arXiv:1305.0961v2 [cs.DM] 18 May 2013

Time-Reversible Random Number Generators : Solution of Our Challenge by Federico Ricci-Tersenghi

Wm. G. Hoover and Carol G. Hoover
Ruby Valley Research Institute
Highway Contract 60, Box 601
Ruby Valley, Nevada 89833

(Dated: May 21, 2013)

Abstract

Nearly all the evolution equations of physics are time-reversible, in the sense that a movie of the solution, played backwards, would obey exactly the same differential equations as the original forward solution. By way of contrast, *stochastic* approaches are typically *not* time-reversible, though they could be made so by the simple expedient of storing their underlying pseudorandom numbers in an array. Here we illustrate the notion of *time-reversible random number generators.* In Version 1 we offered a suitable reward for the first arXiv response furnishing a reversed version of an only slightly-more-complicated pseudorandom number generator. Here we include Professor Ricci-Tersenghi's prize-winning reversed version as described in his arXiv:1305.1805 contribution: "The Solution to the Challenge in 'Time-Reversible Random Number Generators' by Wm. G. Hoover and Carol G. Hoover".

PACS numbers: 05.40.-a, 05.20.-y, 83.10.Rs, 05.10.Gg

Keywords: Time Reversibility, Algorithms, Langevin Equation

I. TIME REVERSIBILITY

The Newtonian, Lagrangian, or Hamiltonian microscopic motion equations ,

$$\{ F = m\ddot{r} \} \ ; \ \{ p = (\partial \mathcal{L}/\partial \dot{q}) \ ; \ \dot{p} = (\partial \mathcal{L}/\partial \dot{q}) \} \ ; \ \{ \dot{q} = +(\partial \mathcal{H}/\partial p) \ ; \ \dot{p} = -(\partial \mathcal{H}/\partial \dot{q}) \} \ ,$$

even when embellished with thermostats, ergostats, or barostats, are typically time-reversible[1]. The Stϕrmer-Verlet time-symmetric "Leapfrog Algorithm" :

$$\{ \ q(t+dt) - 2q(t) + q(t-dt) \equiv (F(t)/m)dt^2 \ \} \ ,$$

which can be iterated either forward or backward once the coordinates are given at two successive times, is the most transparent example of time reversibility. Likewise the Schrödinger equation and Maxwell's electromagnetic field equations can be used to generate movies which obey exactly the same equations whether projected in the "forward" or the "backward" direction of time. Mathematicians have considered more general definitions of time reversibility[2], but in some cases these generalizations would include the damped oscillator among the class of reversible systems[3], which we believe isn't sensible.

The Langevin equation ,

$$\{ \ m\ddot{r} = F - (m\dot{r}/\tau) + \mathcal{R} \ \} \ ,$$

where both the drag coefficient $(1/\tau)$ and the random force $\mathcal{R}$ aren't time-reversible, is often used in molecular simulations[4,5]. In order to make it possible to extend stochastic solutions both forward and backward in time, and to simplify the reproducibility of numerical results by others we think it is desirable to incorporate time-reversible random number generators in our otherwise deterministic algorithms. The following Section illustrates this idea with a simple example algorithm, too simple for serious use in simulation. The final Section of Version 1 challenged the reader to find a time-reversed version of a useful algorithm, with a reward for being "first" with that specific algorithm. In this Version we include the successful algorithm found by Federico Ricci-Tersenghi *within a day* of the challenge's publication.

II. AN OVERSIMPLIFIED PSEUDORANDOM NUMBER GENERATOR AND ITS TIME-REVERSED VERSION

The design of reversible random number algorithms can be illuminated by the study of time-reversible maps. Kum and Hoover[6] considered two-dimensional maps which are time-reversible in the physicist's sense :

$$M(+q,+p) = (+q',+p') \; ; \; M(+q',-p') = (+q,-p) \; .$$

They pointed out that simple shears, with $\delta q \propto \delta p$ or $\delta p \propto \delta q$, as well as certain phase-space reflection operations, are time-reversible and can be combined with periodic boundary conditions so that the points (q,p) remain within the unit square. In addition, if Q, P, and R are time-reversible maps then symmetric combinations of them, like $QPRPQ$, are likewise time-reversible. The simple q and p shears very closely resemble typical algorithms for pseudorandom numbers, such as the FORTRAN example function :

```
function rund(intx,inty)
i = 1029*intx + 1731
j = i + 1029*inty + 507*intx - 1731
intx = mod(i,2048)
j = j + (i - intx)/2048
inty = mod(j,2048)
rund = (intx + 2048*inty)/4194304.0
return
end
```

This generator returns a periodic sequence of 2^{22} pseudorandom numbers, updating the two seed variables `intx` and `inty` as it goes. The least significant 11 binary digits of `rund`'s numerator can be generated by the simpler function :

```
function next(it)
next = mod(1029*it + 1731,2048)
return
end
```

The Figure at the bottom of this page is a plot of the 2048 iterates of `next` , ordered according to the index `it` . The first six entries are the pairs

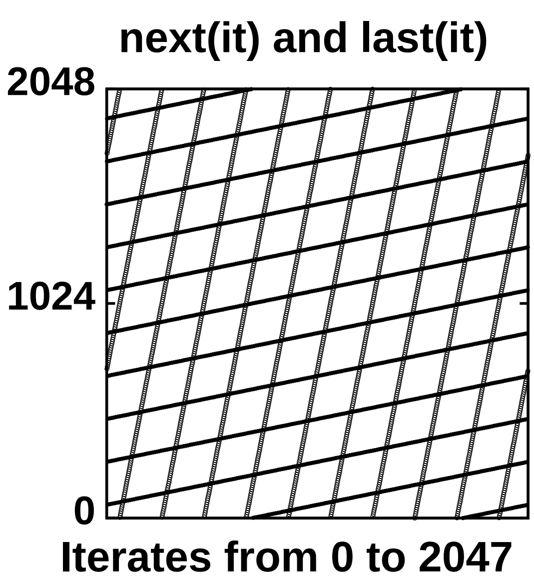
$$\texttt{next} \rightarrow (1,712),(2,1741),(3,722),(4,1751),(5,732),(6,1761)\ .$$

The single-valued plot of these forward iterates gives the (misleading) impression of *continuous* lines with a slope (from either the odd or the even entries) of (5/1) , while the actual function is *discontinuous* between successive entries due to the jumpy nature of the `mod` function. Reflecting the plot ,

$$(\ x,y\ ) \longleftrightarrow (\ y,x\ )\ ,$$

illustrates the output of the time-reversed algorithm `last` . Because the equations are *linear* it is relatively easy to find the analytic form of the reversed function :

```
function last(j)
last = mod(205*j + 1497,2048)
return
end
```



The `last` function, likewise plotted in the Figure, is also single-valued. It *appears* to generate ten separate lines. The values of `last` for $1 \leq j \leq 11$ are just enough to indicate how this function resembles ten continuous lines :

$$\texttt{last} \rightarrow (1,1702),(2,1907),(3,64),(4,269),(5,474),$$

$$(6,679),(7,884),(8,1089),(9,1294),(10,1499),(11,1704) \ .$$

Comparing the first and last entries shows that the apparent slope of the less-steep "lines" is $(1704 - 1702)/(11 - 1) = (1/5)$. The reversed arrays of points have an apparent slope of $(1/5)$ because increasing `j` by 10 is *usually* required in order to increase `last` by 2 . These two functions `next` and `last` go forward and backward, taking in the result of the most recent iteration, in the range $[0, 2047]$, as the abscissa and returning, as the ordinate, either the next or the most recent integer.

III. OUR CHALLENGE [RECENTLY MET!]

We viewed a simple, explicit time-reversible pair of generators analogous to `next` and `last` above as desirable for stochastic computer simulations. We have happily rewarded the first successful FORTRAN algorithm generating the two-argument reversal of `rund(intx,inty)` above with a cash prize of 500 United States dollars, awarded to Federico Ricci-Tersenghi. As was required, his solution was demonstrated to work for the initial seeds `intx = inty = 0` . Here is a program based on his solution:

```
program federico
parameter (items = 4194304)
implicit integer(a-z)
dimension forwx(items),forwy(items),backx(items),backy(items)
intx = 0
inty = 0
do n = 1,items
i = 1029*intx + 1731
j = i + 1029*inty + 507*intx - 1731
intx = mod(i,2048)
j = j + (i - intx)/2048
```

```
inty = mod(j,2048)
forwx(n) = intx
forwy(n) = inty
end do

intx = 0
inty = 0
do n = 1,items
oldx = mod(205*intx + 1497,2048)
inty = inty + items - 1536*oldx - (1029*oldx + 1731 - intx)/2048
inty = mod(205*inty,2048)
intx = oldx
backx(n) = intx
backy(n) = inty
enddo
stop
end
```

The seed variables forward and backward can be verified to satisfy the identities :

$$\texttt{forwx}(\texttt{i}) = \texttt{backx}(\texttt{items} - \texttt{i}) \; ; \; \texttt{forwy}(\texttt{i}) = \texttt{backy}(\texttt{items} - \texttt{i}) \; .$$

IV. ACKNOWLEDGMENTS

We are particularly grateful to the late Ian Snook and our colleague Niels Grϕnbech-Jensen for calling the importance of stochastic algorithms to our attention, to Nathan Hoover for pointing out the disallowed storage shortcut, and to Carl Dettmann for pointing out to us that the damped harmonic oscillator *is* time-reversible in the sense put forward in Reference 2 . We specially thank Professor Ricci-Tersenghi for his prompt solution of our challenge.

V. ANOTHER CHALLENGE?

In 2014 we intend again to offer an Ian Snook Memorial Challenge Prize for solving an interesting problem relevant to computational statistical mechanics. Suggestions welcome!

---

[1] Wm. G. Hoover and Carol G. Hoover, *Time Reversibility, Computer Simulation, Algorithms, and Chaos* (World Scientific, Singapore, 2012) .

[2] J. A. G. Roberts and G. R. W. Quispel, "Chaos and Time-Reversal Symmetry. Order and Chaos in Reversible Dynamical Systems", Physics Reports **216**, 63-177 (1992) .

[3] C. P. Dettmann, Private Communications of February 2013 .

[4] Ian Snook, *The Langevin and Generalised Langevin Approach to the Dynamics of Atomic, Polymeric, and Colloidal Systems* (Elsevier, Amsterdam, 2007) .

[5] N. Grϕnbech-Jensen and O. Farago, "A Simple and Effective Verlet-type Algorithm for Simulating Langevin Dynamics", arXiv 1212.1244 (2013) .

[6] Wm. G. Hoover and O. Kum, "Time-Reversible Dissipative Ergodic Maps", Physical Review E **53**, 213-2129 (1996) .