

# Modeling of Non-polar Particles in Implicit Solvent Using Levelset Approach

Preliminary Test on Two Particle System

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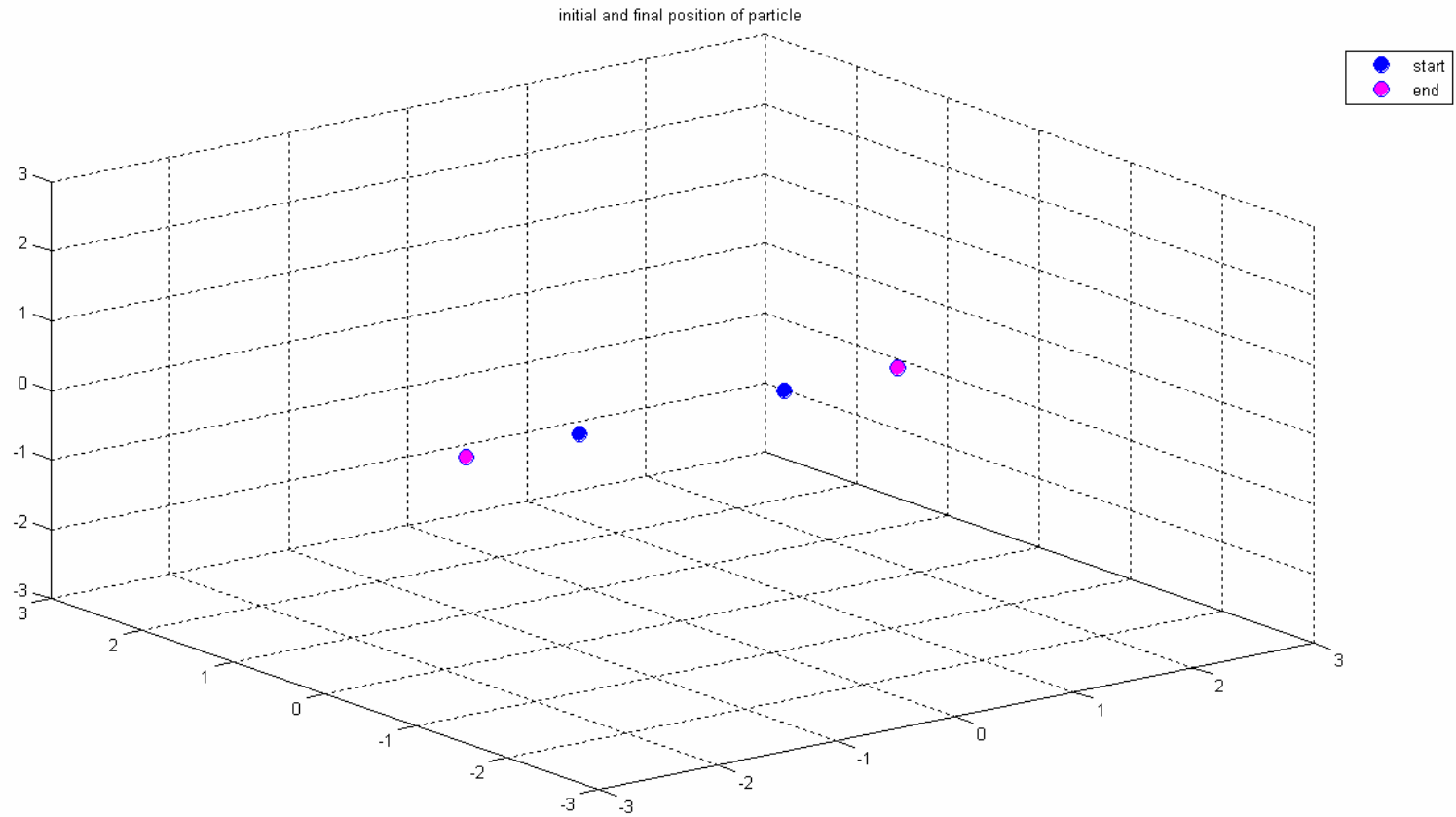
Yang Xie

Jianwei (John) Che

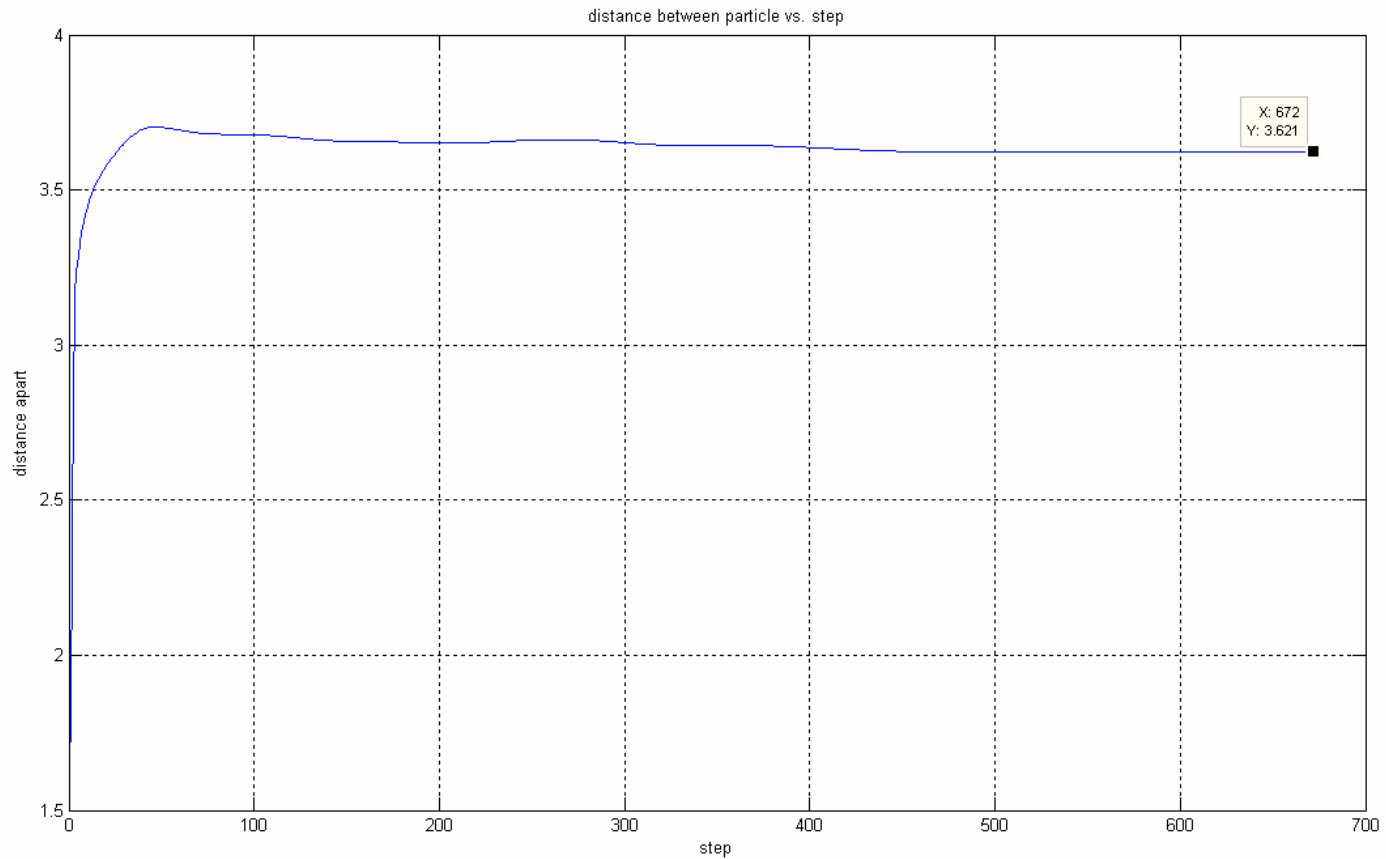
## Simplifications:

- 3D problem. No torsion or bending energy.
- Assume no Bonding between particles for testing purpose. (Allow van der Waal interaction)
- The terms that present in the energy functional are surface tension energy, van der Waals potential between particles, and between particles and solvent.

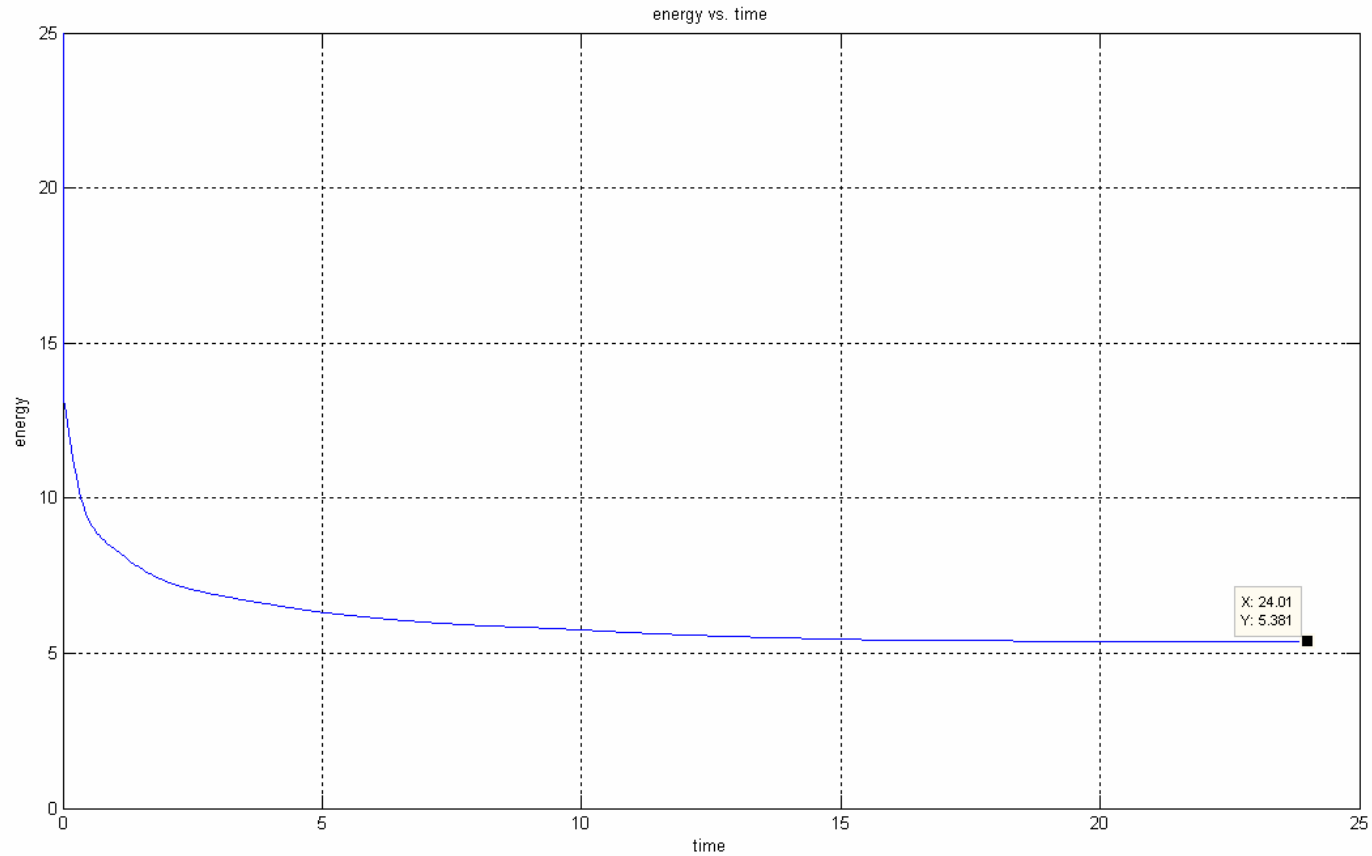
$$X_{\text{initial}} = \pm 0.5$$



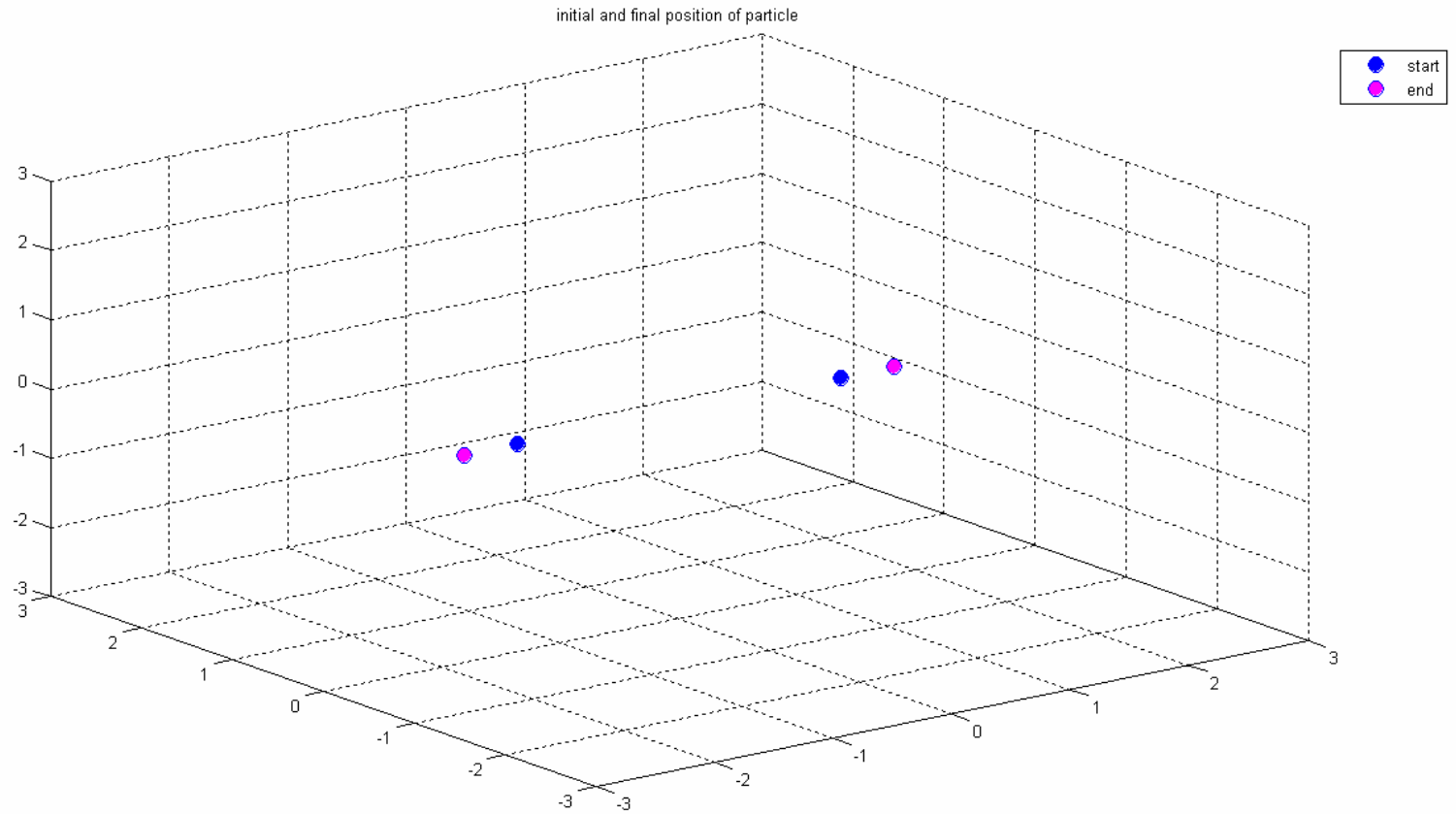
# Final distance apart = 3.621



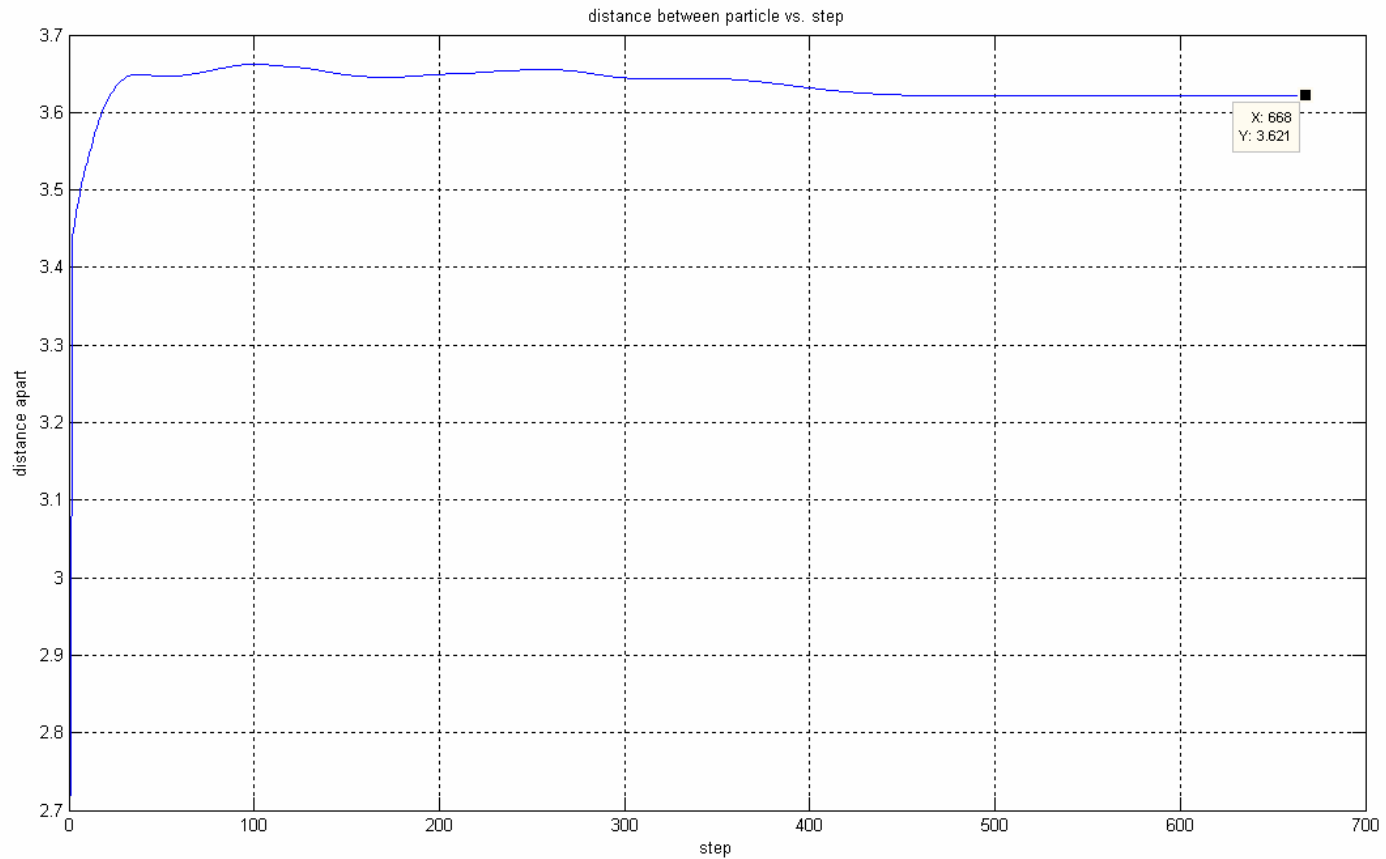
# Minimal Energy = 5.381



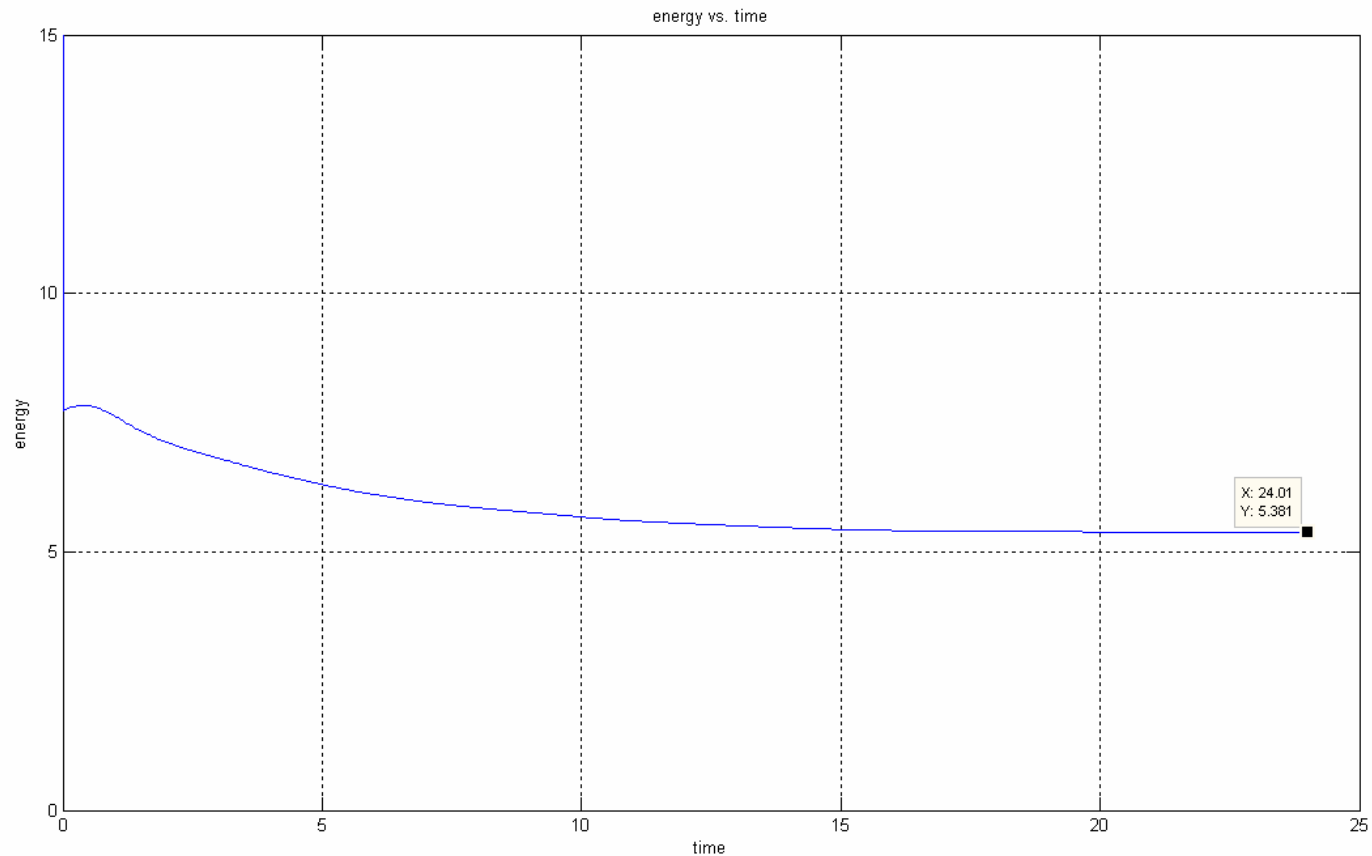
$$X_{\text{initial}} = +/- 1$$



# Final distance apart = 3.621

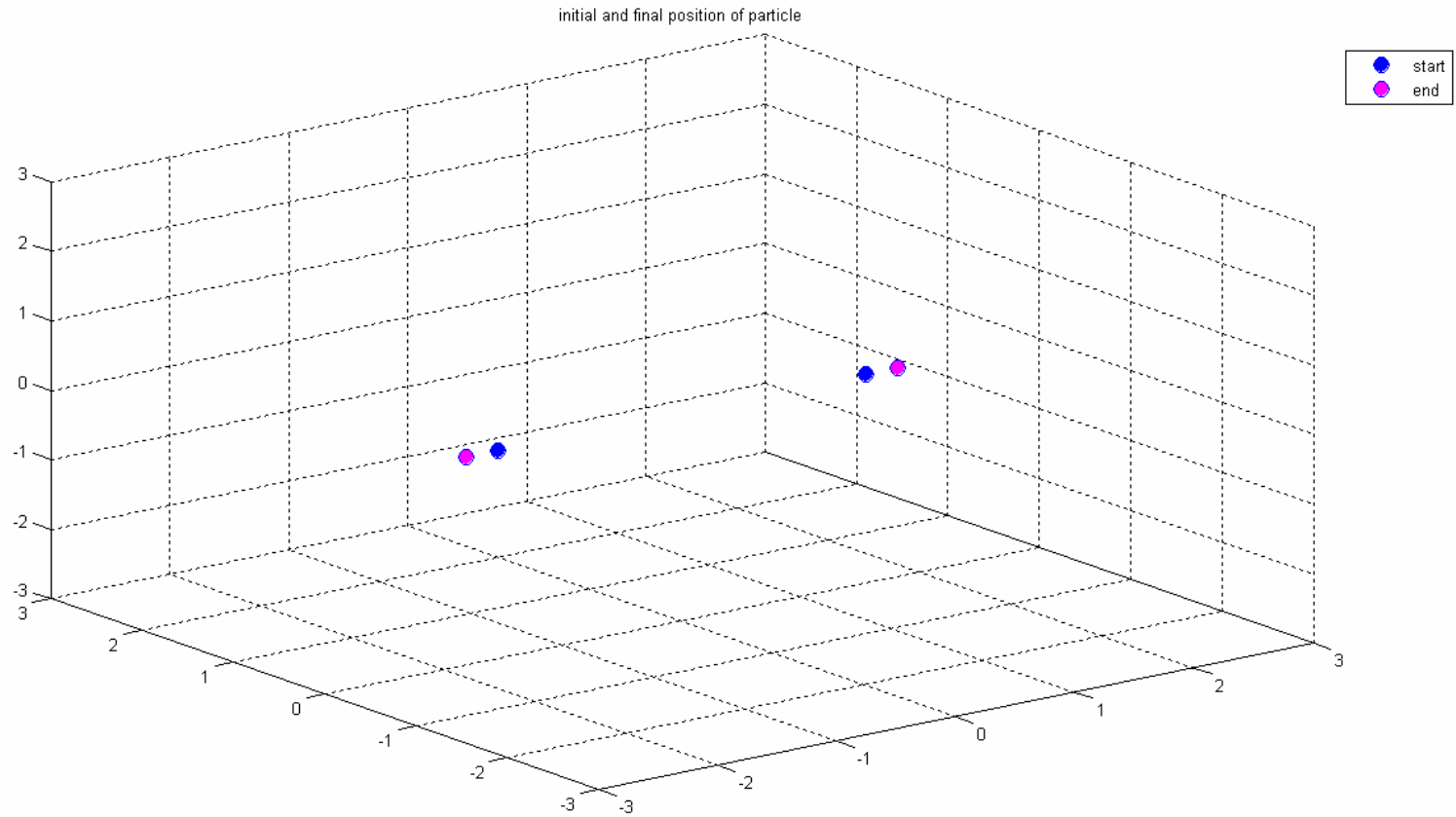


# Minimal Energy = 5.381

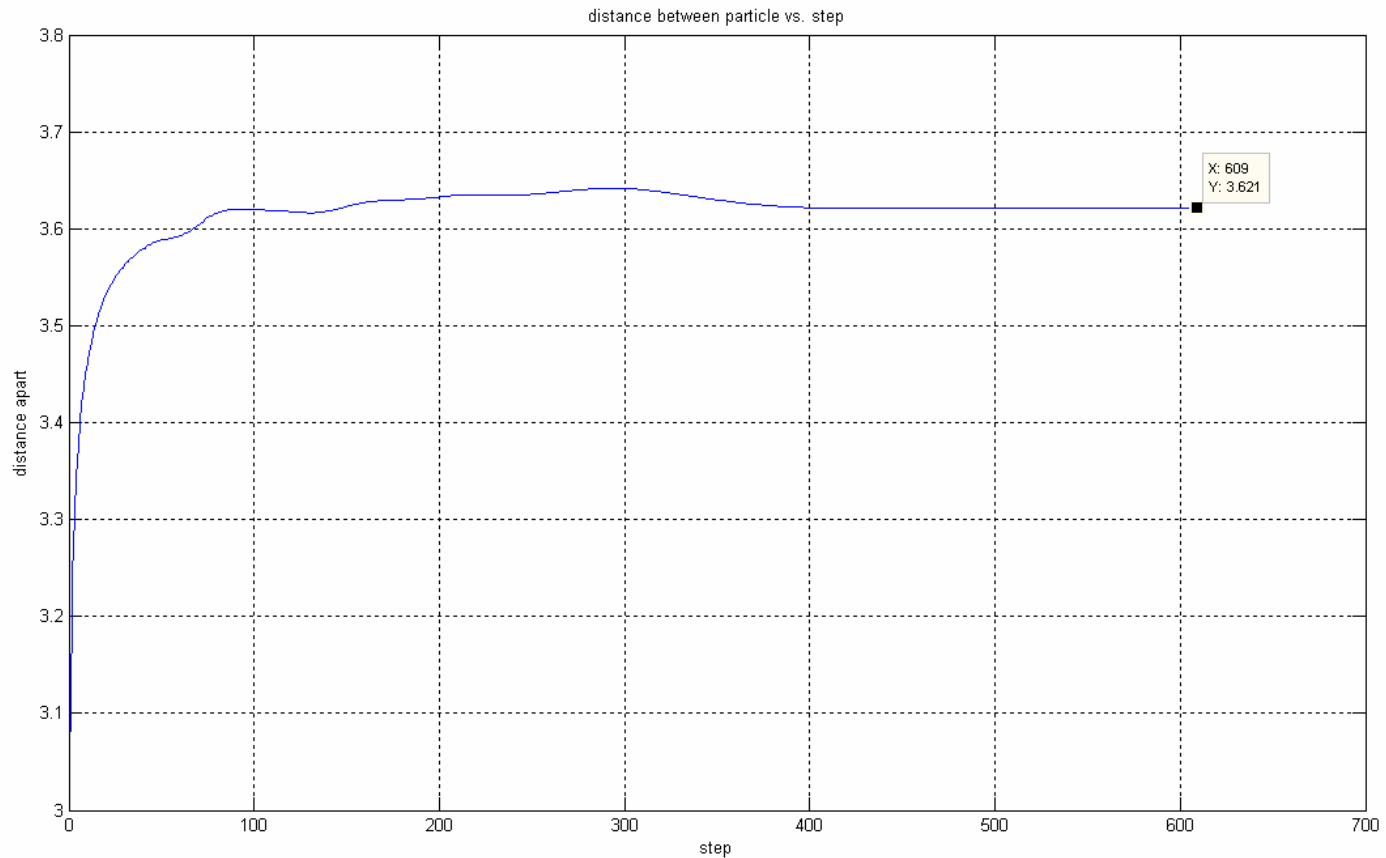




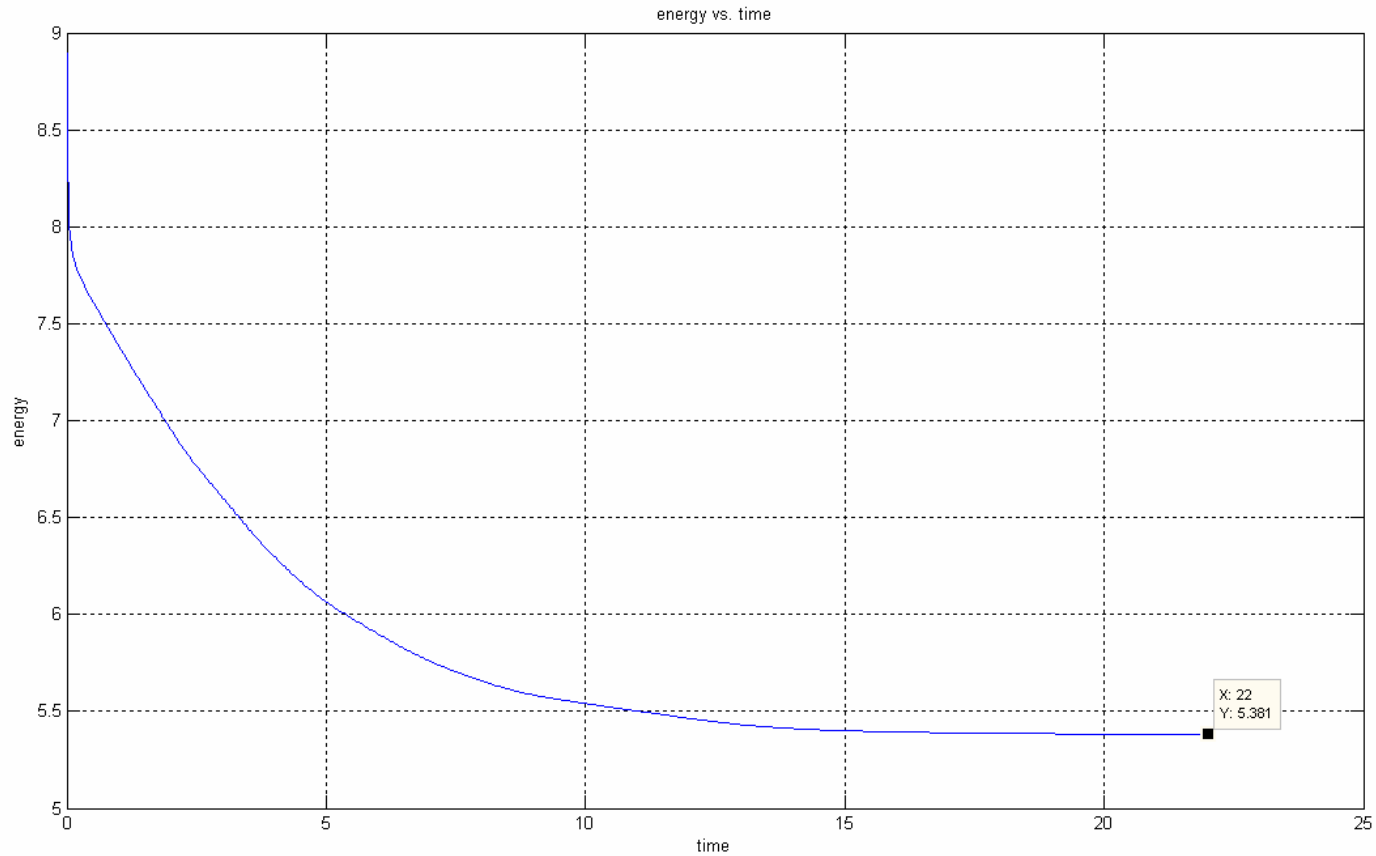
$$X_{\text{initial}} = +/- 1.5$$



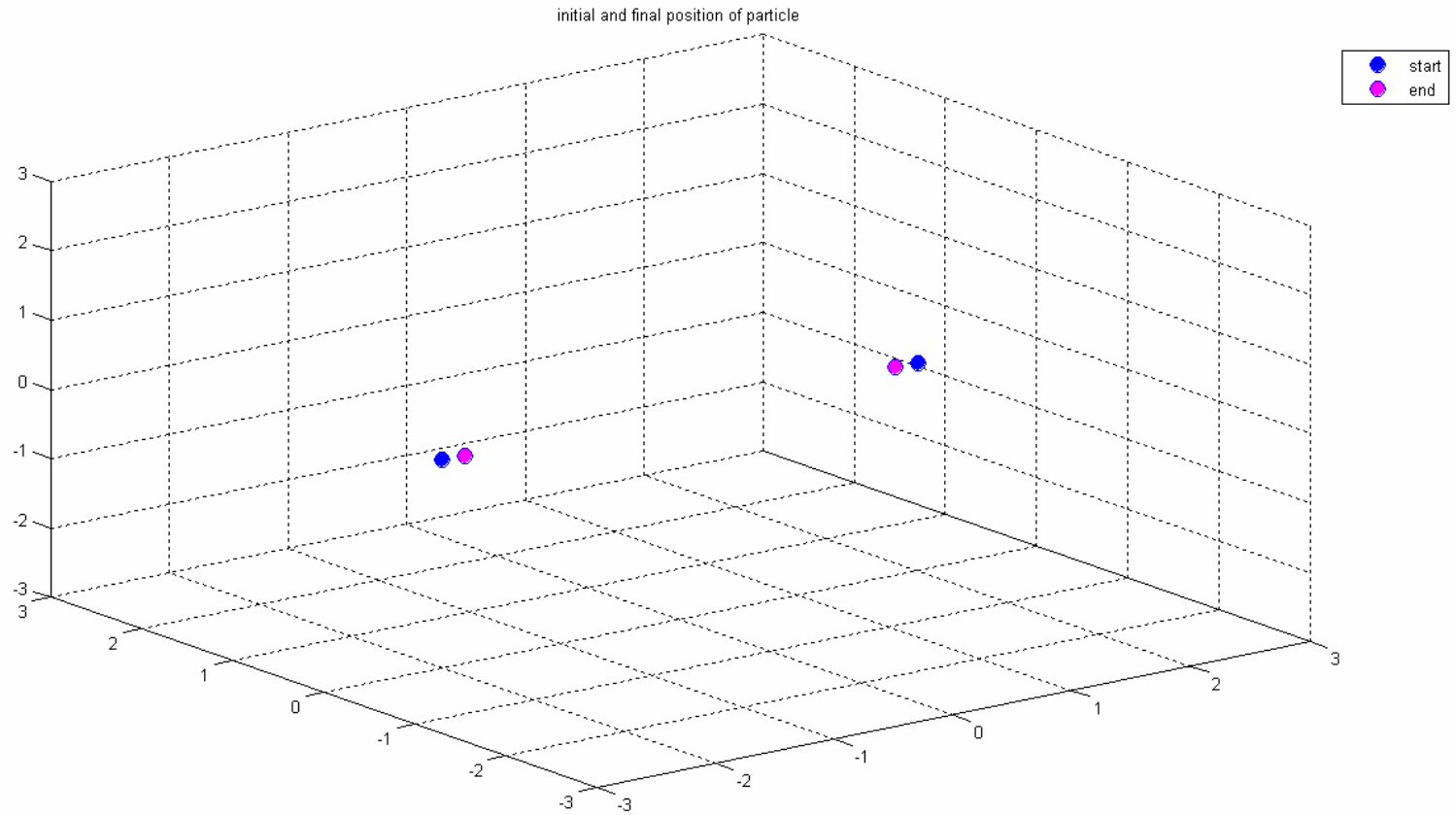
# Final distance apart = 3.621



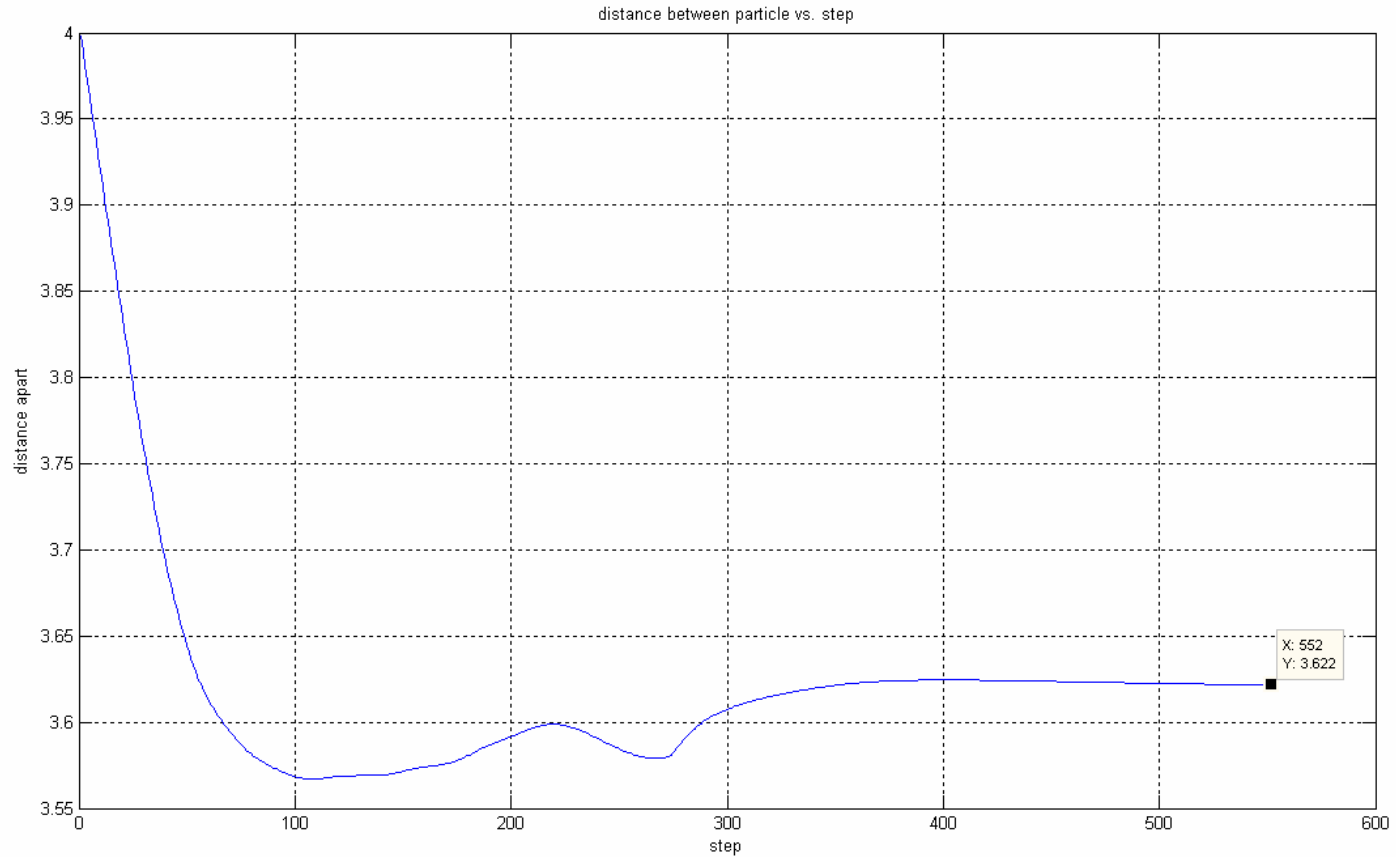
# Minimal Energy = 5.381



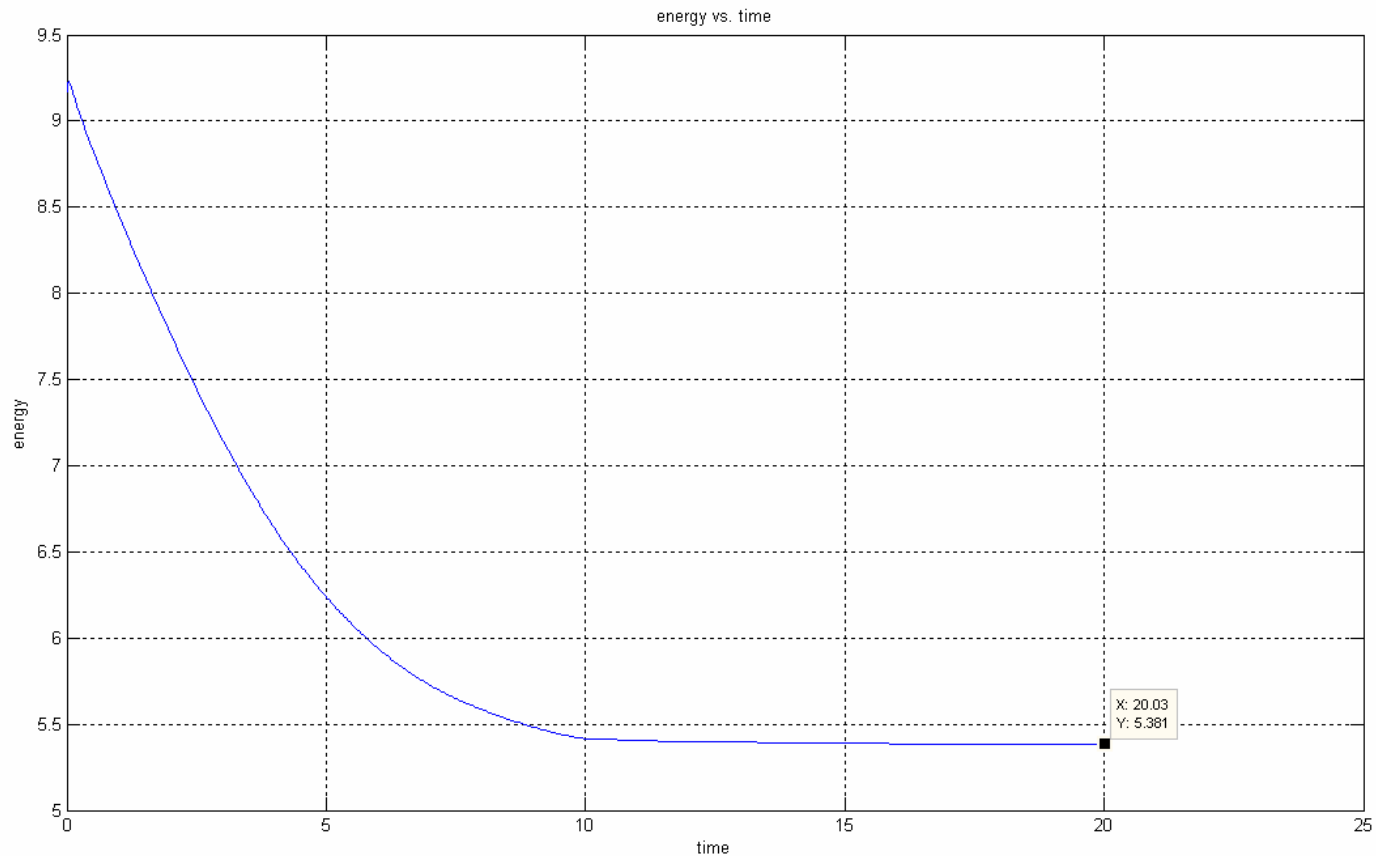
$$X_{\text{initial}} = +/- 2$$



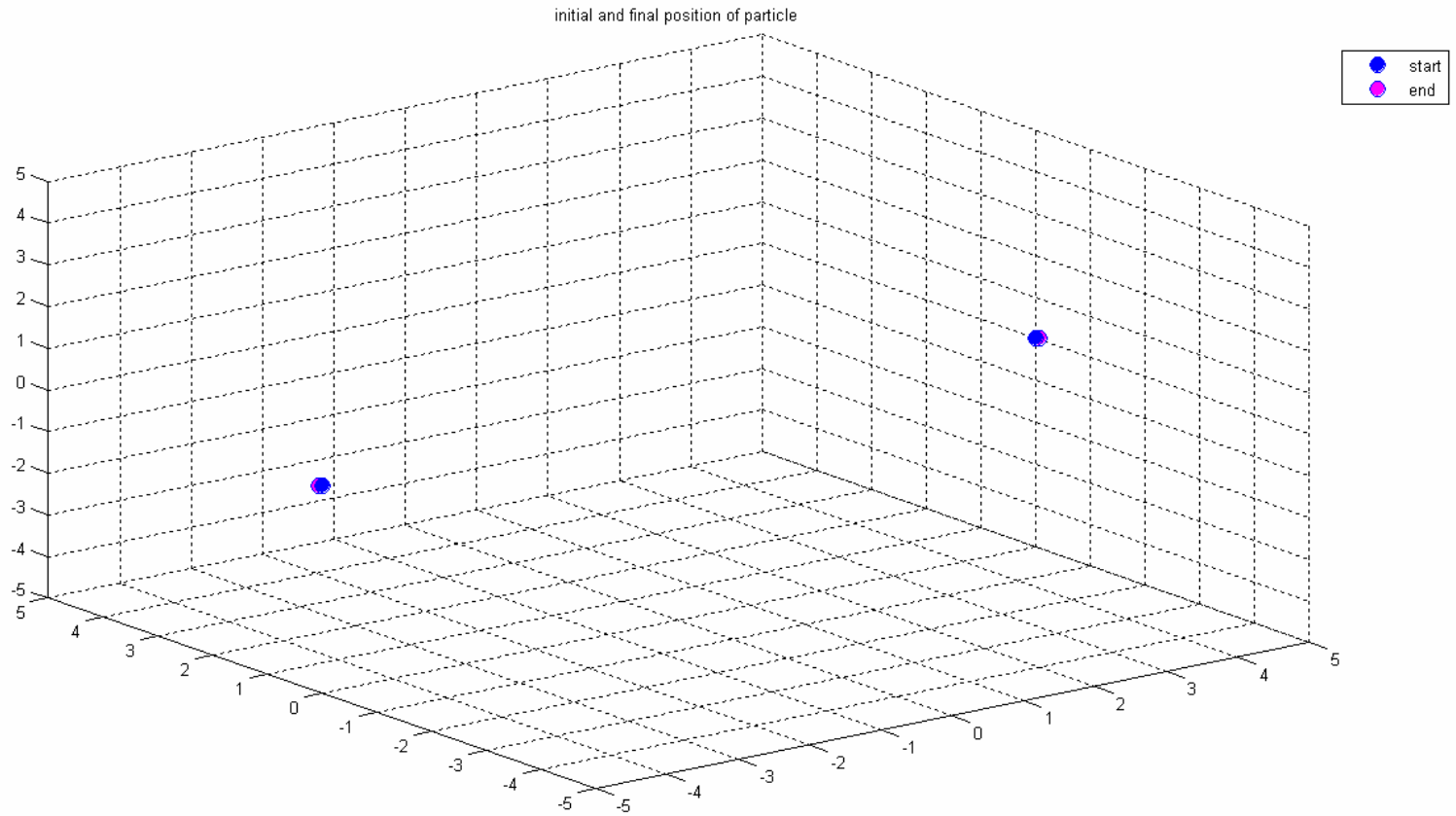
# Final distance apart = 3.622



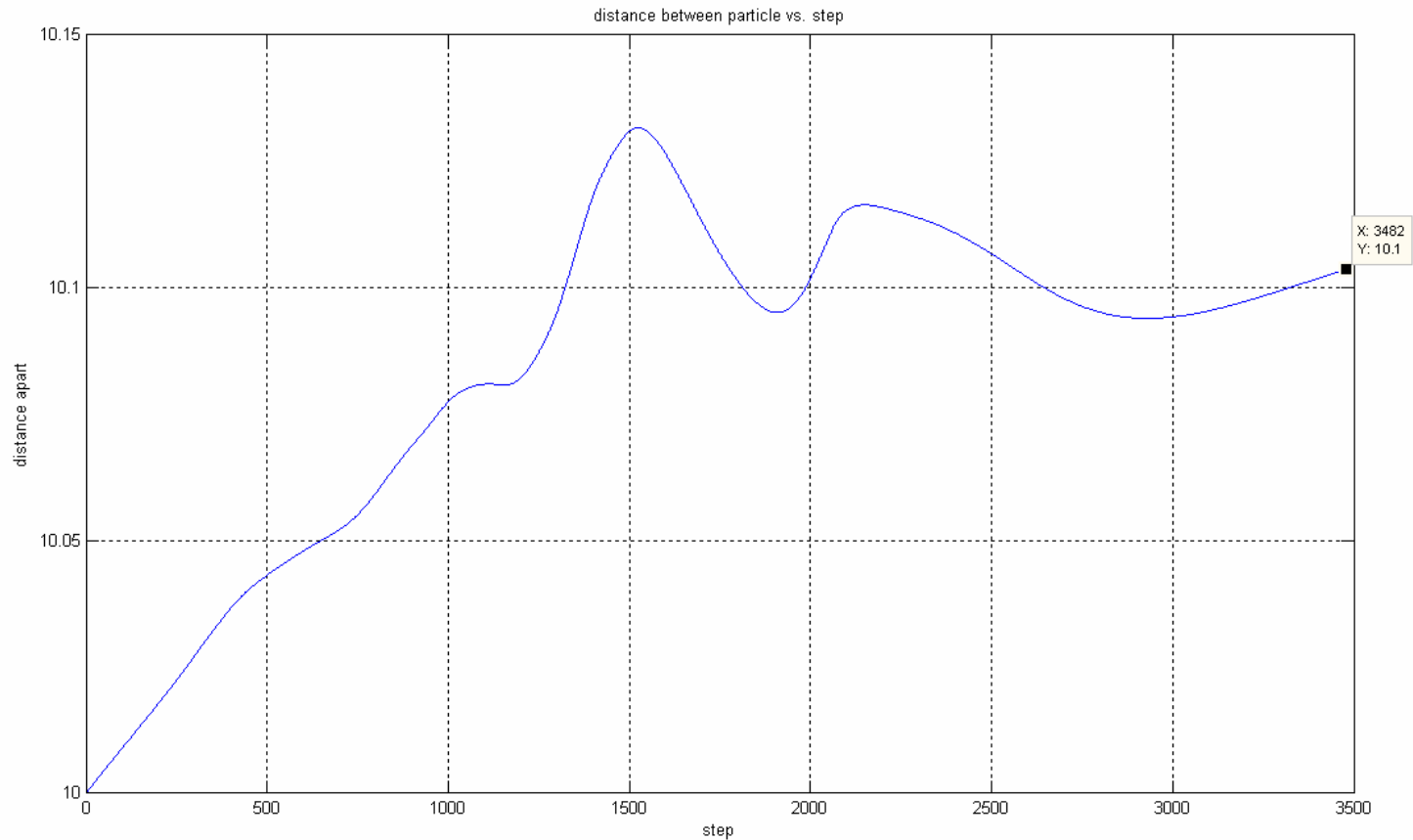
# Minimum Energy = 5.381



$$X_{\text{initial}} = +/- 5$$

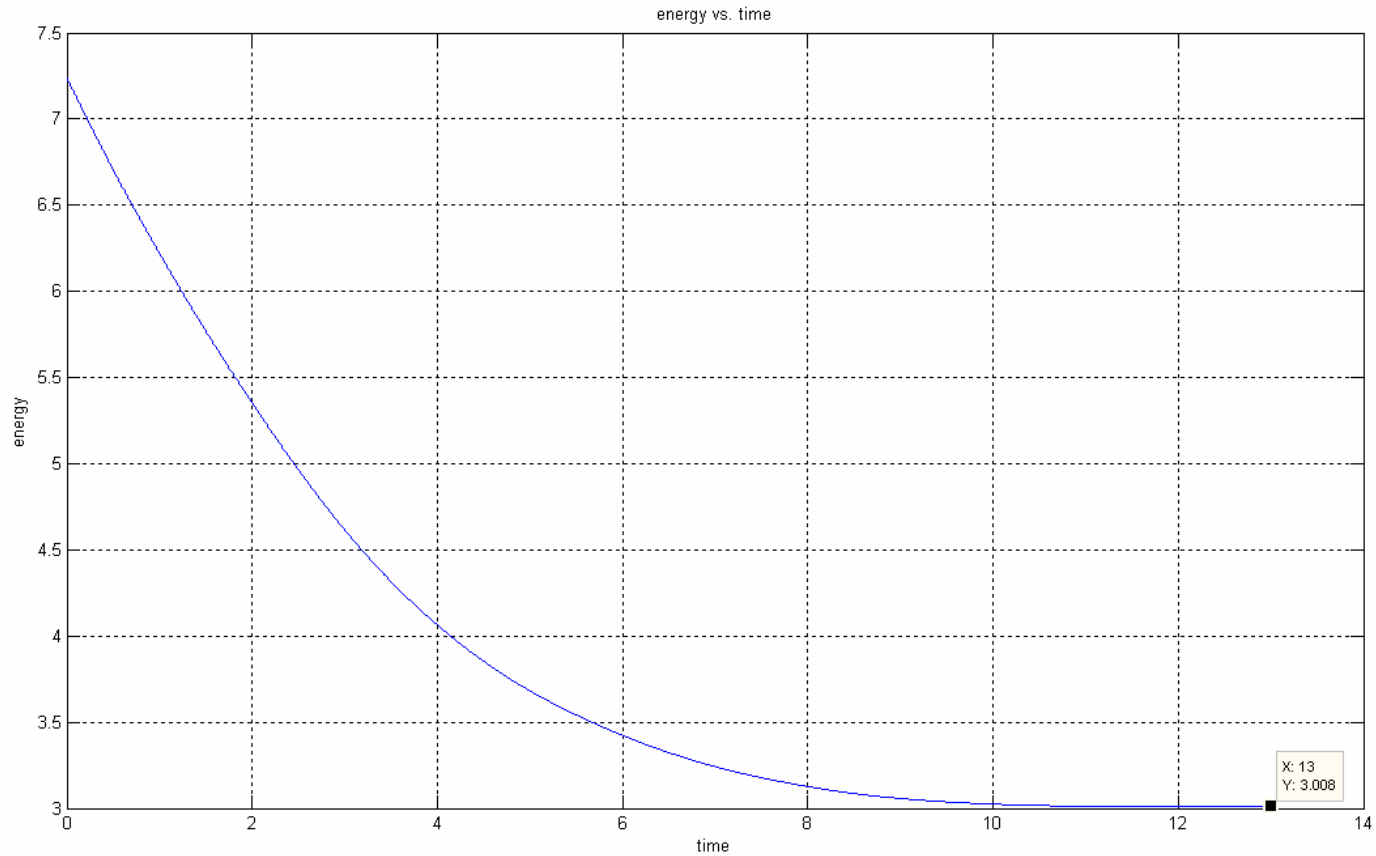


# Final distance apart = 10.01

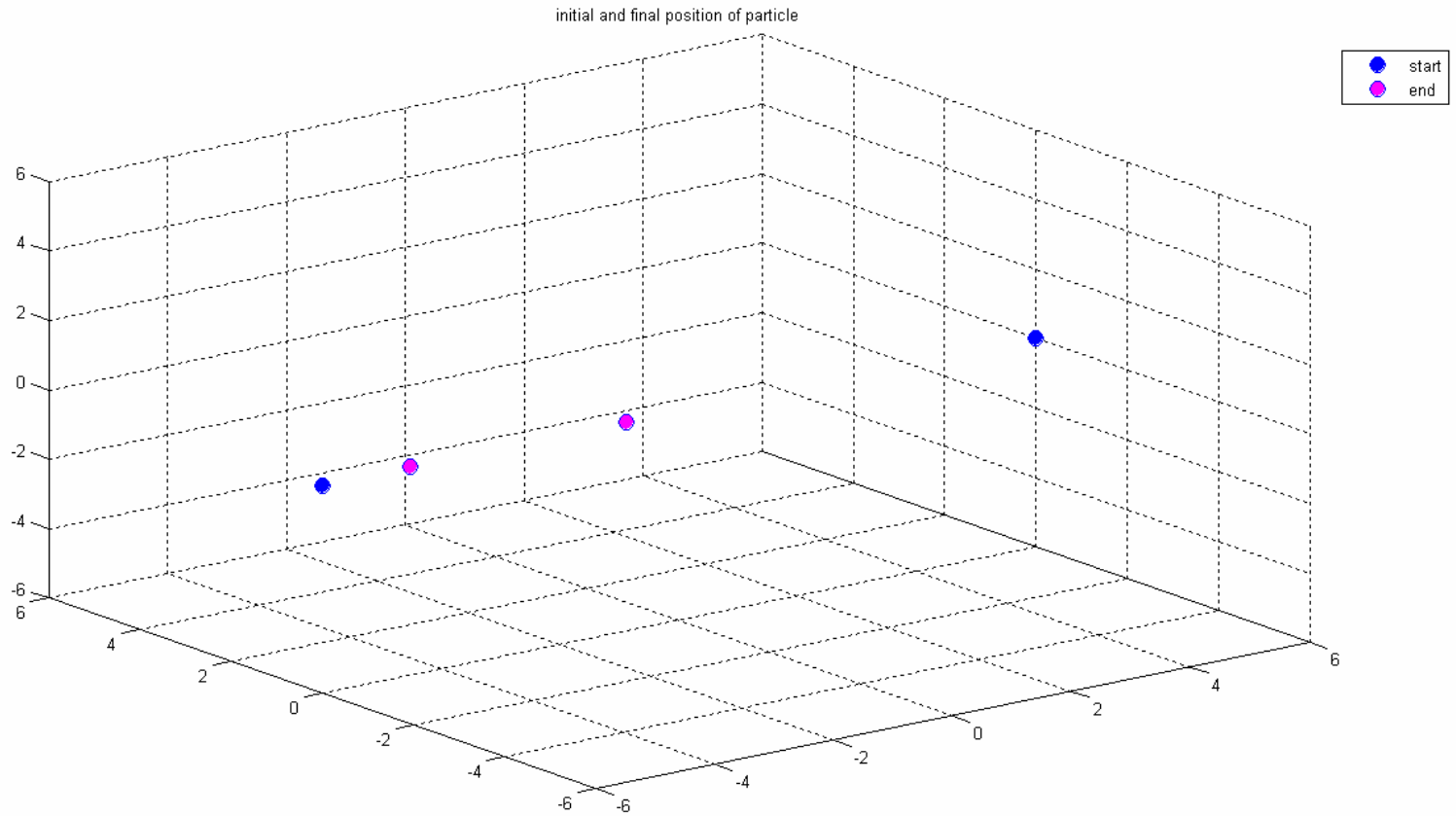




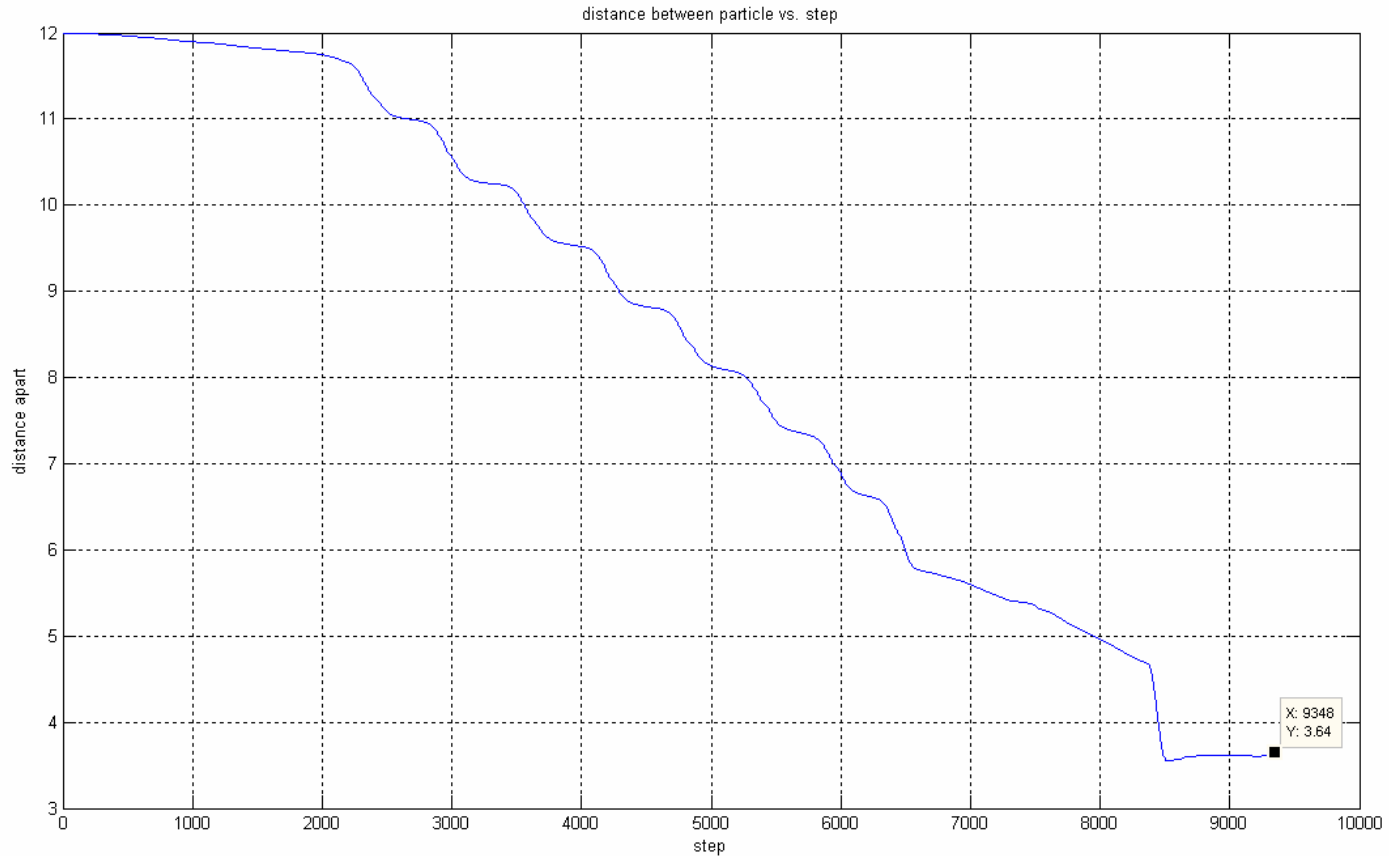
# Minimal Energy = 3.008



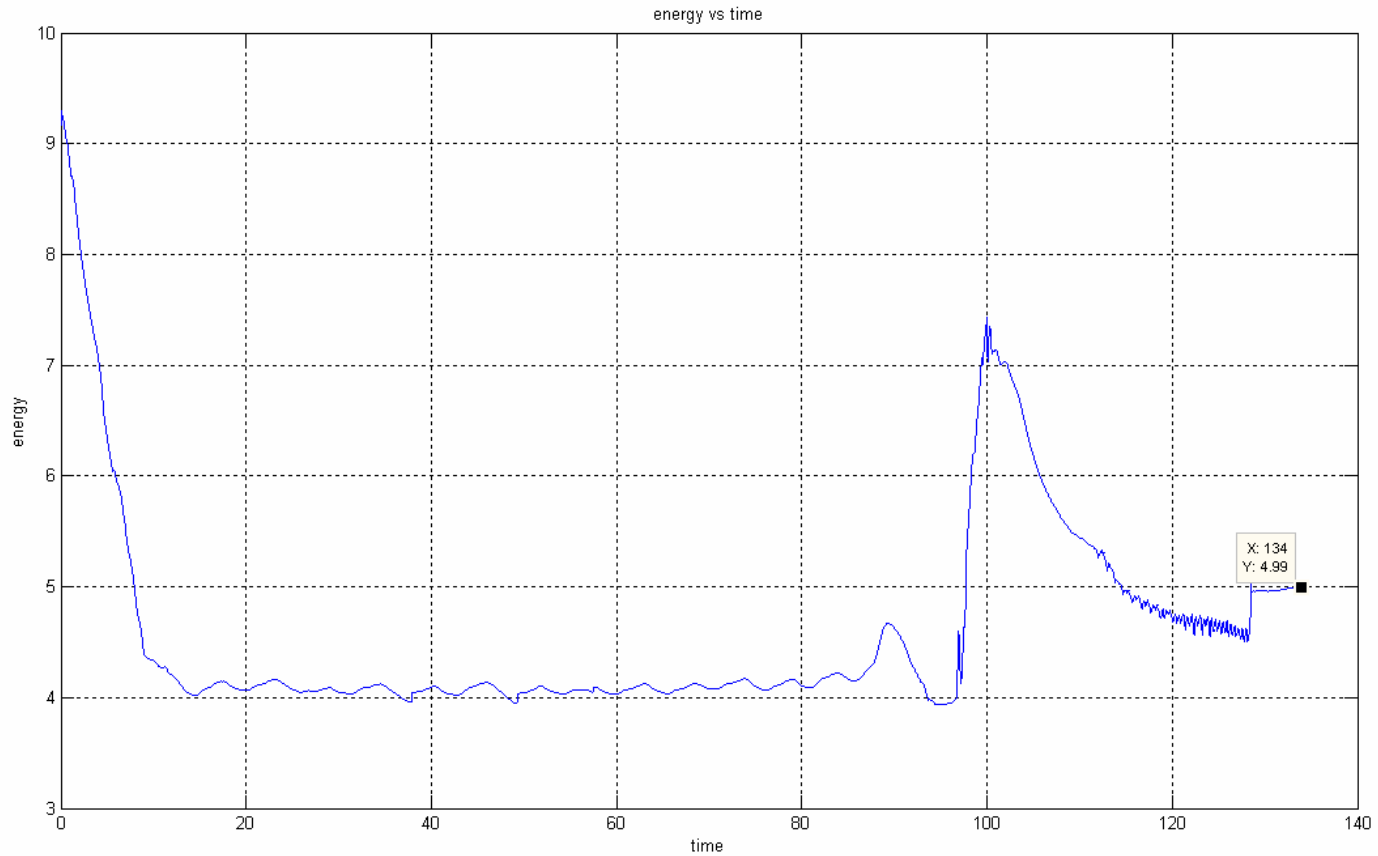
$$X_{\text{initial}} = +/- 6$$



# Final distance apart = 3.640131



# Minimal Energy = 4.98962



# Summary (gamma = 2 joined/unjoined circles with radius of sigma = 3.19 C<sub>60</sub>)

	+0.5 modified dt	+1 modified dt	+1.5	+2	+5	+6 modified dt
convergence	Yes	Yes	Yes	Yes	Yes	Yes
final distance	3.62124	3.62118	3.6212	3.62164	10.10368	3.640131
final energy	5.38091	5.38062	5.38086	5.38057	3.00826	4.98962
steps	672	668	609	552	3482	9348

# Summary (gamma = one circle with radius of sigma = 3.19 C<sub>60</sub>)

	+0.5 modified dt	+1 modified dt	+1.5	+2	+5 r = 2 sigma
convergence	Yes	Yes	Yes	Yes	N/A
final distance	3.6212	3.6212	3.62114	3.62114	N/A
final energy	5.38068	5.3807	5.38043	5.38035	N/A
steps	2250	2248	672	673	N/A