Random walk, self-avoiding random walk

```
IMPLICIT NONE
integer saw
integer i,j,is,weight
integer io,jo
integer ne,nemax,nt,ntmax,vmax
double precision rnd,rnds,r2,t,wnow
parameter(saw=1) ! saw=0, random walk, saw=1, self-avoiding walk
parameter(ntmax=100) ! maximum number of time steps
parameter(nemax=100000)  ! number of walks in ensemble
parameter(vmax=100) ! max size for visit matrix
double precision r2a(ntmax) ! accumulated average of r**2
double precision  wtot(ntmax) ! accumulated "weights" at each step
integer visit(-vmax:vmax,-vmax:vmax)    ! keep track of visited sites
```

Random number generator

```
c initialize random number generator
        call RANDOM_SEED

50        call RANDOM_NUMBER(rnd)
         call RANDOM_NUMBER(rnds)
```

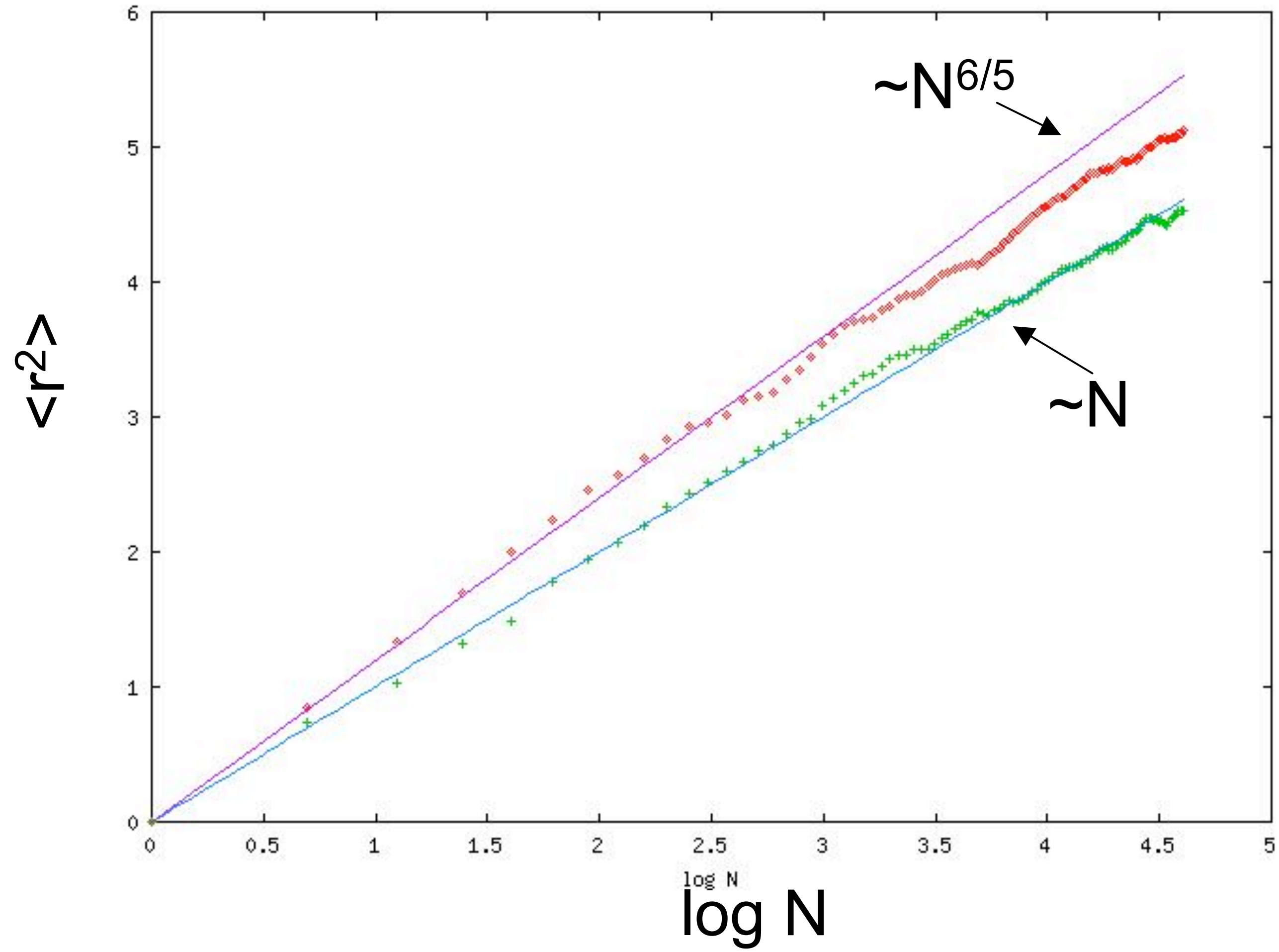
One random number (rnds) can be used to decide on +/- Step

Other random number (rnd) can be used to decide whether we move walker in x,y, or z direction

*Average r**2 for many random walks*

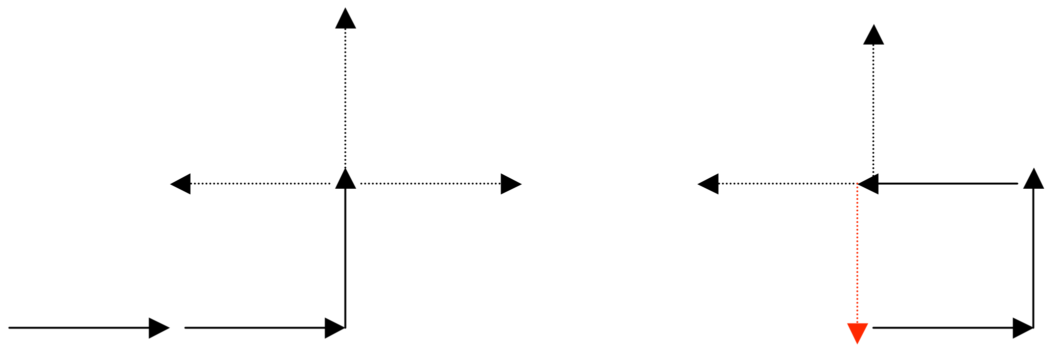
```
  do ne=1,nemax ! Nemax realizations of random walk

   do nt=1,ntmax

  …

60       r2=real(i)**2+real(j)**2+real(k)**2
          r2a(nt)=r2a(nt)+r2/nemax
  enddo

 enddo
```

Random walk, self-avoiding random walk in 3D



SAW not exactly right! What is wrong?

Each path should be equally likely…



Path 1 Path 2

$P_1=(1/4)(1/3)(1/3)(1/3)$ $P_2=(1/4)(1/3)(1/3)(1/2)$

$\mathbf{P_2 > P_1}$

In fact, $P_2 = (3/2)P_1$.

This somewhat surprising result shows that some paths will be overrepresented in a random ensemble due to self-intersecting trajectories. The disallowed red path skews ensemble.

We could throw away entire paths…

- If a self-intersecting step is chosen at random, throw away entire path and start over

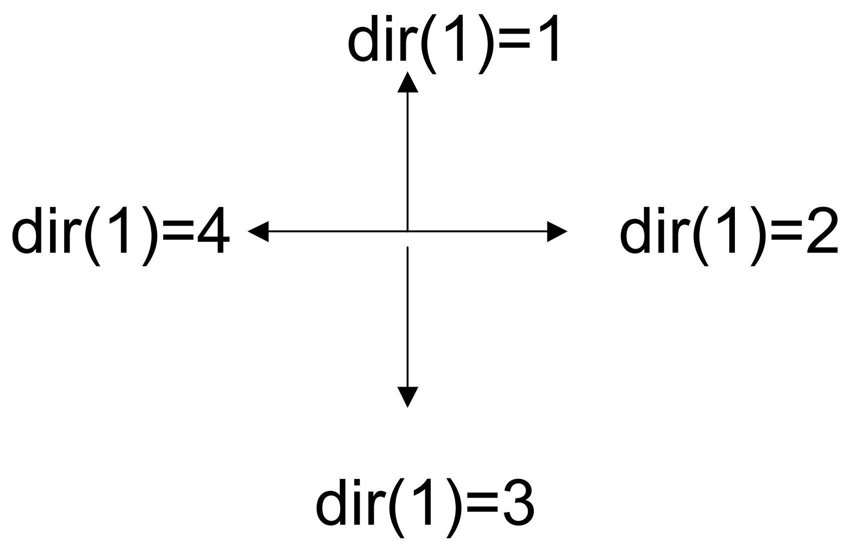
- Correct statistics… terrible sampling…

- For long enough paths, we hardly ever avoid one self-intersecting step…

- We can apply an “enumeration” technique of Giordano

- Another approach is to weight trajectories

Enumeration a la Giordano… consider 2D SAW



- The array dir(n) selects the direction for the nth step
- Predefine length we are searching (ntmax=20)
- Do project in two-dimensions

Enumeration a la Giordano… consider 2D SAW

- Sample **all** paths for some nmax (e.g. ntmax=20)
- For nmax=20, ~10^9 paths!
- Hard to go much further

Outline of approach…

Start with n=1, dir(1)=1 for the first step. Set visit(0,0)=1.

For each site n we are at…

1. Check if we have tested each direction… dir(n)=1,2,3,4
   If yes, then backtrack n=n-1, set visit for site to 0 (unvisited)
   If no, check and see if the next site is unvisited

   When we backtrack, we will consider the next direction from the n-1 site

   Otherwise, if next site unvisited, go to it and mark it as visited, also increment dir(n)

   If next site is visited, go to next direction (increment dir(n)) and again go back to step 1 to see if each direction searched

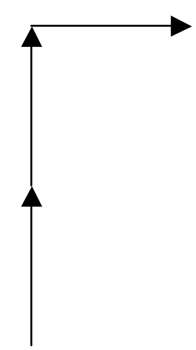
How do we proceed? When do we end?

- Each path that reaches desired limit is included in averages

- When we backtrack to n=0, we are finished (all paths searched)

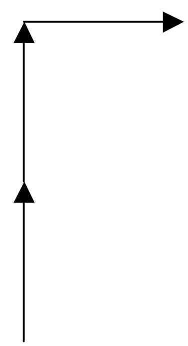
For example… if dir(n)=1 searches “up”, and ntmax=3, we
First sample a path of all up arrows and set dir(1)=2, dir(2)=2

Next path…
after backtrack…

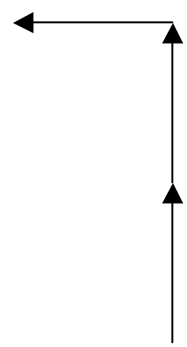


This is for
dir(3)=2…
accept it
then set
dir(3)=3…

Continuing along…

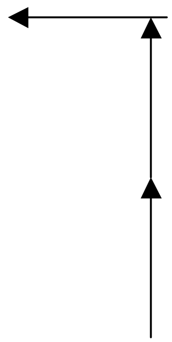


After this step, dir(3)=3, corresponding to a “downward” step which revisits a site… so increment dir(2)=4

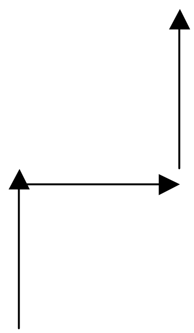


We accept this one and increment dir(2)…. But then dir(2)=5, so we are done with this “family” of paths, so we backtrack…

And more…



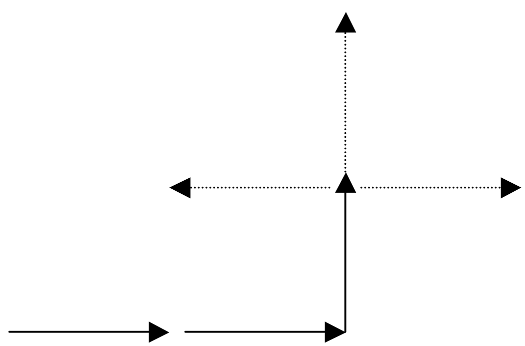
Last step before backtrack…



Since dir(2)=2, we must consider all paths that have an "up" then a "right" step… start with the path at the left which is for dir(3)=1… accept and set dir(3)=2

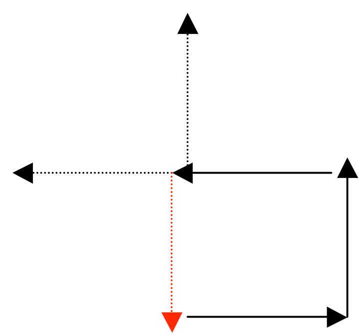
Another approach…

- Random paths with appropriate weights…
- Weight path by factors 4-possible paths



Path 1

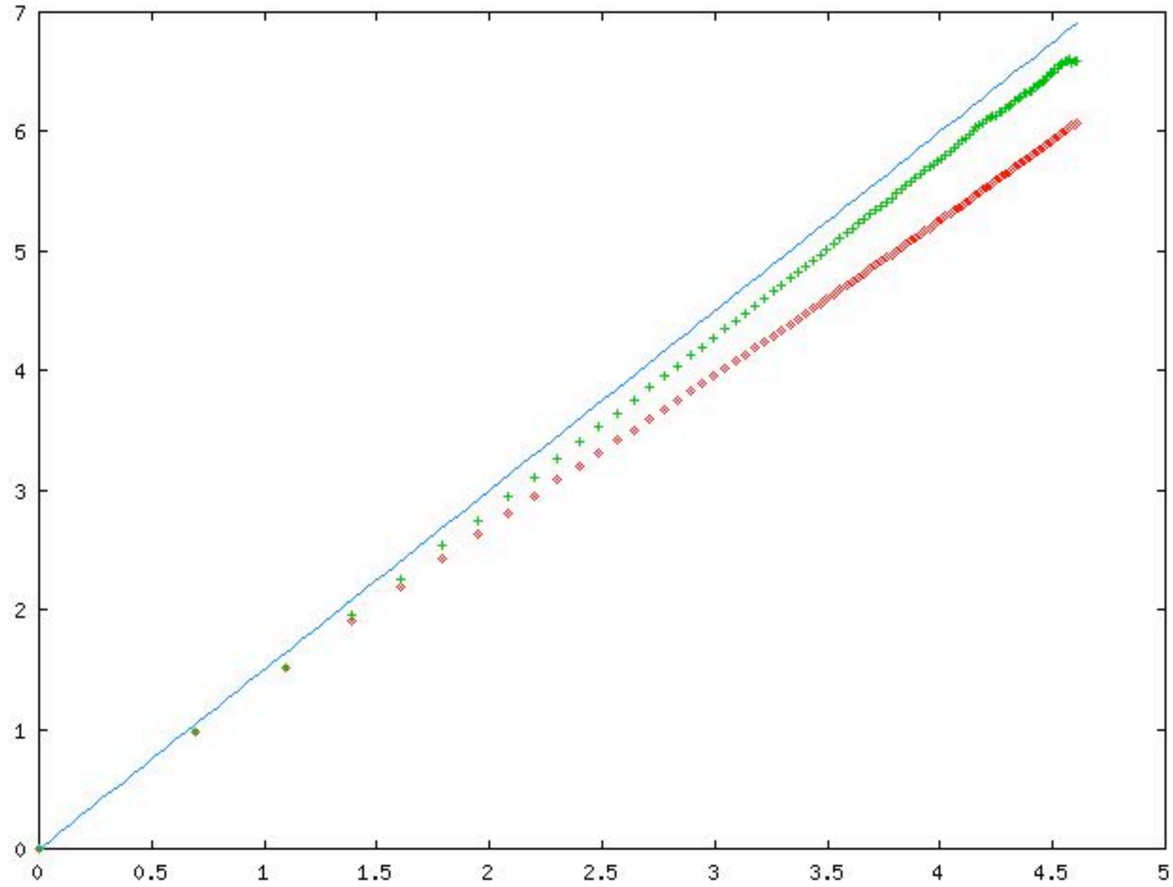
Weight factor 3



Path 2

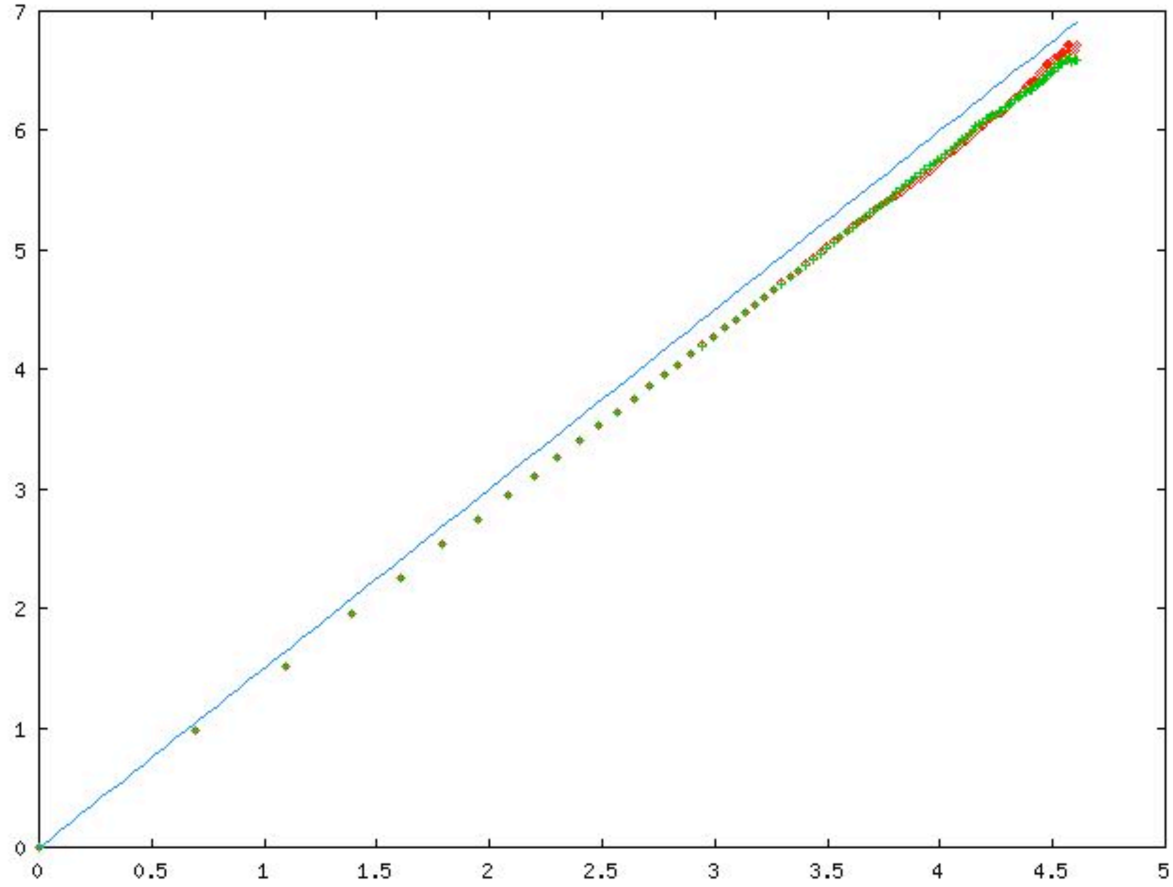
Weight factor 2

Results for 100,000 random walks, with and without weights for N=100 steps…



- Conclusion is that weights approach agrees with ν=3/4
- Can extend to larger walks than enumeration

Effect of step size… 10,000 and 100,000 random paths to compare statistics…



- Statistics reasonable even for 10^4… Giordano does 10^9 for only a 20 step SAW!!

Weight factors in my code…

```
50 weight=4-visit(i+1,j)-visit(i-1,j)-visit(i,j+1)-visit(i,j-1)

 wnow=(1.0d0/3.0d0)*wnow*weight
 wtot(nt)=wtot(nt)+wnow
```

weight= 1,2,3depending on how many paths exist

More possible paths give a higher weight to chosen path

Total weight of path is product of factors for each step

Weight=0 used in case we have a dead end.