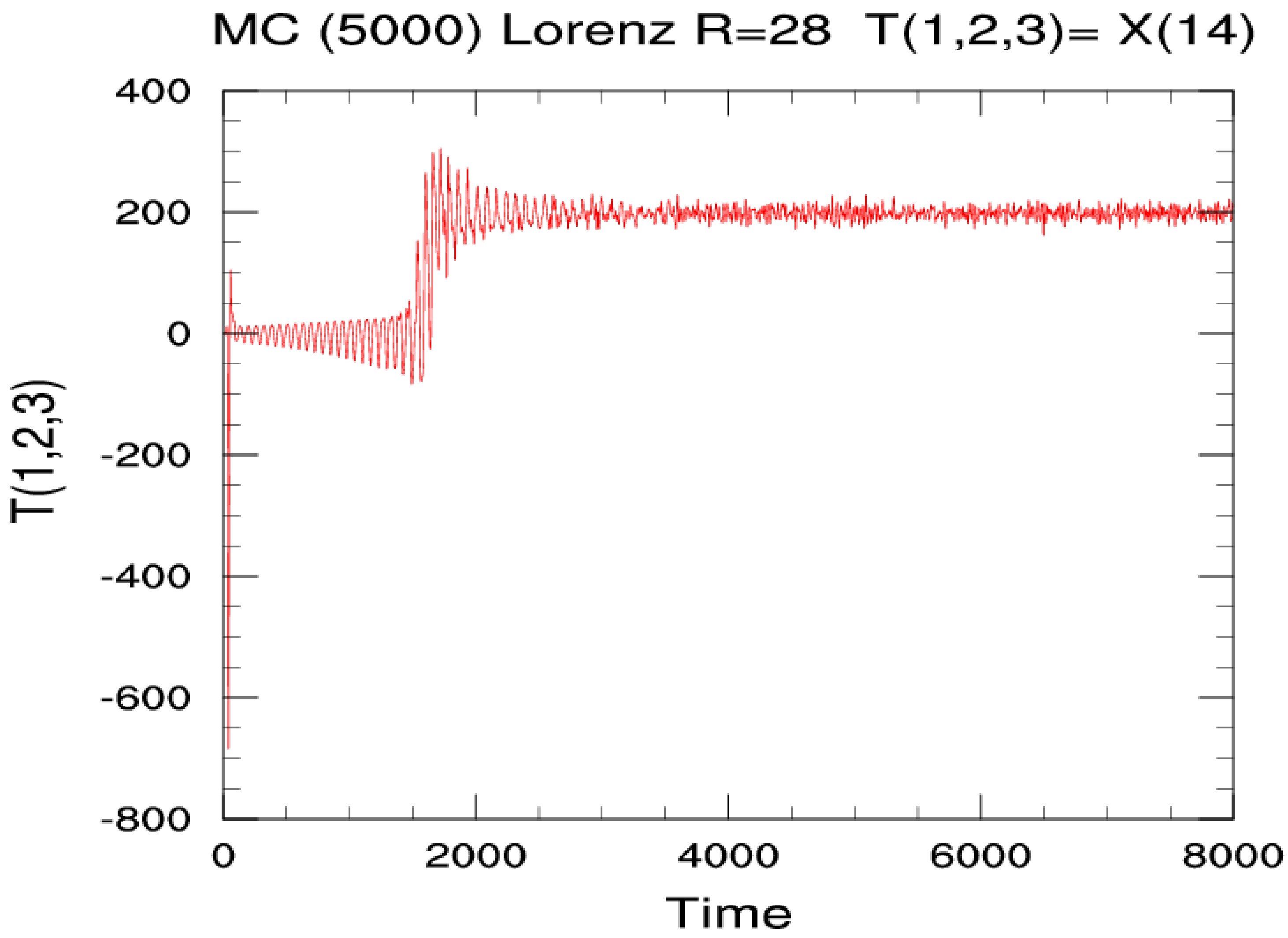
With the proper closure, SD3 provides the correct answers of X3 = 13 but also the correct answer for X1 = X2 = - 2.52



R = 14, X(3) = constant; all moments → to constant values and LHS = 0 in SD3 equations gives relationships: σ(1,1) = σ(1,2) = σ(2,2) = 28.32 which agree with Monte Carlo result – both in final form and in initial explosive randomness



R = 28 (chaos -- a formidable challenge!) X3 is far from constant – wild gyrations and the triple correlation T (1,2,3) is a large number with its own wild gyrations – shown in next slide



MC (5000) run for T (1,2,3): very large initial explosive randomness; some 1500 iterations oscillating about zero; then jumping up to over 300; then a turbulent jostling around the value 200 from 2200 to 8000 iterations

When a system is bounded and dissipative as the Lorenz system, all trajectories eventually tend toward some bounded set of zero volume in phase space.

This led to a discussion of my right side of brain (creative side in pink) with left side of brain (practical side in black)

Lets flood the attractor with Monte Carlo samples! How many? Let’s experiment!

What about that distracting Monte Carlo jostling we see? Let’s time average!

How many iterations do we average over? Let’s experiment!

How do know when we have the right answer? That’s easy – when the numbers stop changing – and we can look at the time variance which should decrease with increased sample size and the length of the time average.

That sounds like a lot of calculations! It is -- but let’s do it anyway!

The mean value of the 3rd moment T(1,1,3) = 400.6

Sample size	Number of	iterations used in	time averages
	250	1000	4000
100	6931	8302	9470
200	1812	1765	1856
500	1011	831	859
1000	453	388	416
2000	258	248	221
5000	89	91	96
40000	8	10	11

Time variance of T(1,1,3) as function of sample size and time averaging in iterations.

Moment	Variable #	MC Value	SD3 Value	Moment	Variable #	MC Value	SD3 Value
μ(1)	X(1)	– . 001	.000	T(1,1,1)	X(10)	.060	.000
μ(2)	X(2)	– .001	.000	T(1,1,2)	X(11)	.060	.000
μ(3)	X(3)	23.55	23.55	T(1,1,3)	X(12)	400.6	400.6
σ(1,1)	X(4)	62.80	62.80	T(1,2,2)	X(13)	.04	.000
σ(1,2)	X(5)	62.80	62.80	T(1,2,3)	X(14)	198.2	198.2
σ(1,3)	X(6)	– .005	.000	T(1,3,3)	X(15)	– .08	.000
σ(2,2)	X(7)	81.20	81.20	T(2,2,2)	X((16)	.009	.000
σ(2,3)	X(8)	.001	.000	T(2,2,3)	X(17)	84.83	84.8
σ(3,3)	X(9)	74.34	74.34	T(2,3,3)	X(18)	– .06	.000
				T(3,3,3)	X(19)	132.4	132.4

Time averaged values from MC sample size of 40,000 and 4000 iterations. SD3 values from equations described in next slide. The statistics of X(1) and X2) are symmetric thus an odd number of 1's and 2's → 0. These exact for large numbers

Monte Carlo results are just numbers – they do not reveal relationships!

Moreover, one needs only 2 of these 19 moments to derive the remaining!

Using the 19 SDE equations with the LHS = 0 (and no assumptions about 4^{th} moments) & just using X(3) = 23.55 and its variance σ(3,3) = X(9) = 74.34 from MC calculations, all the moment values and relationships are derivable – one needs only paper, pencil, and a hand calculator *

From $X(1)^{\blacksquare}$ = 0, we have X(1) = X(2); from $X(2)^{\blacksquare}$ = 0, we have X(1) { X(3) + R – 1} = 0

but X(3) ≠ R - 1, thus X(1) = X(2) = 0

From $X(3)^{\blacksquare}$ and $X(4)^{\blacksquare}$ = 0, we know that X(4) = X(5) = B X(3) = (8/3) (23.55) = 62.80

From $X(9)^{\blacksquare}$ = 0 ; 2 [X(1) X(8) + X(2) X(6) + T(1,2,3) - B X(9)] = 0 thus,

T(1,2,3) = B σ(3,3) = B X(9) = (8/3) (74.34) = 198.24

One can continue to use one result to build upon another, and many other interesting relationships can be shown; thus, the full nonlinearity of the variables and their relationships is revealed by the SD3 equations.

•Only ten of 15 possible 4th moment terms are in the SD3 equations; of these ten, 8 can be found by the above procedure – other two need MC calculations.

One more Relationship and Summary

$\sigma(2,2) = \sigma(1,1)\,[\,R - \mu(3)\,] - B\,\sigma(3,3)$ involves all 3 variances

$81.20 = (62.8)\,[\,28 - 23.5503] - (8/3)\,(74.34)$

$= 279.44 - 198.24 = 81.20$

The full stochastic dynamic equations (without any assumptions) represent a perfect blend of physics and statistical relationships.

Together with Monte Carlo calculations, this allows one to delve more deeply into the nonlinear nature of bound and dissipative physical systems - all the vital statistics of the strange attractor lay before us

Thank you Edward S. Epstein for your insight !

Several other relationships

$\sigma(2,2) = \sigma(1,1)\,[\,R - \mu(3)\,] - B\,\sigma(3,3)$ – a relationship involving all 3 variances

or

$\sigma(2,2) = \sigma(1,1)\,[\,R - \mu(3)\,] - T(1,2,3)$

$$81.20 = (62.8)\,[\,28 - 23.5503\,] - (8/3)\,(74.34)$$
$$= (62.8)\,(4.4497) - 198.24 = 279.44 - 198.24 = 81.20$$

$T(1,1,3) = \sigma(1,1)\,[\,R - P - 1 - \mu(3)\,] + P\,\sigma(2,2)$

$$400.64 = (62.8)\,[\,28 - 10 - 1 - 23.5503\,] + (10)\,(81.2)$$
$$= (62.8)\,(-\,6.5503) + 812.0 = 812.0 - 411.36 = 400.64$$

$\lambda(1,1,1,2) = (B + 2\,P)\,T(1,1,3) - 2\,P\,T(1,2,3) + \sigma(1,1)\,\sigma(1,2)$

$$9060.1 = [\,8/3 + (2)(10)\,]\,(400.64) - (2)\,(10)\,(198.24) + (62.8)(62.8)$$
$$= 9081.17 - 3964.80 + 3943.84 = 9060.2$$

Further Relationships among the moments

The 1st from σ(3,3)˙, the remainder from T(3,3,3)˙ , λ(3,3,3,3)˙ , and f (3,3,3,3,3)˙

3rd moment: $T(1,2,3) = B\,\sigma(3,3)$

$198.24 = (8/3)\,(74.34) = 198.24$

4th moment: $\lambda(1,2,3,3) = B\,T(3,3,3) + \sigma(1,2)\,\sigma(3,3)$

$5021.6 = (8/3)\,((132,43) + (62.8)\,(74.34) = 5021.6$

5th moment: $f\,(1,2,3,3,3) = B\,\lambda(3,3,3,3) + \sigma(1,2)\,T(3,3,3)$

$39{,}874 = (8/3)\,(11{,}837) + (62.8)\,(132.4)$

$= 31{,}565 + 8{,}315 = 39{,}880$ $1\text{x}\,10^{-5}$ error

6th moment: $f\,(1,2,3,3,3,3) = B\,f\,(3,3,3,3,3) + \sigma(1,2)\,\lambda(3,3,3,3)$

$856{,}366 = (8/3)\,(42{,}341) + (62.8)\,(11{,}838)$

$= 112{,}909 + 743{,}426 = 856{,}335$ $1\text{x}10^{-5}$ error

Kurtosis B_2 for X(1) and X(2) = $\lambda(1,1,1,1) / [\sigma(1,1)]^2 = 9060 / 62.8^2 = 9060 / 3943.8 = 2.3 < 3$

Therefore these are platykurtic.

X(3) is positively skewed with coefficient $T(3,3,3) / \sigma^{3/2}$

$S = T(3,3,3) / [\sigma(3,3)^{1/2}]^3 = T(3,3,3) / \sigma(3,3)^{3/2} = 132 / (74.3)^{3/2} = 132 / 641 = 0.206$

Table 2. Calculated MC values and computed SD3 values from full equations

Moment	Variable #	M C Value	SD3 Value	Moment	Variable #	M C Value	SD3 Value
λ(1,1,1,1)	X(20)	9060.1	9060.1	λ(1,1,3,3)	X(25)	6712.5	6713.0
λ(1,1,1,2)	X(21)	9060.2	9060.1	λ(1,2,2,2)	X(26)	13774	13774
λ(1,1,1,3)	X(22)	-0.14	0.0	λ(1,2,2,3)	X(27)	- 0.15	0.0
λ(1,1,2,2)	X(23)	10735	10735	λ(1,2,3,3)	X(28)	5021.5	5021.1
λ(1,1,2,3)	X(24)	-0.003	0.0	λ(1,3,3,3)	X(29)	- 1.2	0.0

The 4^{th} moments: X(20) and X(30) through X(34) are not in the SD3 equation set

The five 4^{th} moments in blue are active in four 3^{rd} moment prediction equations

Four of the 4^{th} moment terms → 0.0 due to the symmetry of X(1) and X(2)

The Lorenz Equations – a simplified model of fluid convection in the X-Z plane with the fluid heated from below and cooled from above

$\dot{X} = P(Y - X)$ $\dot{Y} = -XZ + RX - Y$ $\dot{Z} = XY - BZ$

X __ proportional to the convective overturning
Y __ measures the horizontal temperature variation between currents
Z __ measures the distortion of the vertical temperature profile from linearity

P = Prandtl number = kinematic viscosity / thermal conductivity = 10 (~ twice that of water)
B = describes the flow conditions = 8/3 (~ ratio of horizontal wavelength to depth of fluid)
R = Rayleigh number; (after Lord Rayleigh's investigation of convection in 1916)

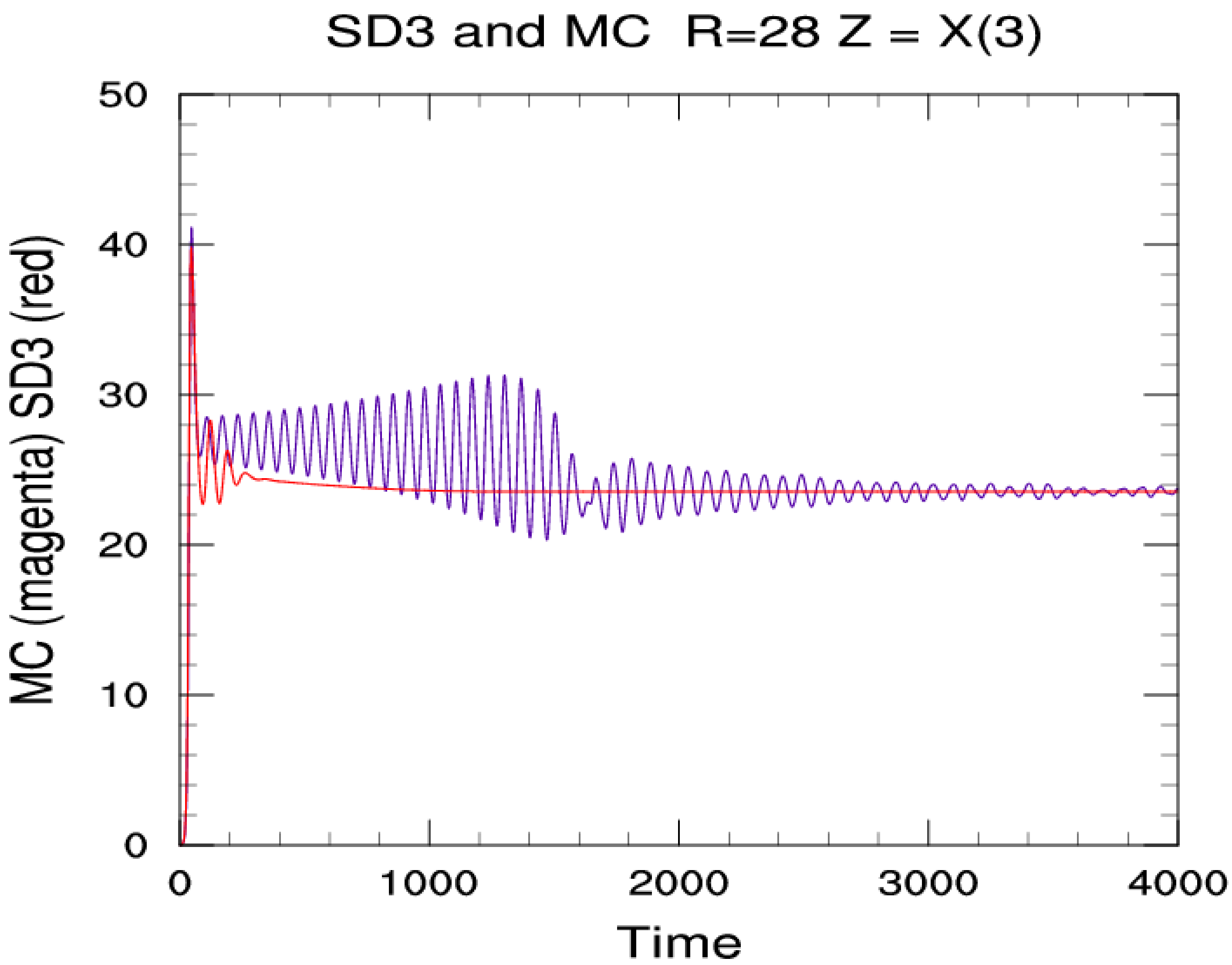
The stability of the equations are investigated by linearizing the equations and analyzing the roots of the characteristic equation of the resulting matrix for each solution

R = 1 is criteria for convection (otherwise if R < 1 then X = Y = Z = 0 and no convection)
R > 1 has two additional steady state solutions $X = Y = \pm[b(r-1)]^{1/2}$, $Z = r - 1$

the steady state solutions become unstable when

$R_{Critical} = (P)(P + b + 3) / (P - B - 1) = (10)(47/3) / (19/3) = (10)(47/19) = 24.74$

which results in the chaotic flow



Eventually X(3) = 23.55 over time: MC and SD3 in excellent agreement