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Comment on "Chaotic Advection in Quiet Discharges in Tokamaks"

S. Tian and W. Horton
Institute for Fusion Studies
The University of Texas at Austin
Austin, Texas 78712

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S. Tian and W. Horton
Institute for Fusion Studies and
Department of Physics
The University of Texas at Austin
Austin, Texas 78712

Fradkin and Nex[1] have recently re-examined the computational aspect of the HCYuP model[2] for turbulent electron diffusion in 'quiet' discharges in tokamaks. They first experimented with the 4-5th order Runge-Kutta algorithm with an adaptive time step and then with the implicit leap-frog or mid-point algorithm with a constant time step. By using the half-way time-reversal tests, they concluded that "When this symplectic algorithm is run with accuracy comparable with that of the ordinary Runge-Kutta algorithm, the time of execution falls by a factor of 10 to 20!" Unfortunately, this seemingly good news does not seem to be universal. In particular, we have performed the same numerical experiments with the 5-6th order Runge-Kutta algorithm with an adjustable time step (referred to IVPRK hereafter),[3] the implicit mid-point algorithm with a constant time step (referred to IRK2 hereafter),[4] and the implicit 4th order Runge-Kutta algorithm with a constant time step (referred to IRK4 hereafter).[4] Note that IVPRK is non-symplectic while both IRK2 and IRK4 are symplectic. Our results do not support the conclusions drawn by Fradkin and Nex.[1]

Our Hamiltonian model and computational procedure are exactly the same as those by HCYuP[2] and Fradkin and Nex.[1] All the computations were performed on the Cray Y-MP. We averaged over 64 particles instead of averaging over an ensemble of Hamiltonian realizations since particle average seems physically more realistic than the ensemble average in tokamaks.

For clarity, we only show two instances of the results, e.g, $\tilde{\phi} = 2$ and $\tilde{\phi} = 10$. The Lyapunov exponents are estimated to be $0.6/2\pi$ and $1.0/2\pi$ for $\tilde{\phi} = 2$ and $\tilde{\phi} = 10$, respectively.

Before we proceed we shall first define how to compare two different algorithms. Fradkin and Nex[1] resolved this by comparing time-reversal diffusivities. Our approach is that given a roughly equal CPU time, we compare both the normal and time-reversal curves produced by three different integrators, that is, we compare both the standard relative error and time-reversal estimation of the error. Once we have defined the terms for comparison of different integrators we will use it to estimate the relative accuracy. We found that for time step of $0.1 \times 2\pi$, the three integrators consume comparable CPU time. The real timing (excluding time-reversal CPU time) is given in Table I. Figs. 1 and 2 show the dependence of diffusion coefficients D on time t, while Figs. 3 and 4 show their time-reversal counterparts D_{rev}. Since the computed D_{rev} for $\tilde{\phi} = 2$ by IVPRK is so small compared with that by IRK2 and IRK4, it is replotted in Fig. 3(b) in an expanded scale. From Figs. 1 and 2, we see that the results by three integrators agree with each other quite well. If we take the average of the three curves as the standard reference diffusion coefficients (this makes sense because the computed diffusivities oscillate around this values at much smaller time steps,) then the relative error for each of three integrators is within 30% for $\tilde{\phi} = 2$ and within 15% for $\tilde{\phi} = 10$. We call this estimate of error the "standard error estimate."

Let us first suppose that the time-reversal coefficients are good indicator for the numerical diffusion. Then from Fig. 3 and 4, we would estimate that the numerical diffusion error is more than 100% (except for $\tilde{\phi} = 2$ by IVPRK, which we will discuss later) if we use the recipe by Fradkin and Nex.[1] So the numerical error estimated by the time reversal procedure is much greater than that by standard error estimate. It is hard to believe this is the case since the results by the three completely different integrators are in good agreement (within 30%). On the order hand, Figs. 3 and 4 would suggest that IVPRK may be 100 times more accurate than other two symplectic integrators for $\tilde{\phi} = 2$ and equally accurate for $\tilde{\phi} = 10$.

This is undoubtedly beyond reasonable ground.

Thus, in our opinion, non-symplectic Runge-Kutta 5-6th order integrator with adequate error control may be competitive with symplectic integrators since it produces similar curves in a comparable CPU time, in particular, we do not find the 20 times faster speed-up by symplectic integrators than that by non-symplectic integrators as suggested by Fradkin and Nex.[1] Although the half-way time reversal procedure is theoretically plausible, in practice it may give a poor indication of the error in the numerical diffusion coefficient.

References

[1]L.J. Fradkin and F. Nex, Plasma Phys. Control. Fusion **36**, 25 (1994).

[2]W. Horton, D.-I. Choi, P.N. Yushmanov, and V.V. Parail, Plasma Phys. and Control. Fusion **29**, 901 (1987).

[3]International Math. and Stat. Library (Version 3.2).

[4]W. Ye, private communications.

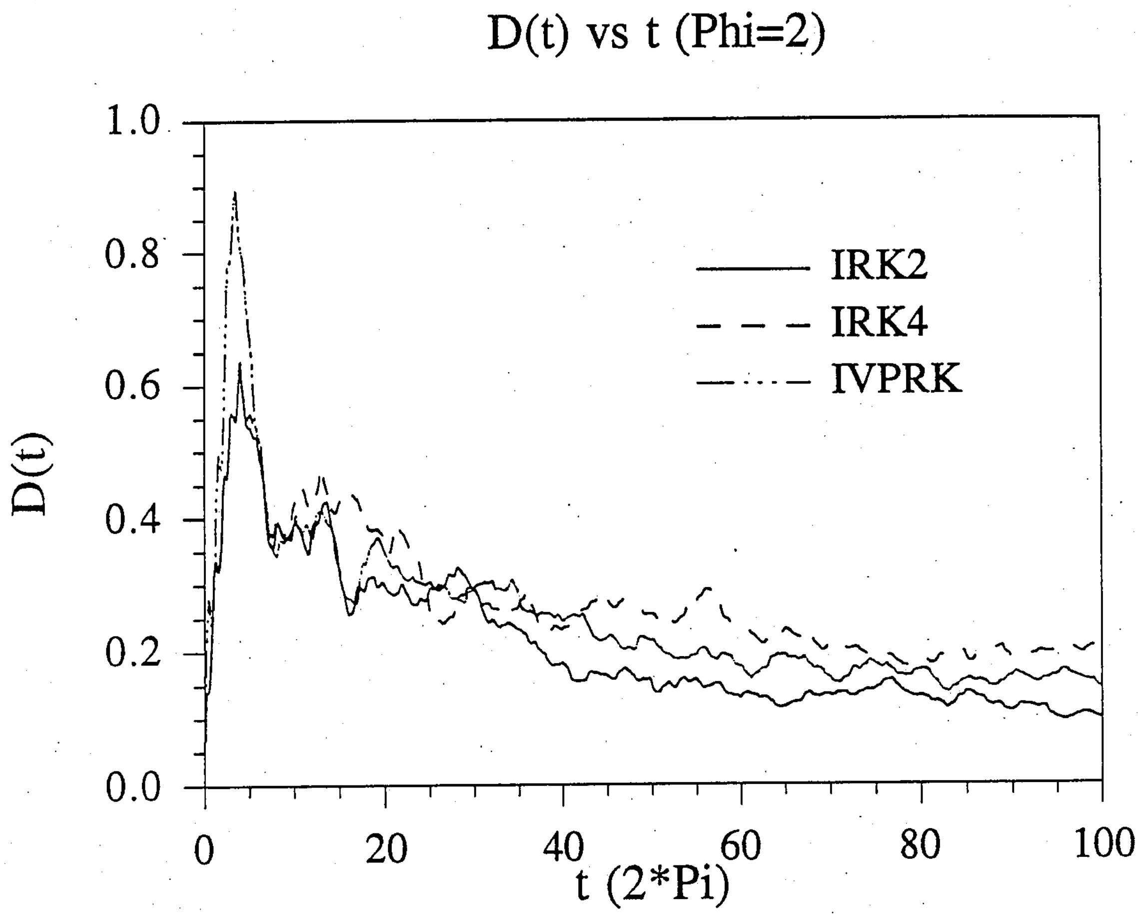

D(t) vs t (Phi=2)
1.0
0.8
0.6
0.4
0.2
0.0
D(t)
IRK2
IRK4
IVPRK
0
20
40
60
80
100
t (2*Pi)

Fig. 1

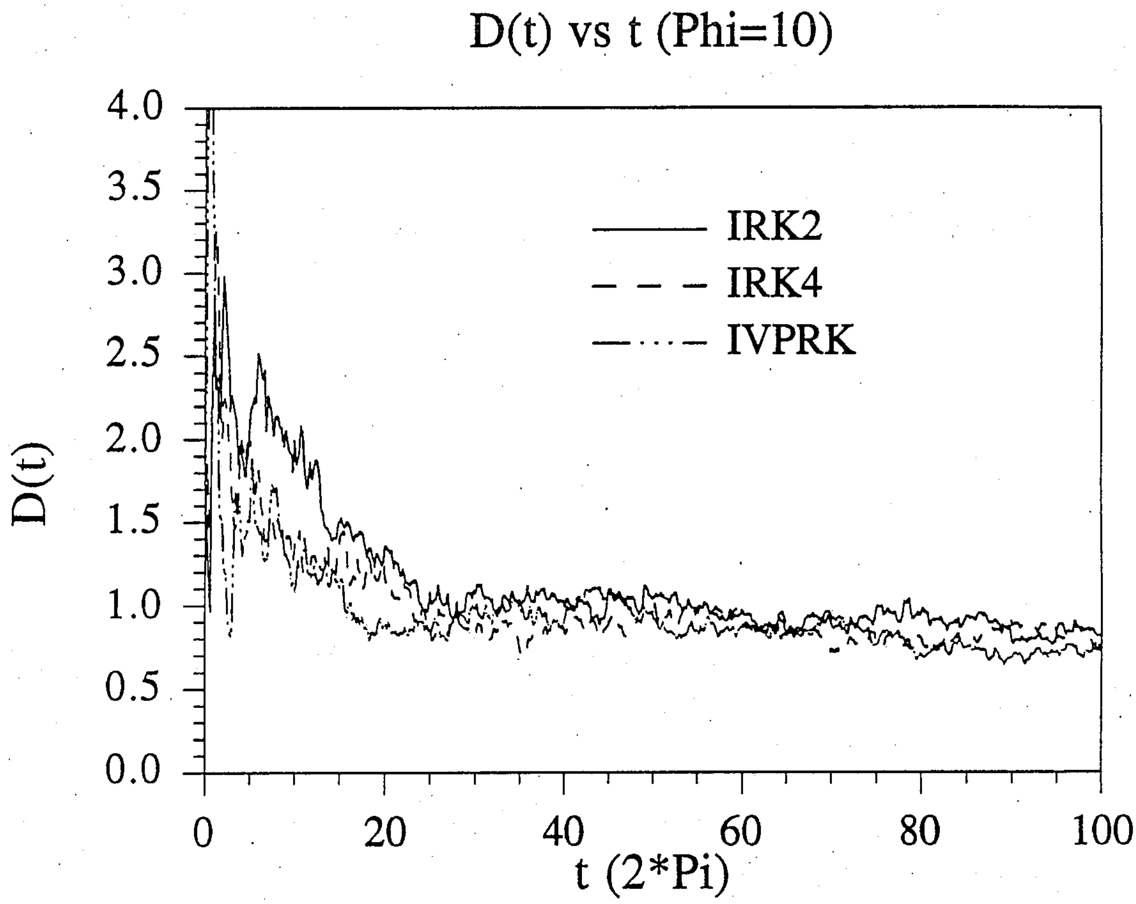
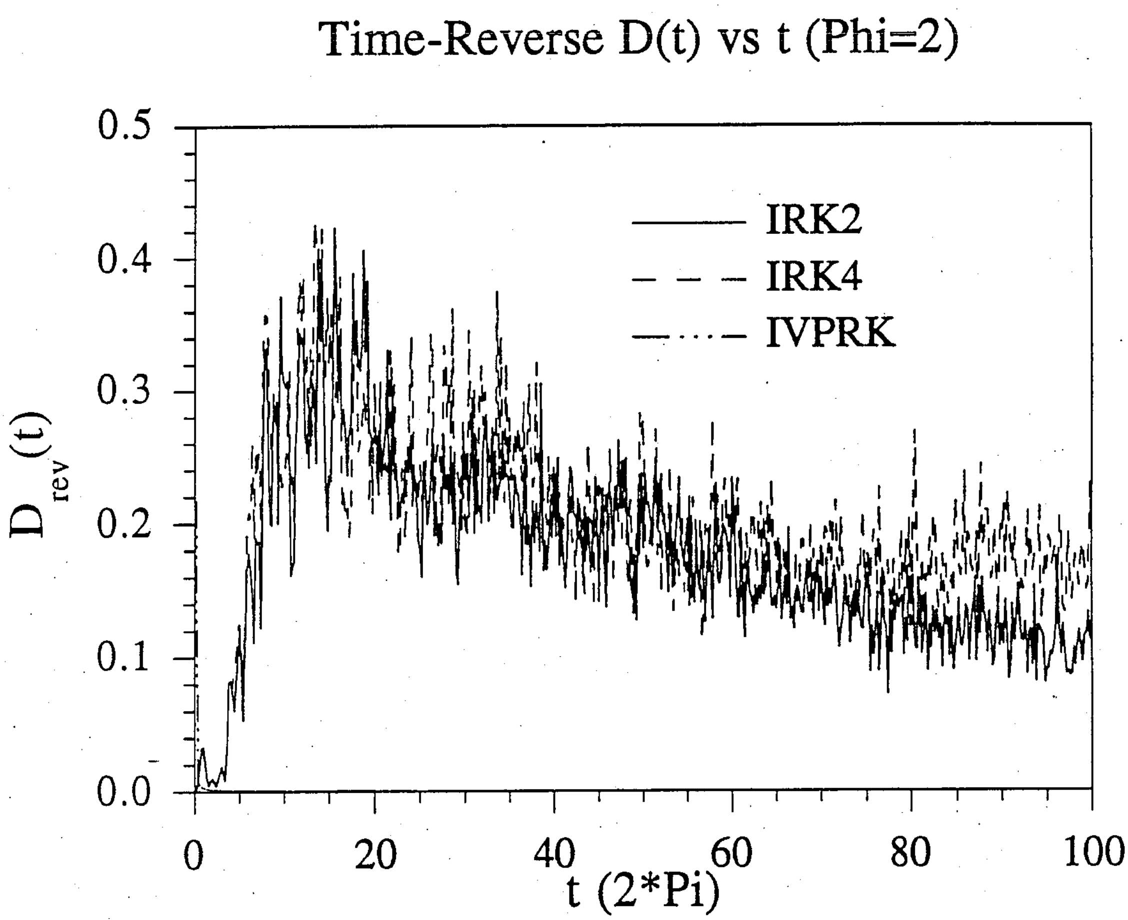

D(t) vs t (Phi=10)
IRK2
IRK4
IVPRK
D(t)
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
t (2*Pi)

Fig. 2



Time-Reverse D(t) vs t (Phi=2)
0.5
0.4
0.3
0.2
0.1
0.0
D_rev(t)
IRK2
IRK4
IVPRK
0
20
40
60
80
100
t (2*Pi)

Fig. 3(a)

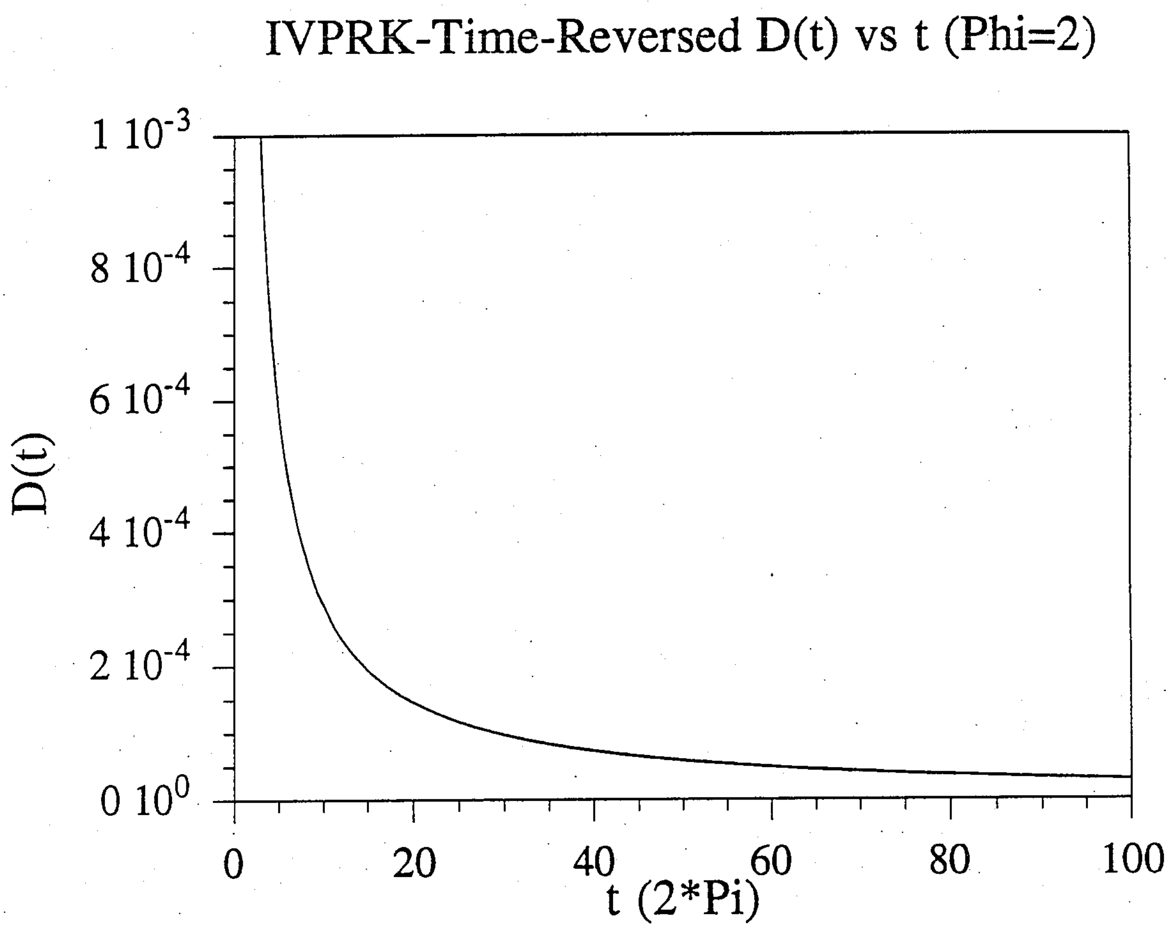

IVPRK-Time-Reversed D(t) vs t (Phi=2)
1 10-3
8 10-4
6 10-4
4 10-4
2 10-4
0 100
D(t)
0
20
40
60
80
100
t (2*Pi)

Fig. 3(b)

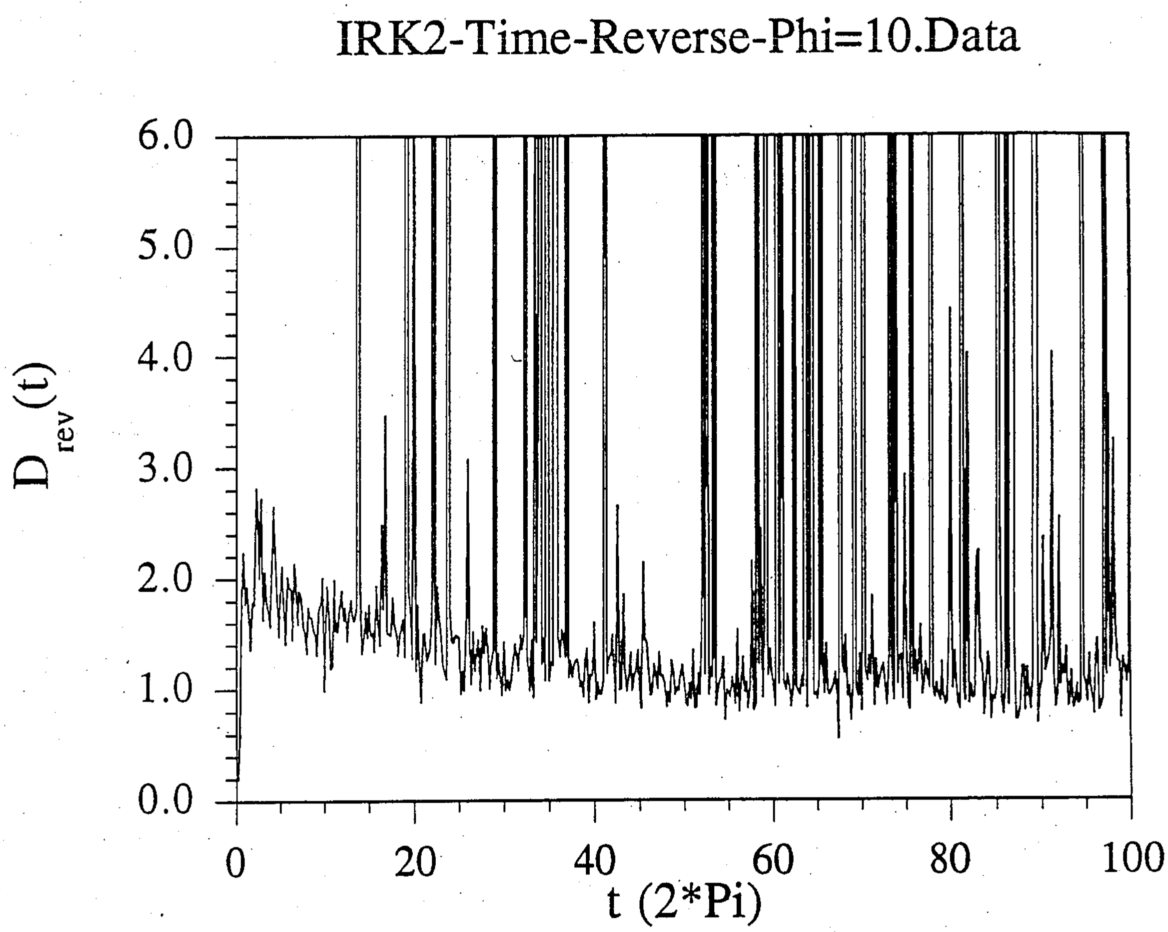

IRK2-Time-Reverse-Phi=10.Data
6.0
5.0
4.0
3.0
2.0
1.0
0.0
$D_{rev}(t)$
0
20
40
60
80
100
t (2*Pi)

Fig. 4(a)

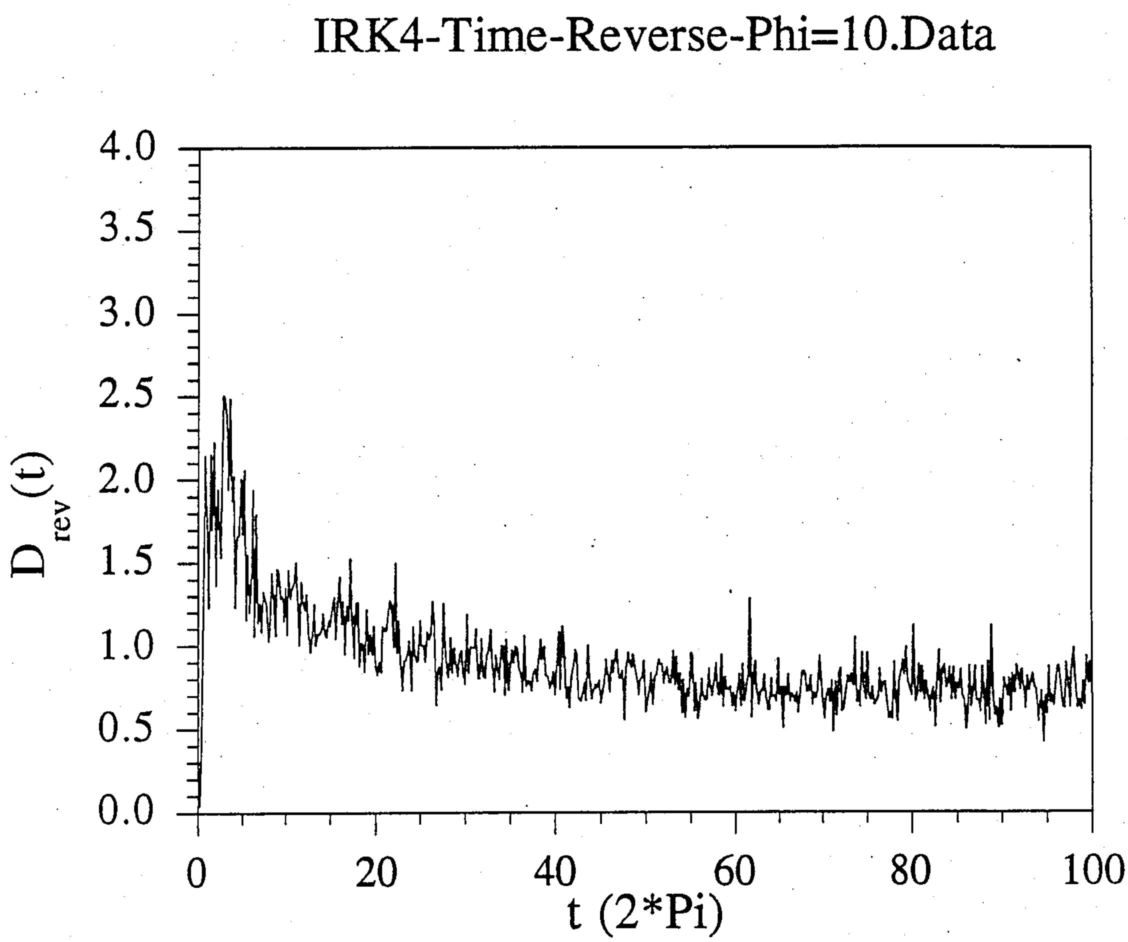

IRK4-Time-Reverse-Phi=10.Data
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
$D_{rev}(t)$
0
20
40
60
80
100
t (2*Pi)

Fig. 4(b)

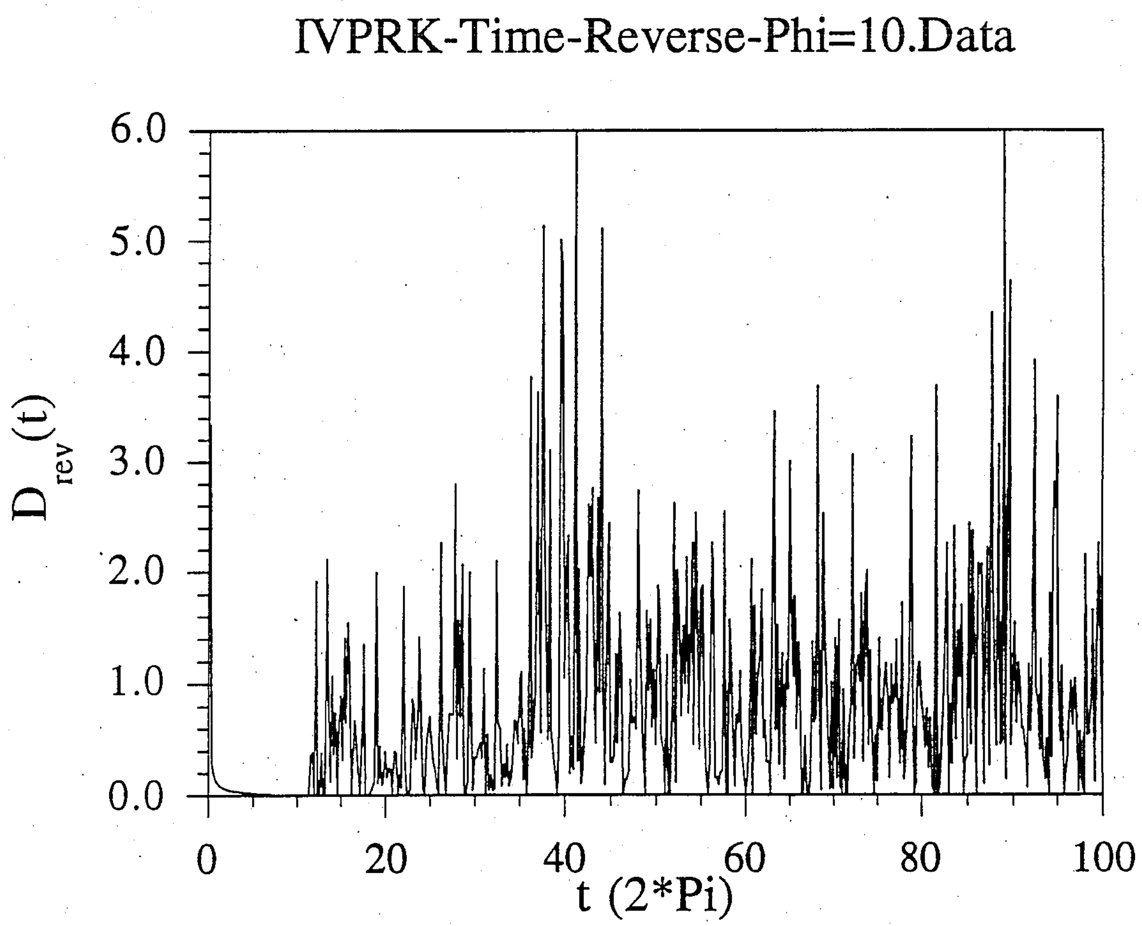

IVPRK-Time-Reverse-Phi=10.Data
6.0
5.0
4.0
3.0
2.0
1.0
0.0
$D_{rev}(t)$
0
20
40
60
80
100
t (2*Pi)

Fig. 4(c)

Figure Captions

1. Comparison of computed diffusivities D as a function of time t by three different integrators (IRK2, IRK4, and IVPRK) for $\tilde{\phi} = 2$. Relative error is 10^{-5} to terminate the iterations for IRK2 and IRK4. And the tolerance for error control is also 10^{-5} for IVPRK.

2. Same as Fig. 1 except for $\tilde{\phi} = 10$.

3. (a) Comparison of computed time-reversal diffusivities D_{rev} as a function of time t by three different integrators for $\tilde{\phi} = 2$. (b) Expanded scale for IVPRK.

4. Same as Fig. 3 except for $\tilde{\phi} = 10$. (a) IRK2, (b) IRK4, and (c) IVPRK. Note that the irregular points are due to the convergent failures after the maximum iterations.

Comparison of CPU Time

	$\widetilde{\phi} = 2$	$\widetilde{\phi} = 10$
IRK2	54.7	116
IRK4	109	187
IVPRK	57.9	141

Table I: Comparison of CPU time (excluding time-reversal part) for time step of $0.1 \times (2\pi)$. Note that since IVPRK is an adaptive integrator, $0.1 \times (2\pi)$ is just the initial time step. Note also that the relative error is 10^{-5} for IRK2 and IRK4 to terminate iteration, and the tolerance for error control is also 10^{-5} for IVPRK.