



993SM – Laboratory of Computational Physics Unit VII November 7, 2024

Maria Peressi

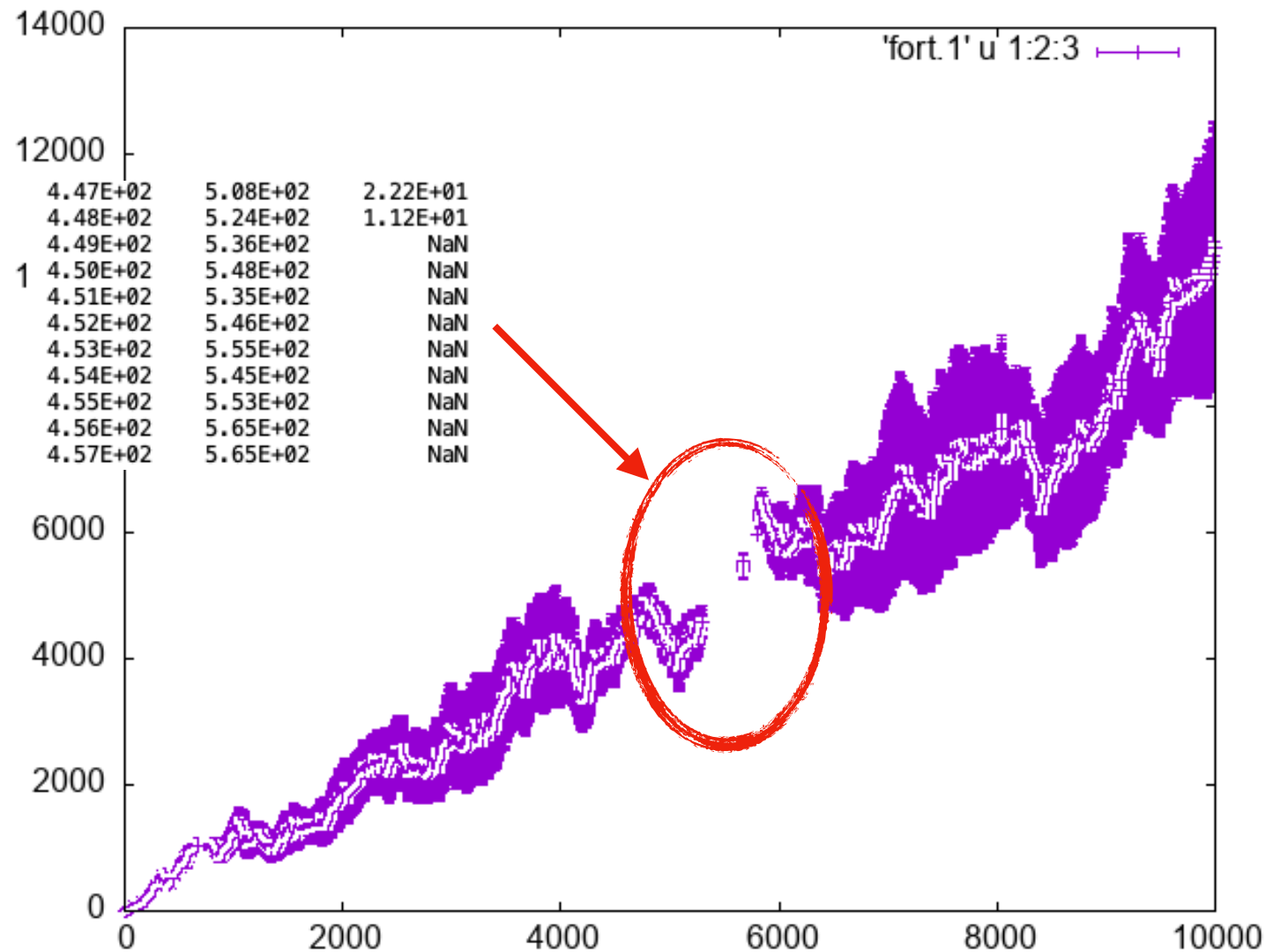
Università degli Studi di Trieste – Dipartimento di Fisica
Sede di Miramare (Strada Costiera 11, Trieste)

e-mail: peressi@units.it

tel.: +39 040 2240242

con il codice “latticegas-modified.f90” :

```
# Density  $N_p/L^2 = 3.24999988E-02$  ;  $N_p = 13$  ;  $L = 2$   
#  $t, drsqave(t), \sqrt{\text{var}(drsqave(t))/N_p}, D(t), \langle D \rangle_T$ 
```



“latticegas-modified.f90”

sbagliato!

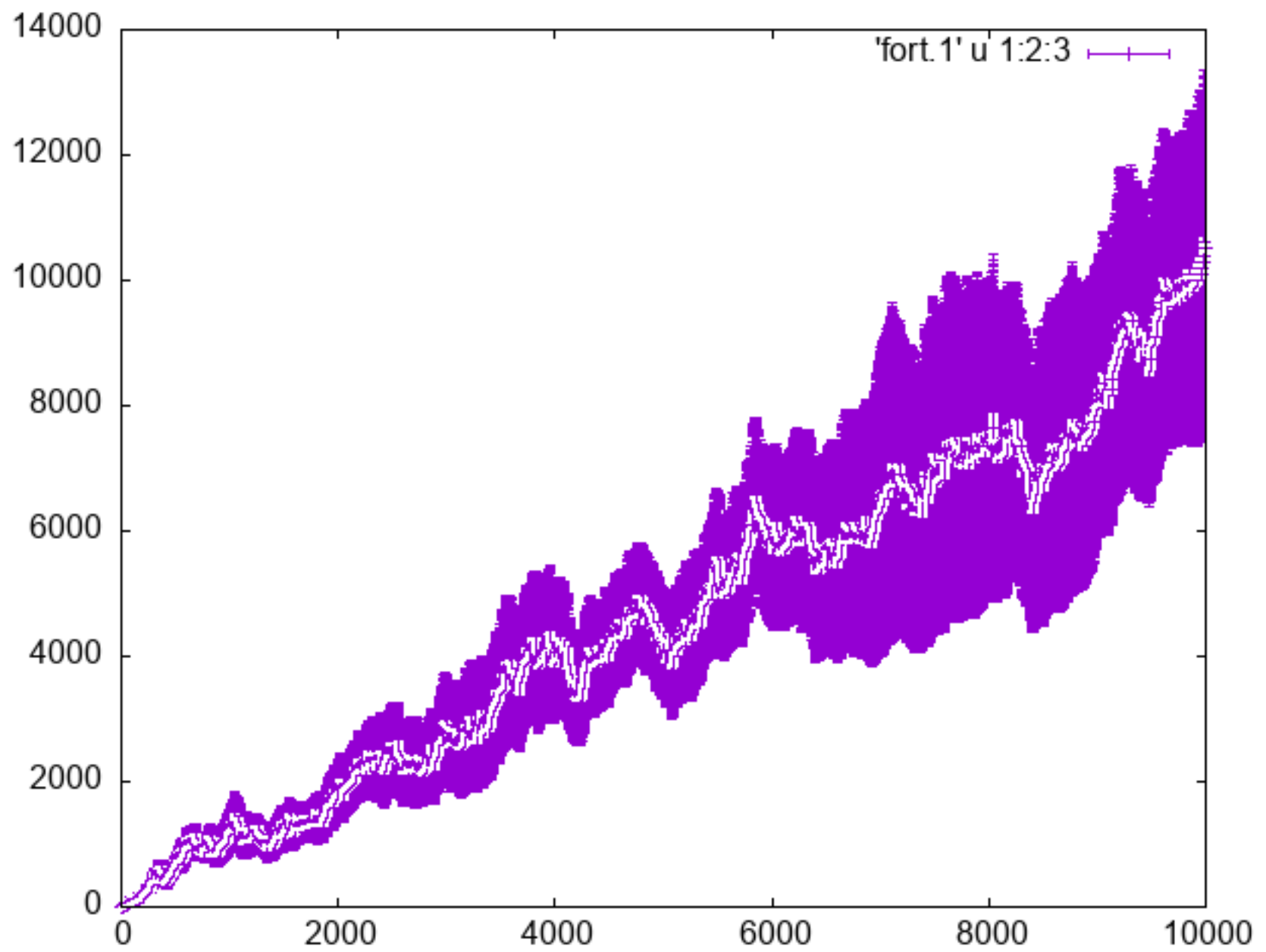
```
dxsum=0.0d0; dysum=0.0d0;
dxsqsum=0.0d0; dysqsum=0.0d0;
dx4thsum=0.0d0; dy4thsum=0.0d0;
do i=1,Np
  dxsum=dxsum+dx(i); dysum=dysum+dy(i);
  dxsqsum=dxsqsum+dx(i)*dx(i);
  dysqsum=dysqsum+dy(i)*dy(i);
  dx4thsum=dx4thsum+dx(i)**4; ! INUTILI!
  dy4thsum=dy4thsum+dy(i)**4; ! INUTILI!
enddo
drsqave=(dxsqsum+dysqsum)/Np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

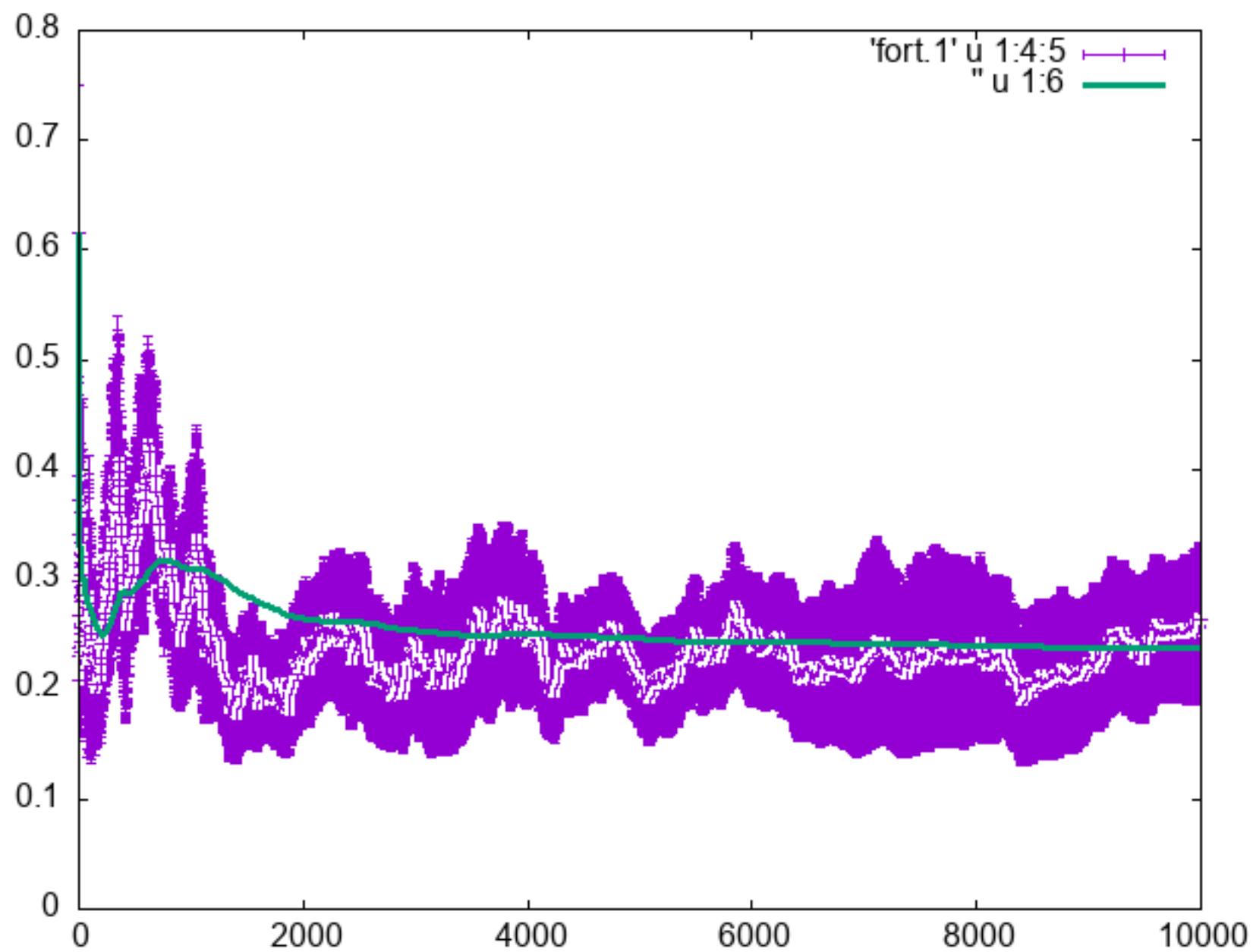
“latticegas-modified-2024.f90”

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
```





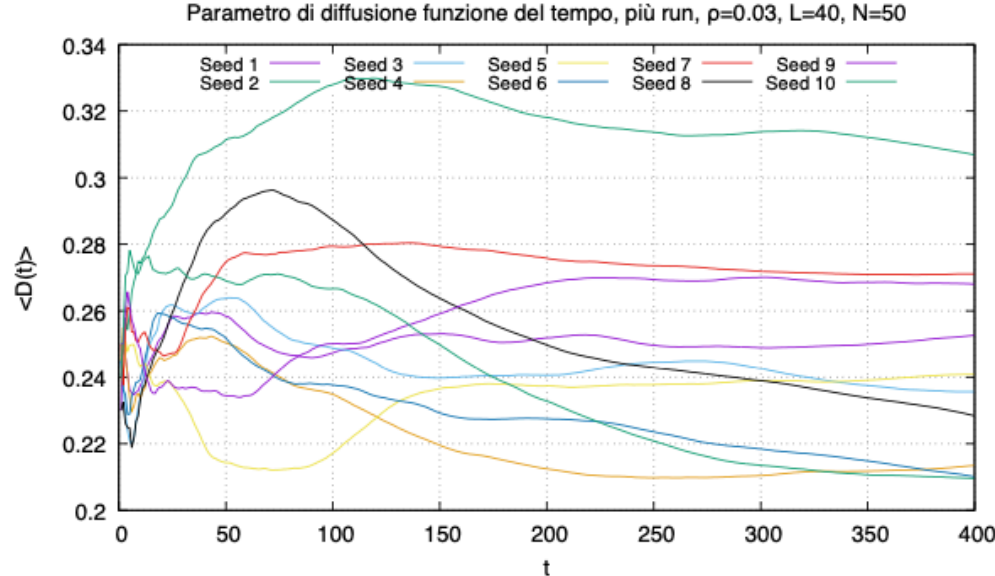


Figura 21: Valori medi di 10 run del parametro di diffusione in funzione del tempo, $L = 40$, $\rho = 0.03$

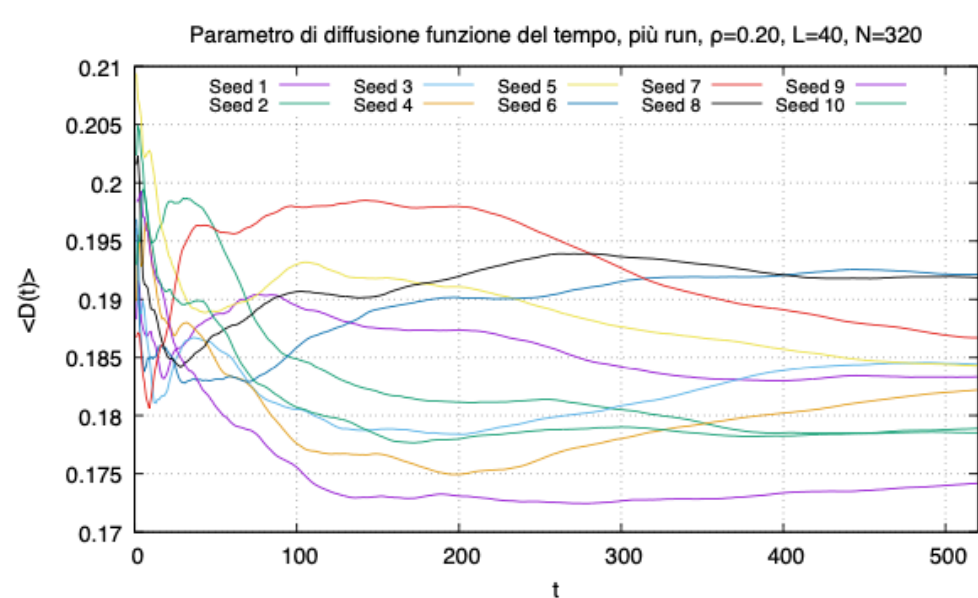


Figura 22: Valori medi di 10 run del parametro di diffusione in funzione del tempo, $L = 40$, $\rho = 0.3$

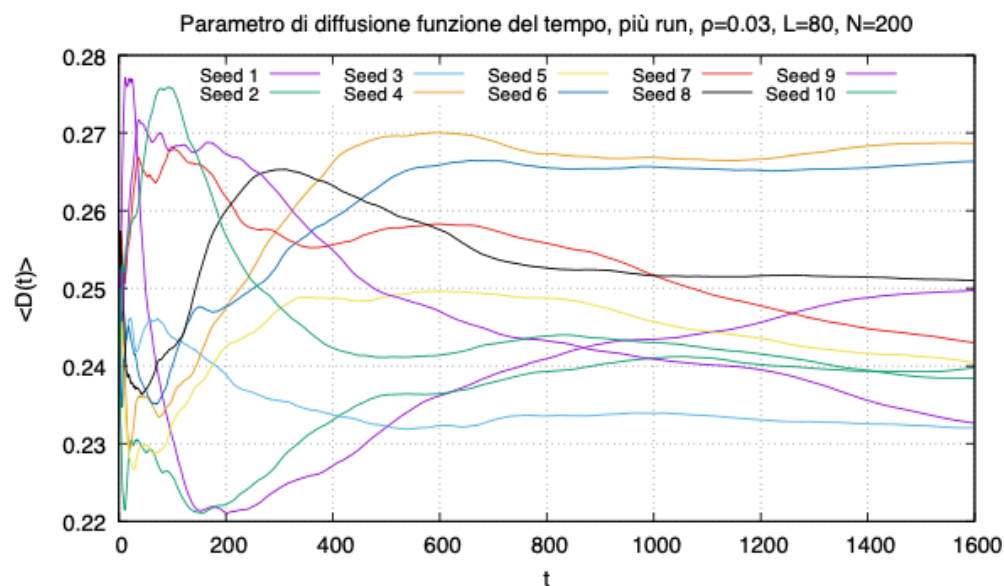


Figura 23: Valori medi di 10 run del parametro di diffusione in funzione del tempo, $L = 80$, $\rho = 0.03$

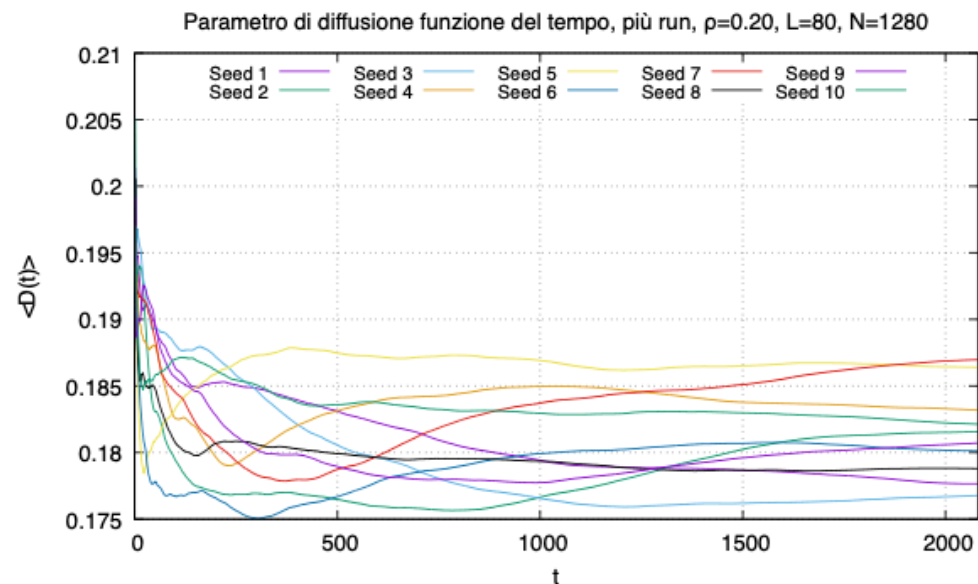


Figura 24: Valori medi di 10 run del parametro di diffusione in funzione del tempo, $L = 80$, $\rho = 0.3$

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

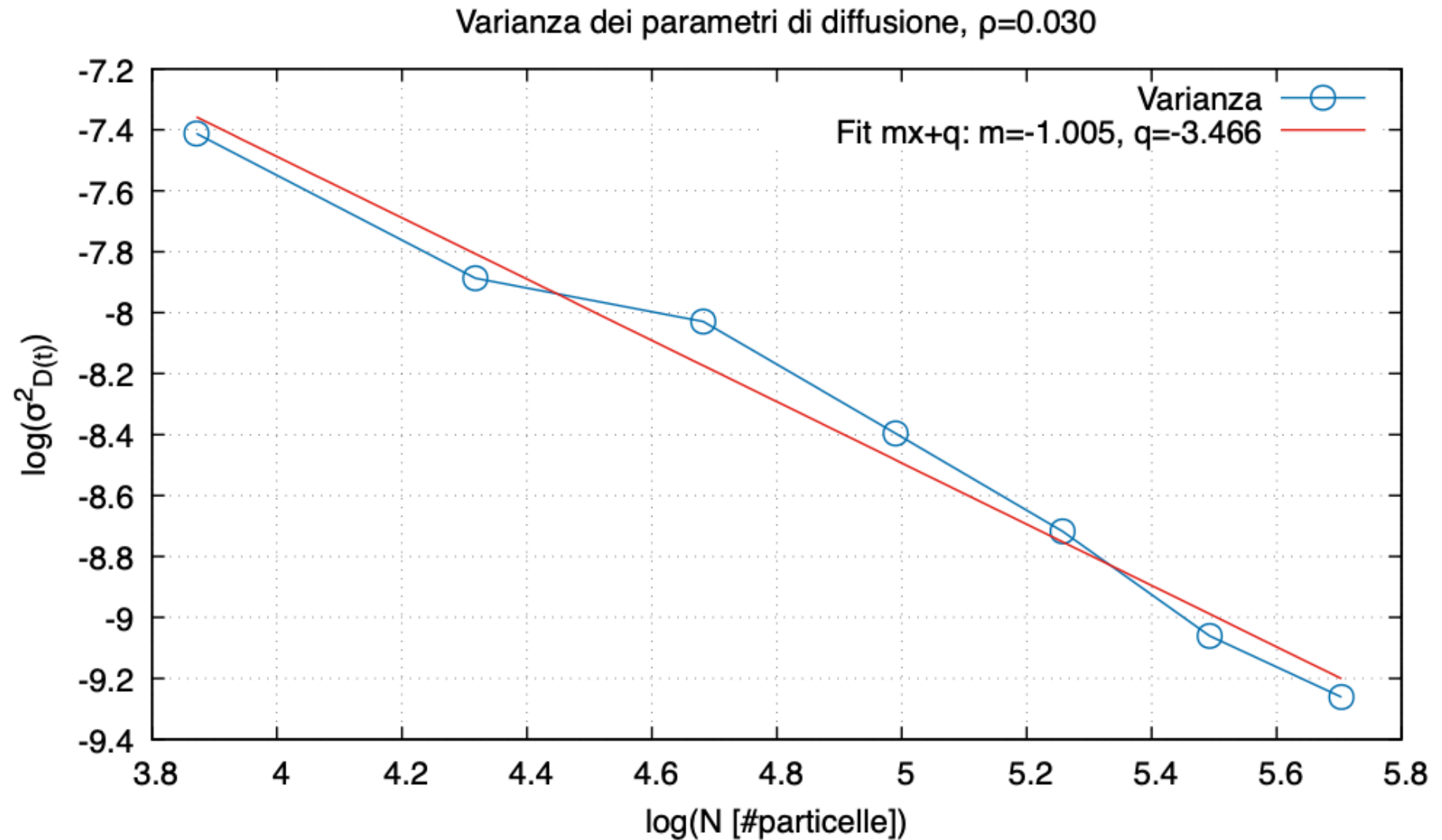


Figura 25: Varianza di $D(t)$ rispetto al valore medio in funzione del numero di particelle N del sistema, $\rho = 0.03$

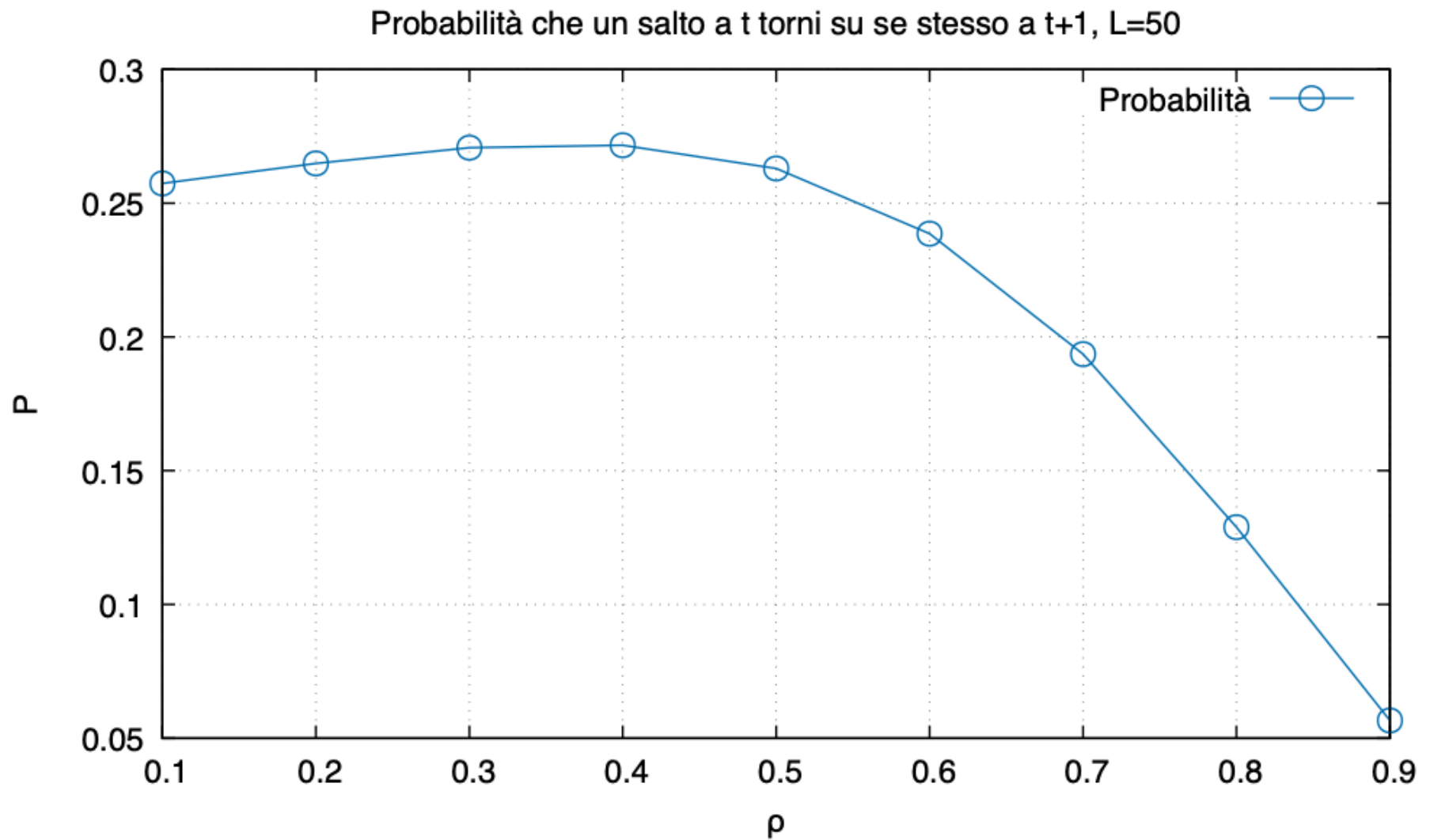


Figura 28: Probabilità che una particella che si sposta in un sito libero al tempo t torni sul sito di partenza al tempo $t + 1$ in funzione della densità ρ

(risultati di Nicolas Bau')