993SM - Laboratory of Computational Physics
Unit XI
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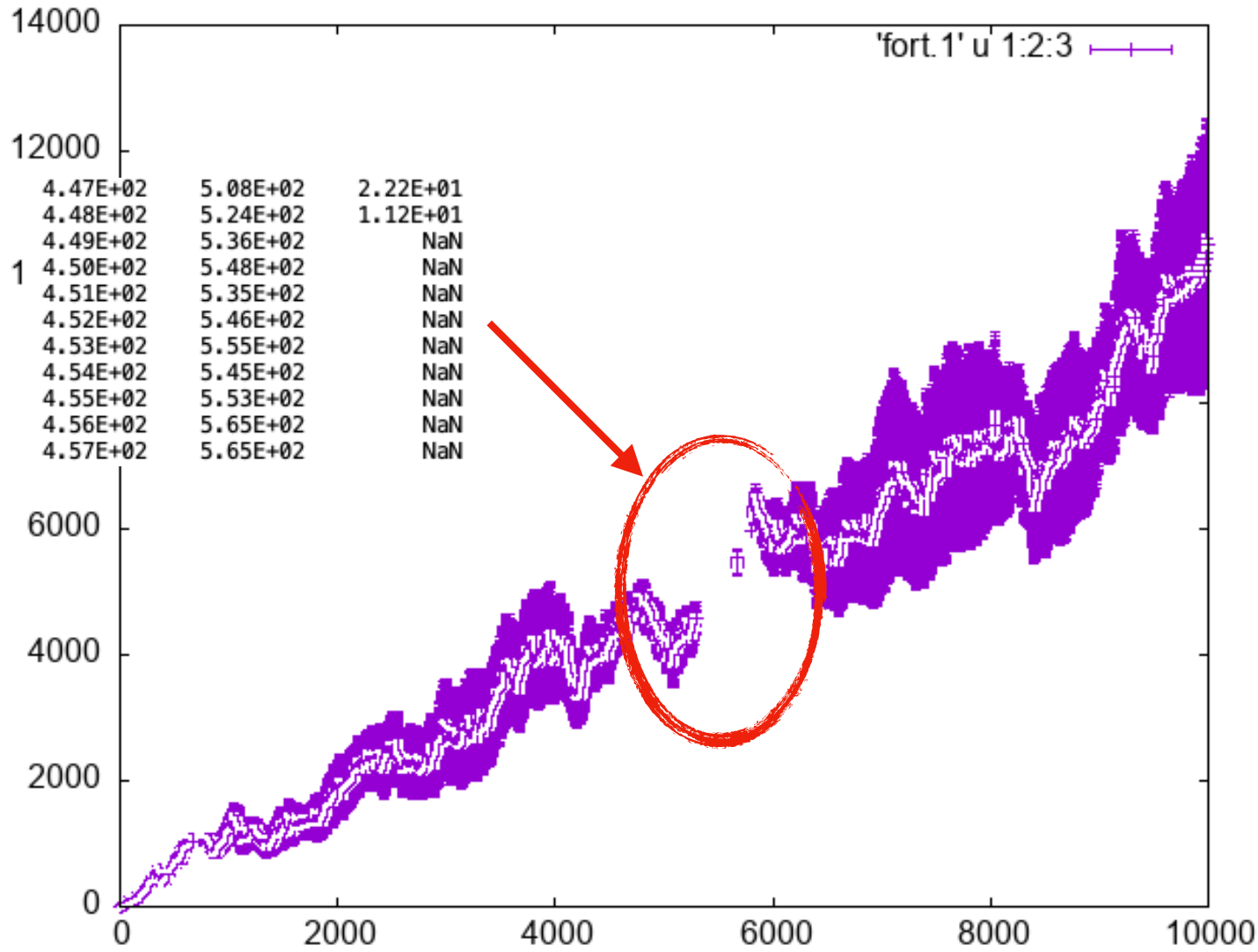
con il codice “latticegas-modified.f90” :

Density Np/L^2= 3.24999988E-02 ; Np= 13 ; L= 2
t, drsqave(t), sqrt(var(drsqave(t))/Np), D(t), <D>_T



"latticegas-modified.f90"

sbagliato!

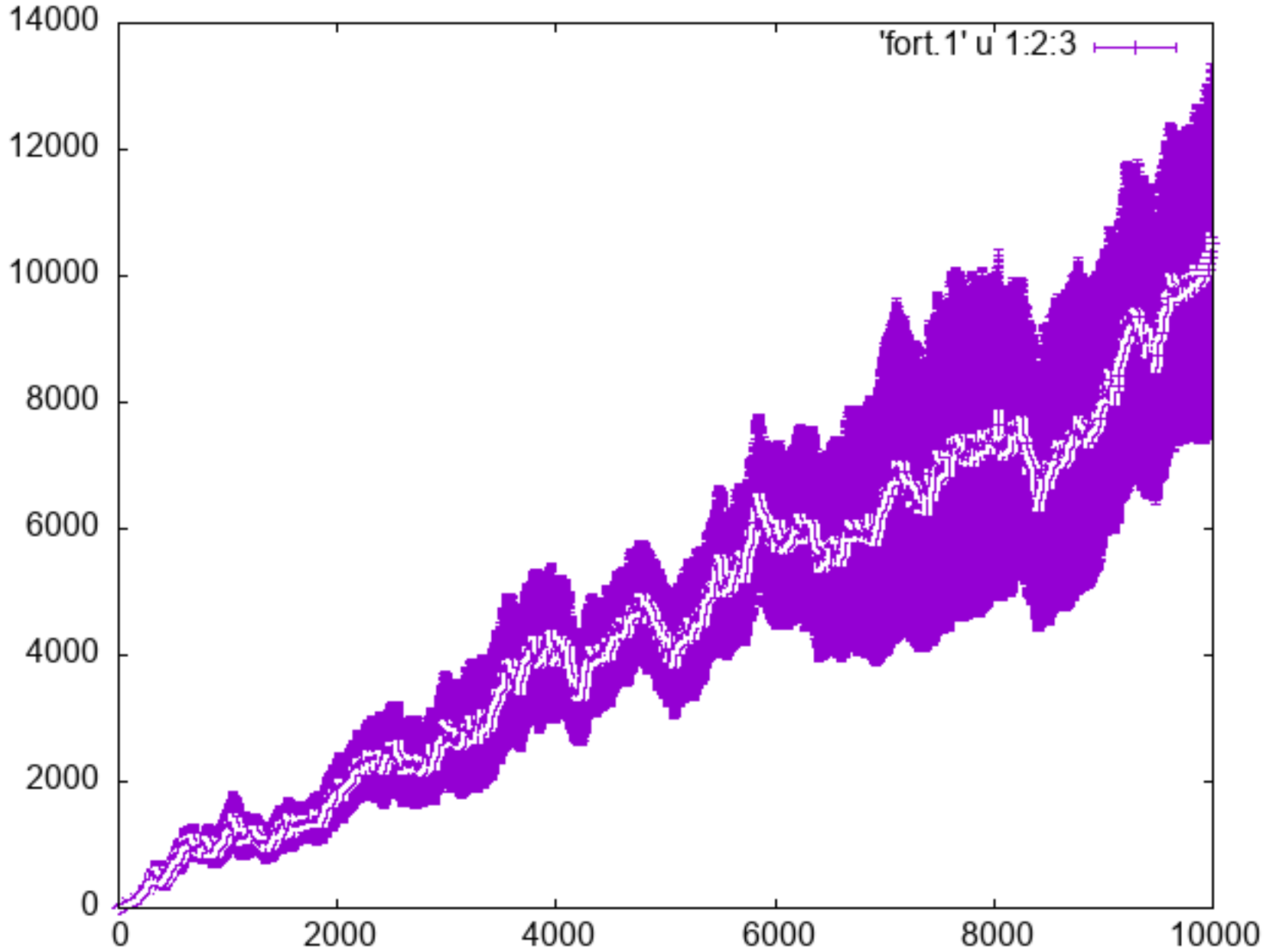
```
    dxsum=0.0d0; dysum=0.0d0;
    dxsqsum=0.0d0; dysqsum=0.0d0;
    dx4thsum=0.0d0;  dy4thsum=0.0d0;
    do i=1,Np
       dxsum=dxsum+dx(i);   dysum=dysum+dy(i);
        dxsqsum=dxsqsum+dx(i)*dx(i);
        dysqsum=dysqsum+dy(i)*dy(i);
        dx4thsum=dx4thsum+dx(i)**4;  ! INUTILI!
        dy4thsum=dy4thsum+dy(i)**4;  ! INUTILI!
    enddo
drsqave=(dxsqsum+dysqsum)/Np
vardrsqave=(dx4thsum+dy4thsum)/Np - ((dxsqsum+dysqsum)/Np)**2  !CHECK SE VIENE >0!  NO!!!
```

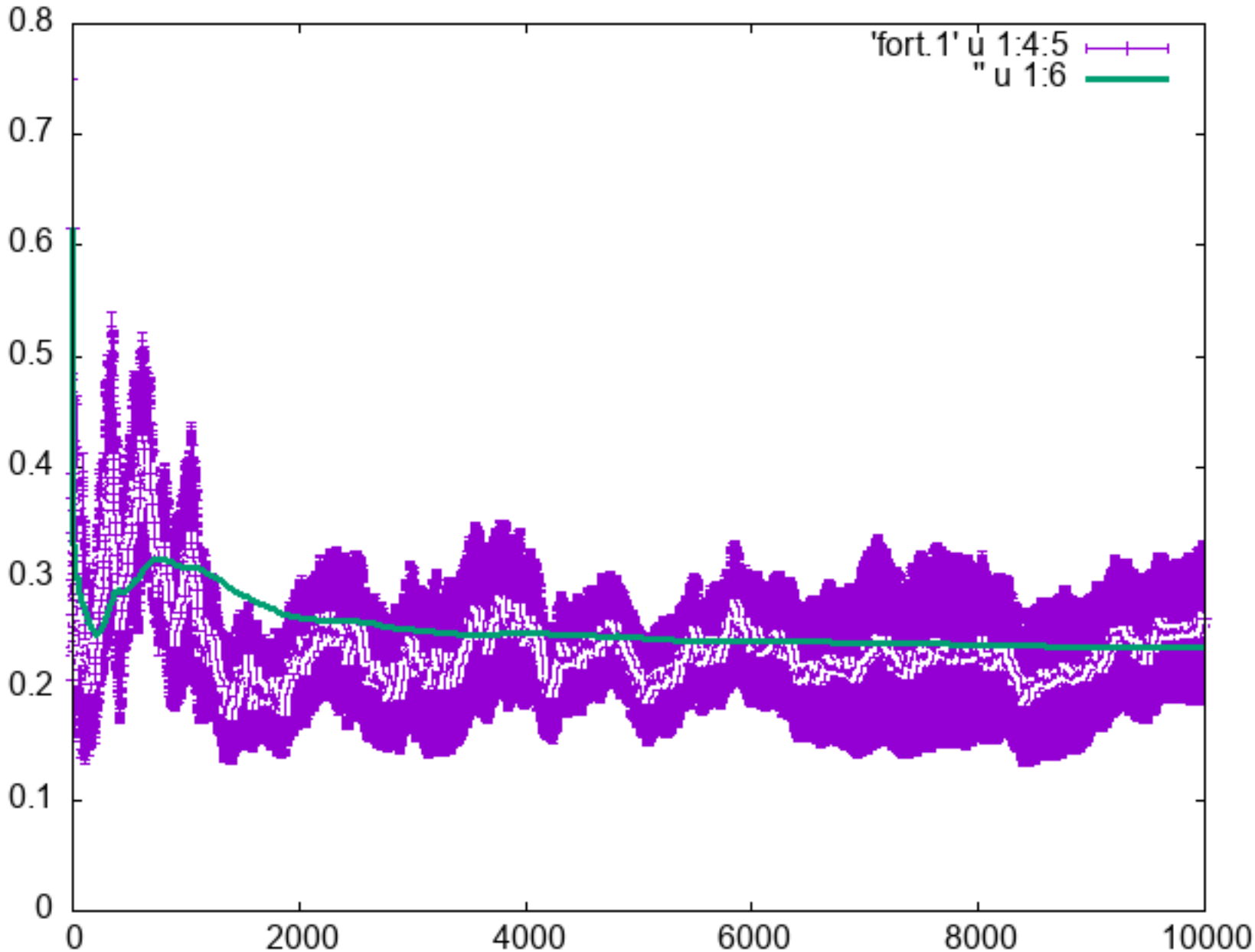
"latticegas-modified-2024.f90"

corretto!

```
dxsum=0.0d0; dysum=0.0d0;
dxsqsum=0.0d0; dysqsum=0.0d0;
drsqsqave=0.0
do i=1,Np
   dxsum=dxsum+dx(i);   dysum=dysum+dy(i);
    dxsqsum=dxsqsum+dx(i)*dx(i);
    dysqsum=dysqsum+dy(i)*dy(i);
    drsqsqave = drsqsqave + (dx(i)*dx(i)+dy(i)*dy(i))**2
enddo
drsqave=(dxsqsum+dysqsum)/Np
drsqsqave=drsqsqave/Np
vardrsqave=drsqsqave-drsqave**2  ! VARIANZA di <deltaR^2(t)>  (ISTANTANEO, media su Np)

if (t>0.0) then   ! avoid the first point that should be divided by zero
   !  Get  diffusion coefficient  by  proper scaling
   D=drsqave*a*a/(4*t)
   Dave_in_t=Dave_in_t+D
   write(1,fmt='(6(1pe10.2,2x))')t,drsqave,sqrt(vardrsqave/Np),&
        & D,sqrt(vardrsqave/Np)*a*a/(4*t),Dave_in_t/t
endif
```


'fort.1' u 1:2:3
14000
12000
10000
8000
6000
4000
2000
0
0
2000
4000
6000
8000
10000


'fort.1' u 1:4:5
" u 1:6
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
2000
4000
6000
8000
10000

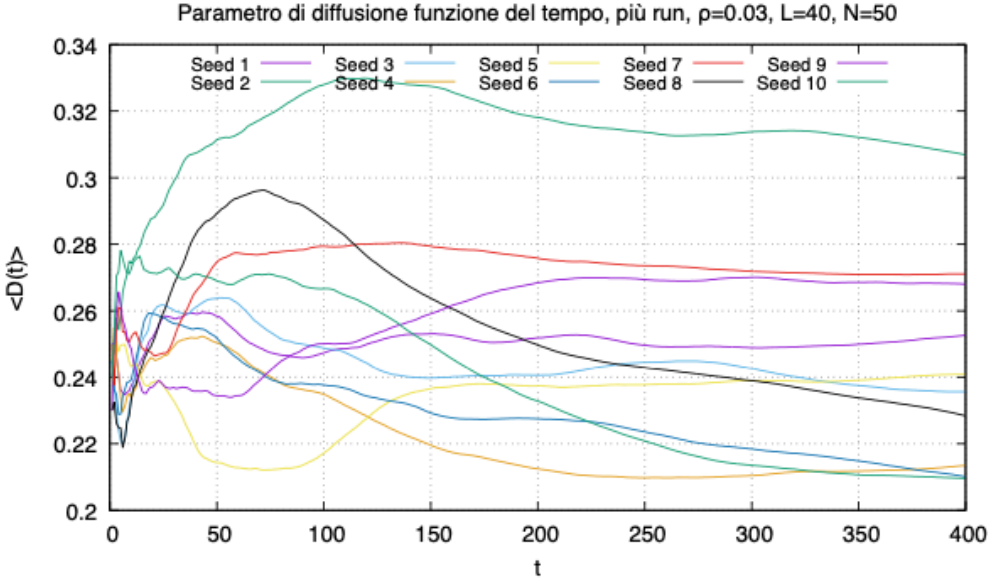


Figura 21: Valori medi di 10 run del parametro di diffusione in funzione del tempo, $L = 40$, $\rho = 0.03$

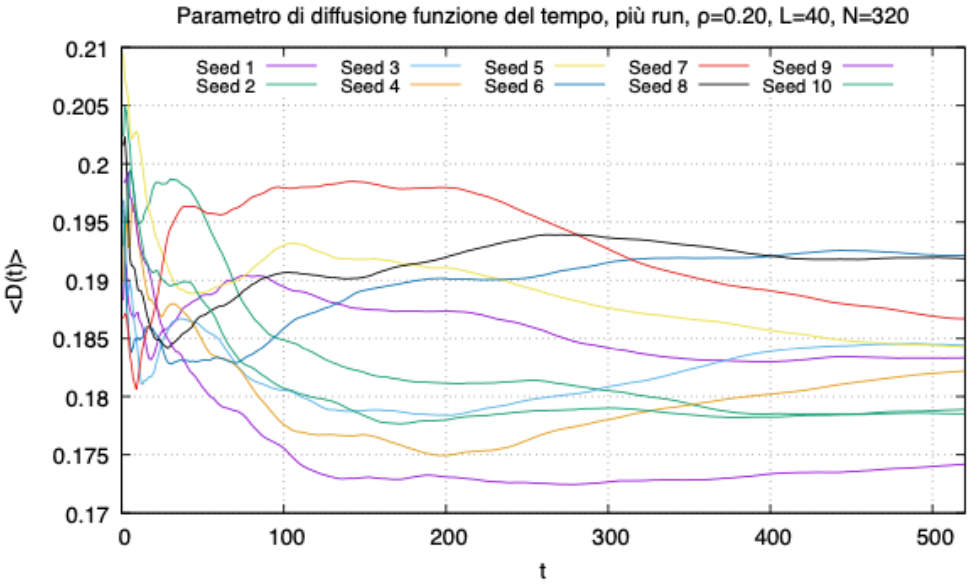


Figura 22: Valori medi di 10 run del parametro di diffusione in funzione del tempo, $L = 40$, $\rho = 0.3$

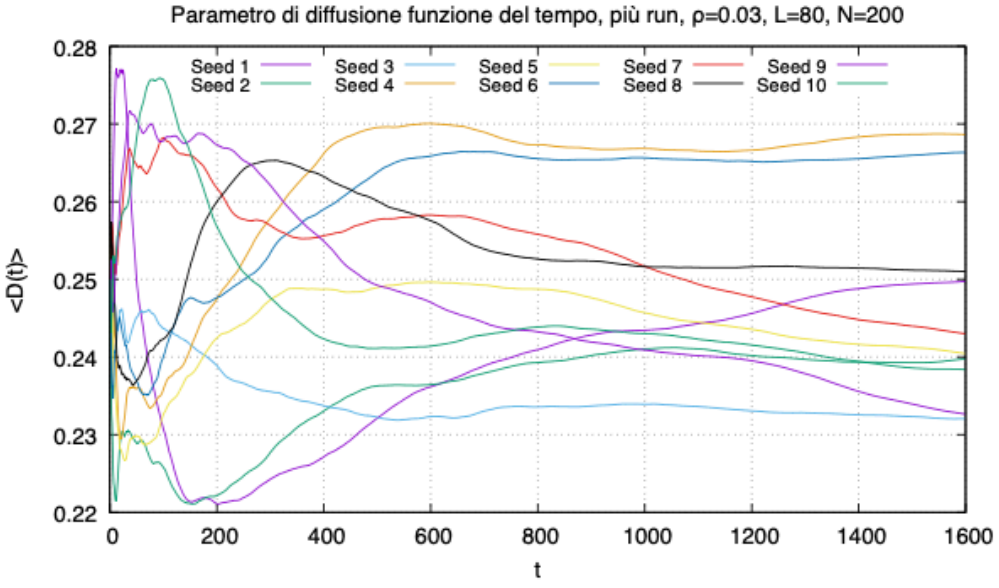


Figura 23: Valori medi di 10 run del parametro di diffusione in funzione del tempo, $L = 80$, $\rho = 0.03$

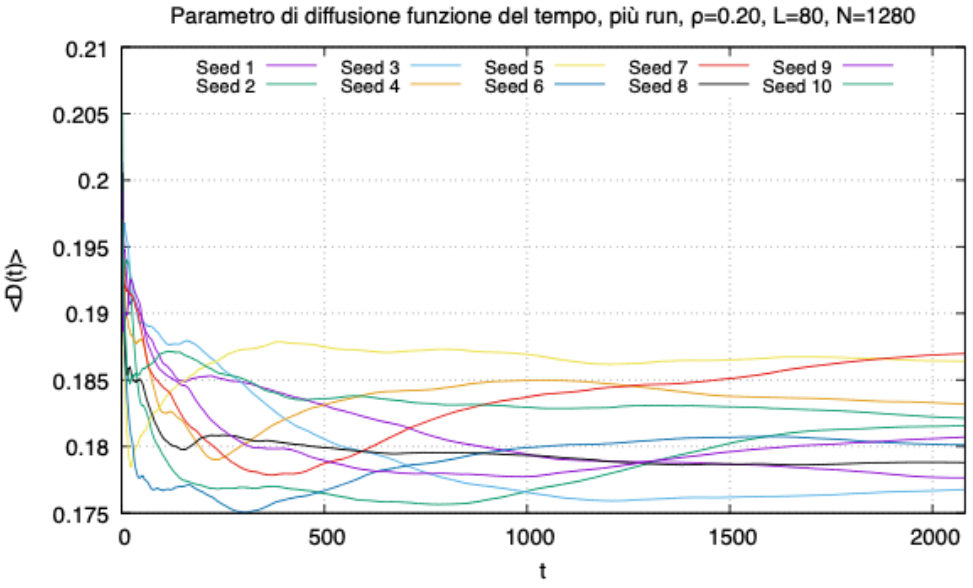


Figura 24: Valori medi di 10 run del parametro di diffusione in funzione del tempo, $L = 80$, $\rho = 0.3$

$\sigma^2_{D(t)}$ calcolato come spread (v plot precedenti) di D(t) per diversi seeds

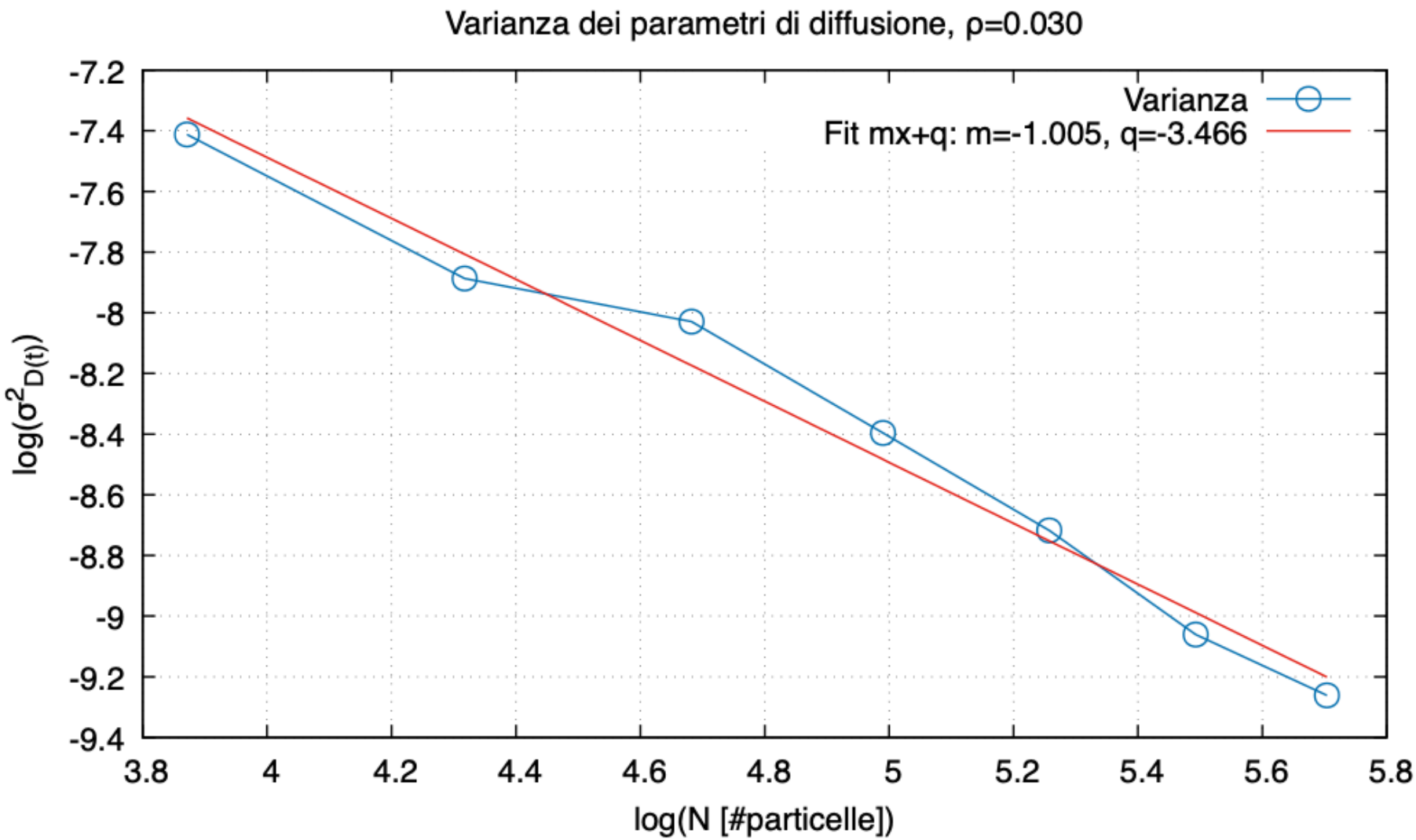


Figura 25: Varianza di $D(t)$ rispetto al valore medio in funzione del numero di particelle N del sistema, $\rho = 0.03$

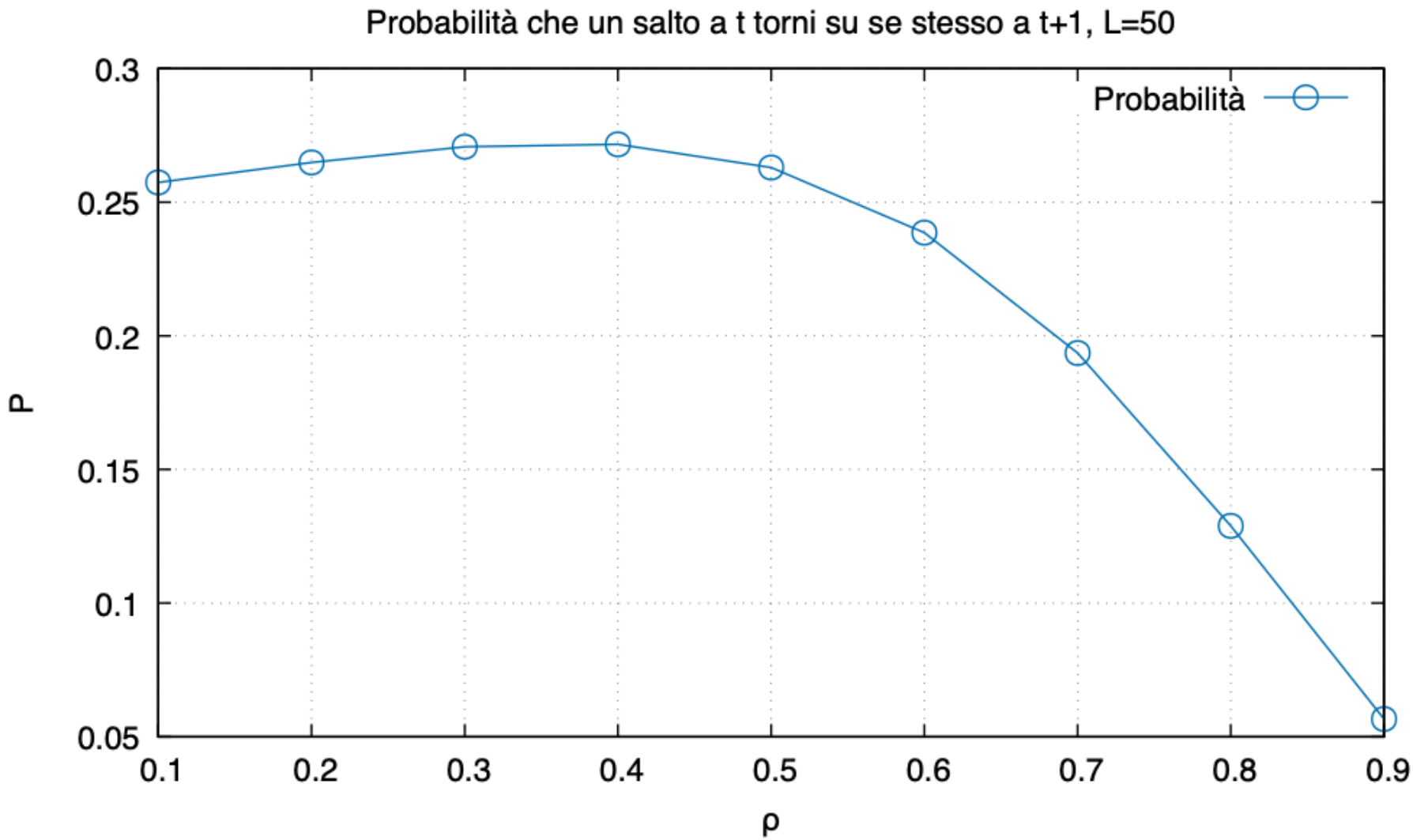


Figura 28: Probabilità che una particella che si sposta in un sito libero al tempo t torni sul sito di partenza al tempo $t+1$ in funzione della densità ρ

(risultati di Nicolas Bau')