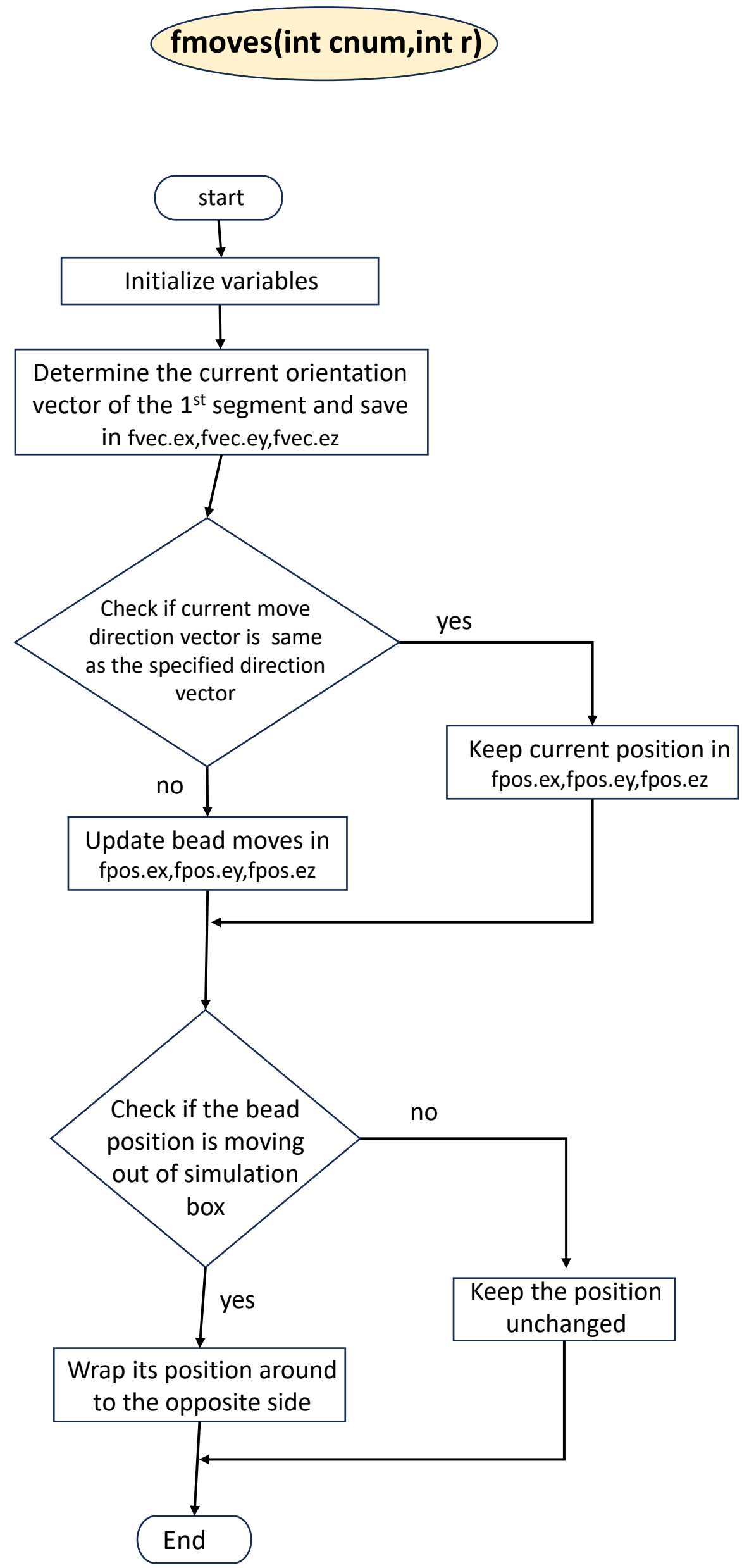
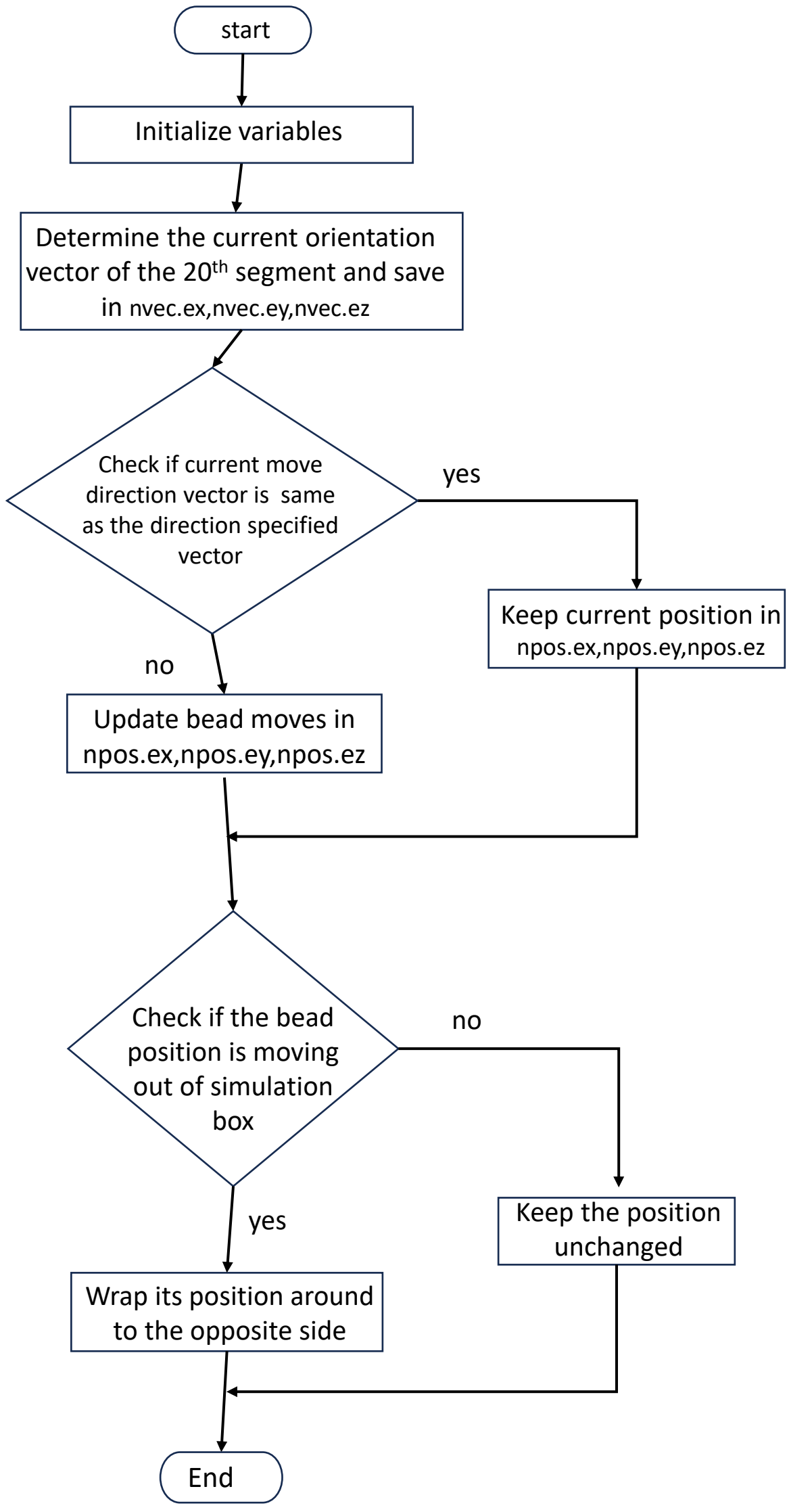
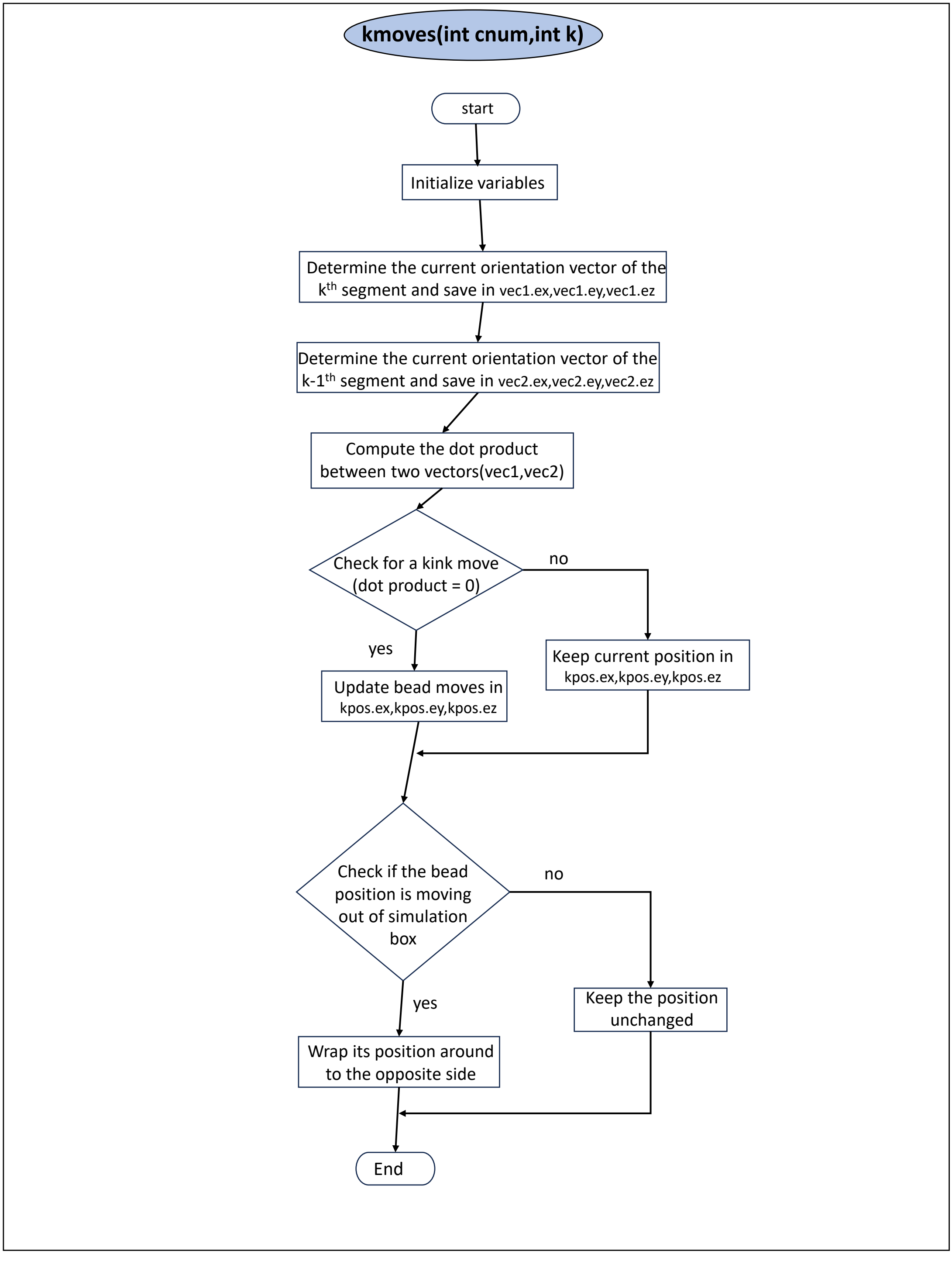
Subroutines for the PBC:

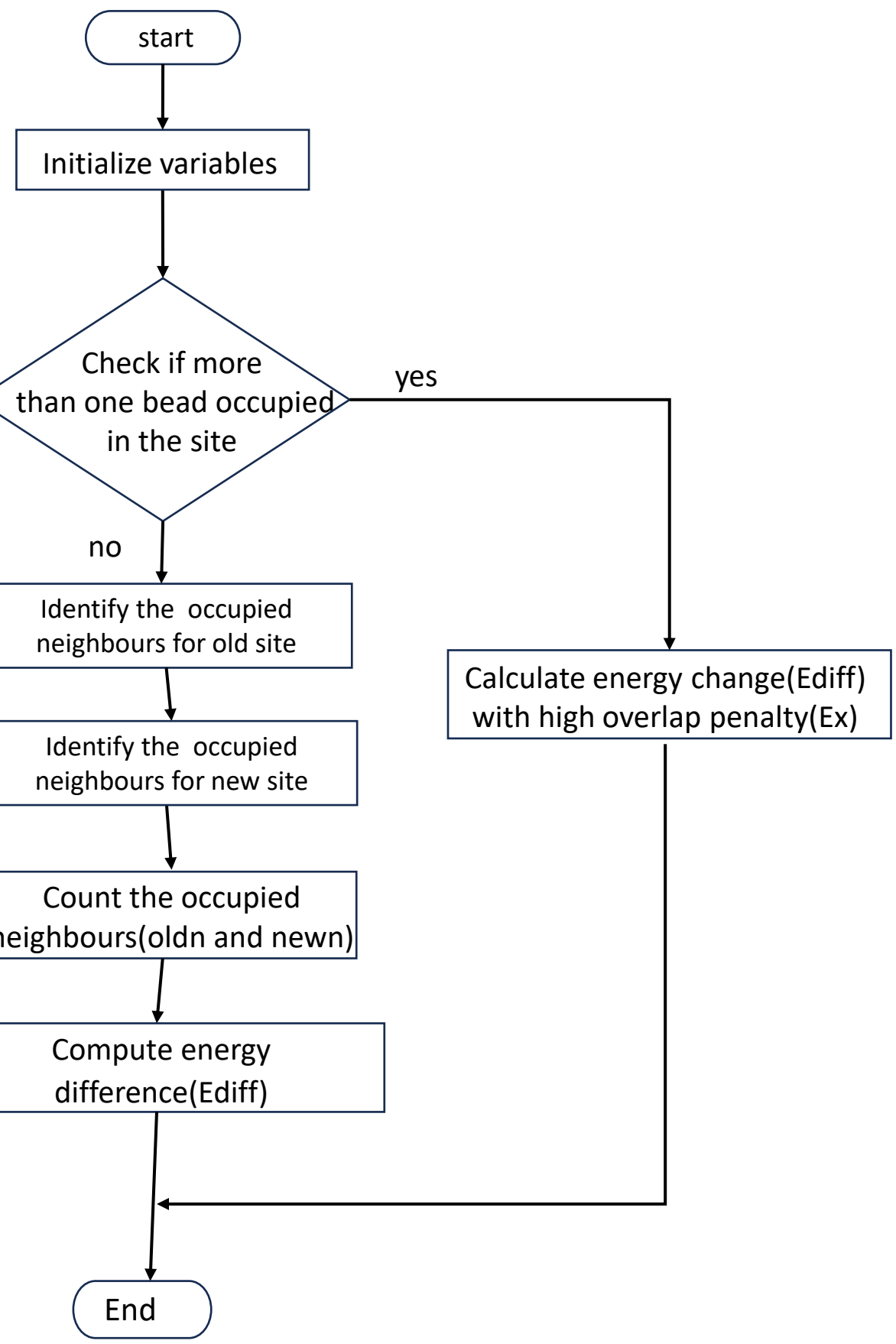

fmoves(int cnum,int r)
start
Initialize variables
Determine the current orientation vector of the 1st segment and save in fvec.ex,fvec.ey,fvec.ez
Check if current move direction vector is same as the specified direction vector
yes
Keep current position in fpos.ex,fpos.ey,fpos.ez
no
Update bead moves in fpos.ex,fpos.ey,fpos.ez
Check if the bead position is moving out of simulation box
no
Keep the position unchanged
yes
Wrap its position around to the opposite side
End

nmoves(int cnum,int r)

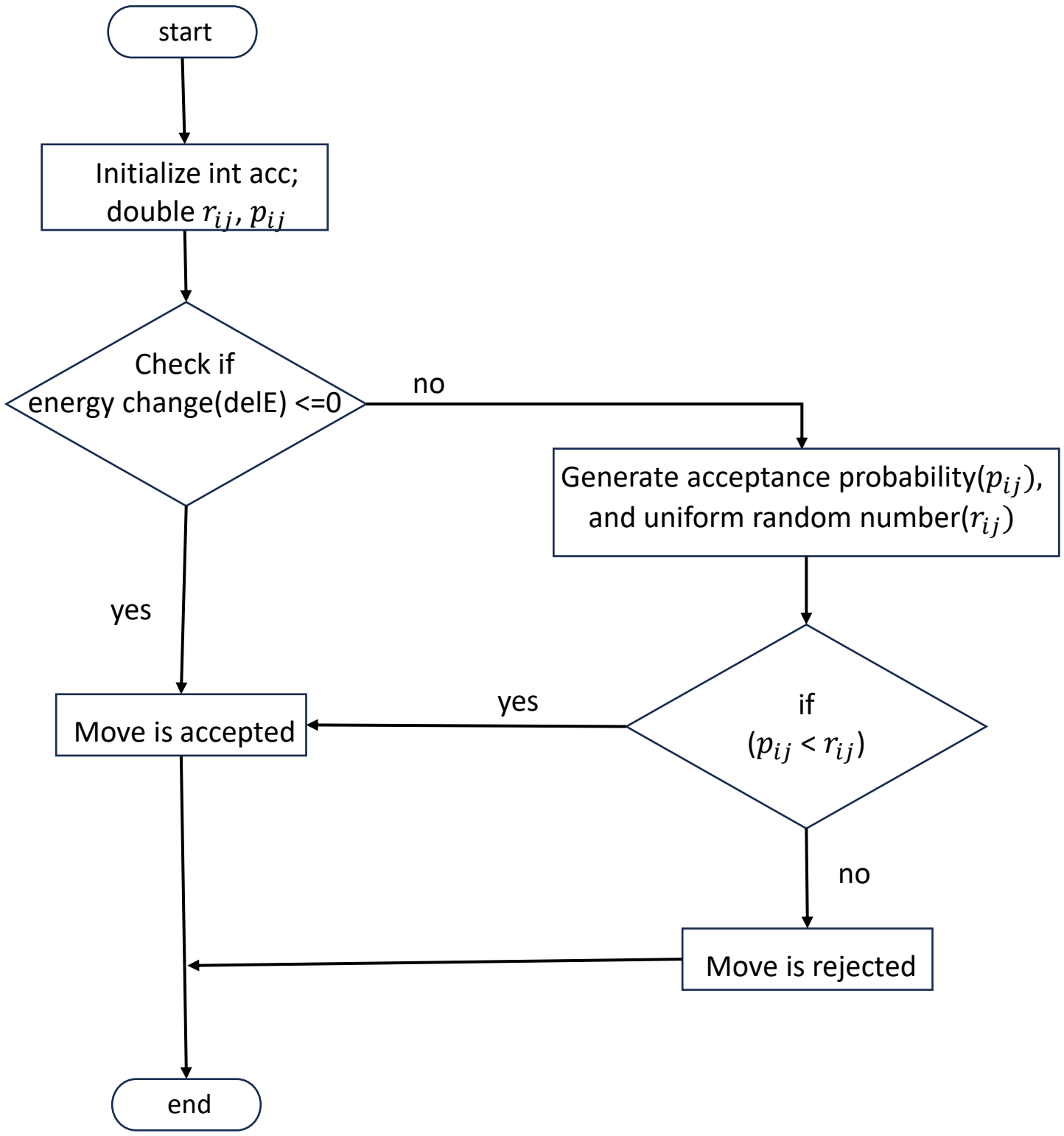



kmoves(int cnum,int k)
start
Initialize variables
Determine the current orientation vector of the k^th segment and save in vec1.ex,vec1.ey,vec1.ez
Determine the current orientation vector of the k-1^th segment and save in vec2.ex,vec2.ey,vec2.ez
Compute the dot product between two vectors(vec1,vec2)
Check for a kink move (dot product = 0)
no
yes
Keep current position in kpos.ex,kpos.ey,kpos.ez
Update bead moves in kpos.ex,kpos.ey,kpos.ez
Check if the bead position is moving out of simulation box
no
yes
Keep the position unchanged
Wrap its position around to the opposite side
End

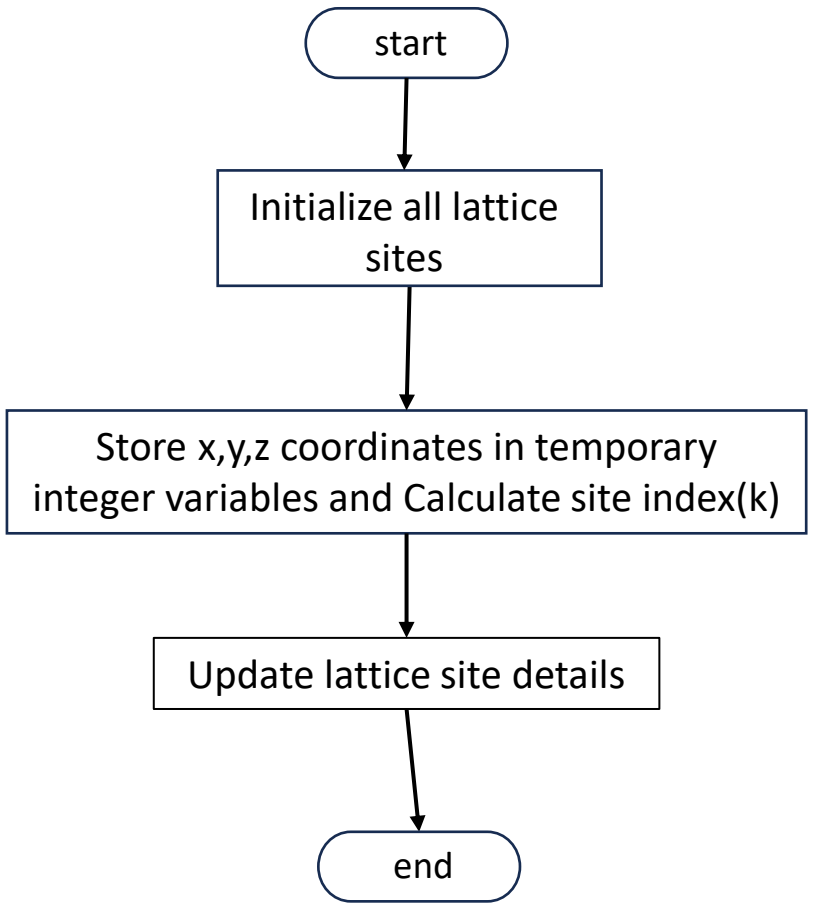
deltaE(int olds,int news)



metrop(double delE)



Sstate()



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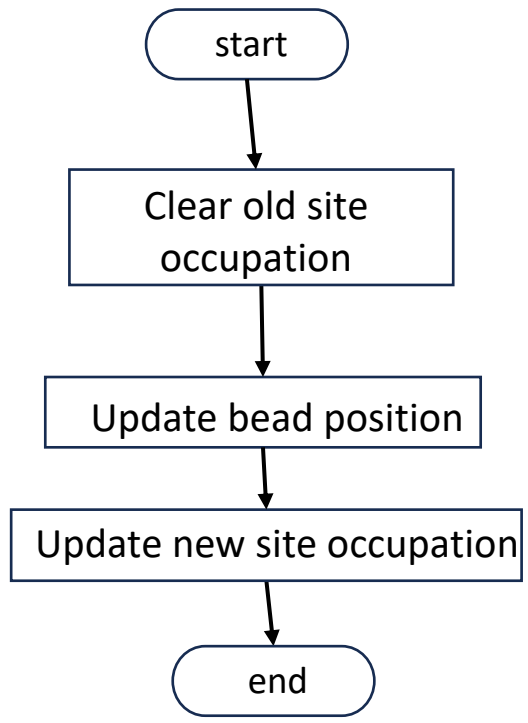
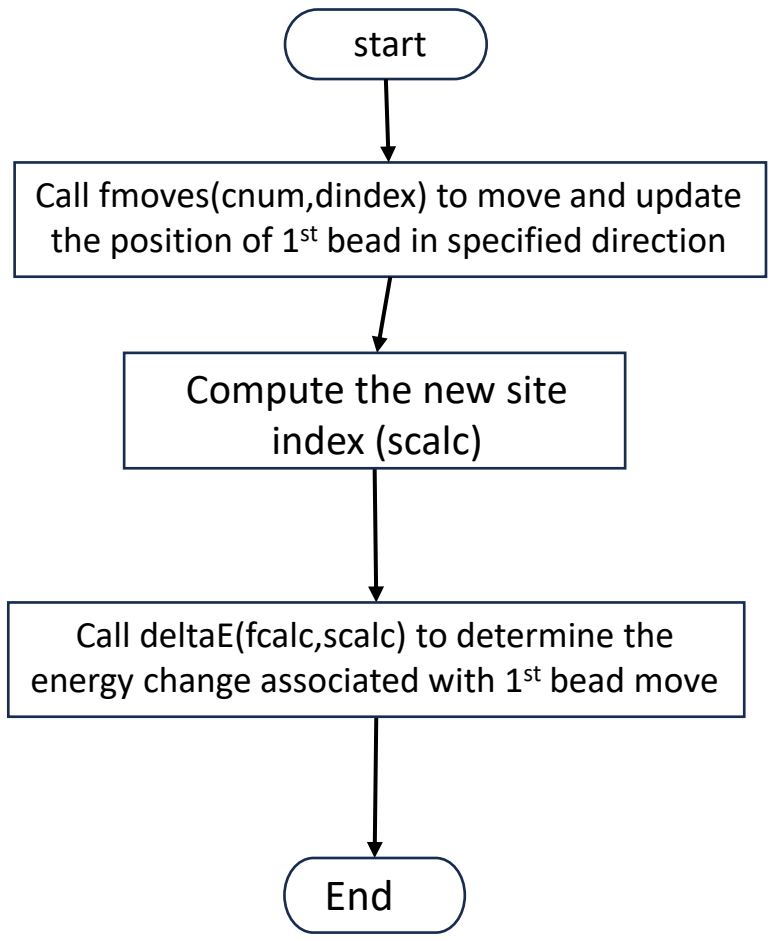
accmov(int cnum,int bnum,int pcalc,int scalc,struct vec mpos)



fmeval(int cnum,int dindex,int fcalc)



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lmeval(int cnum,int dindex,int lcalc)