

Contact curve based simulation of side chains from two amino acids in a protein molecule

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Motivation

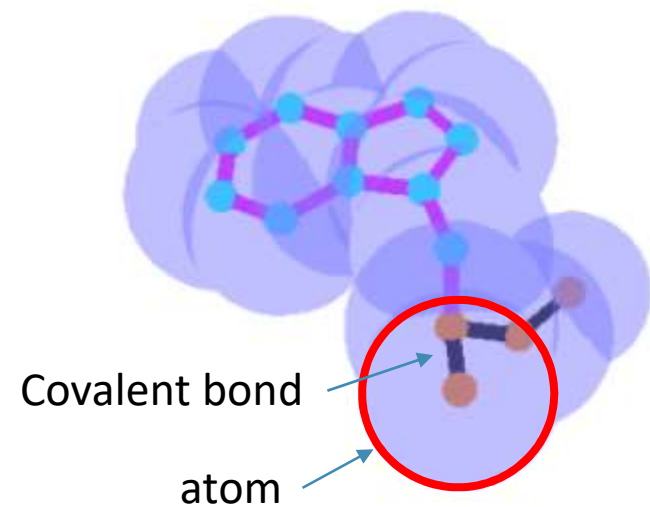
- Protein molecules have flexibility
- Simulating flexible molecules requires heavy computation efforts
- Efficient simulating method is needed
- We propose an efficient simulation method based on contact curve computation

Problem Definition

- Find a method to efficiently simulate two flexible amino acids
- Assumption
 - Fixed main chain and rotating side chains
 - Often used method for simplifying flexibility

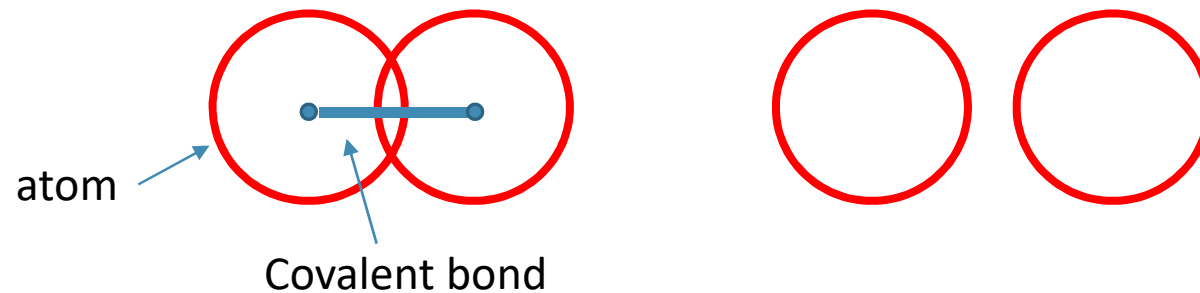
Preliminaries (1)

- A protein is composed of amino acids
- Amino acids are composed of atoms
- Each atom can be represented as van der Waals spheres
- Only covalent bonded atoms have sphere intersections

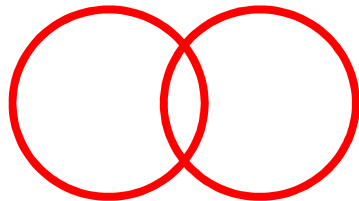


Preliminaries (2)

- No collision cases

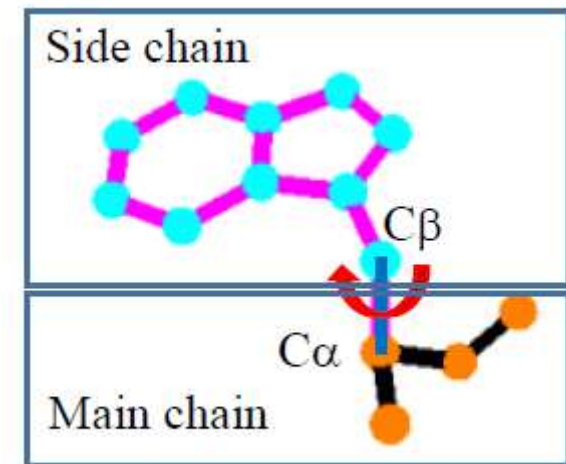


- Collision case

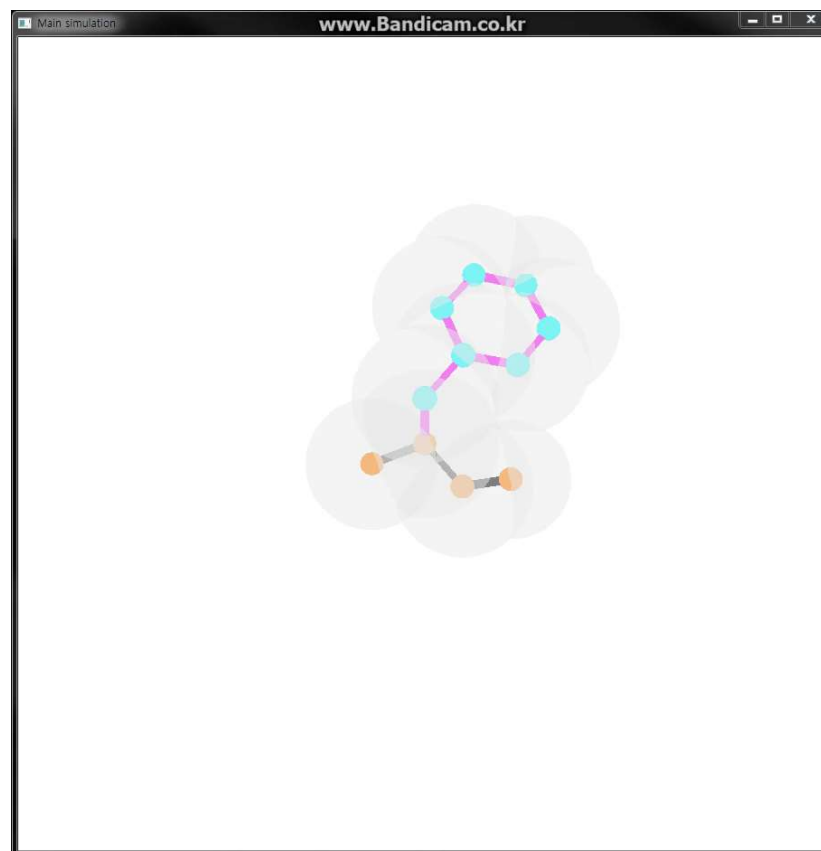


Preliminaries (3)

- An amino acid has two parts
 - Main chain
 - Side chain
- Main chain is fixed
- Side chain rotates along the axis containing centers of $C\alpha$ and $C\beta$

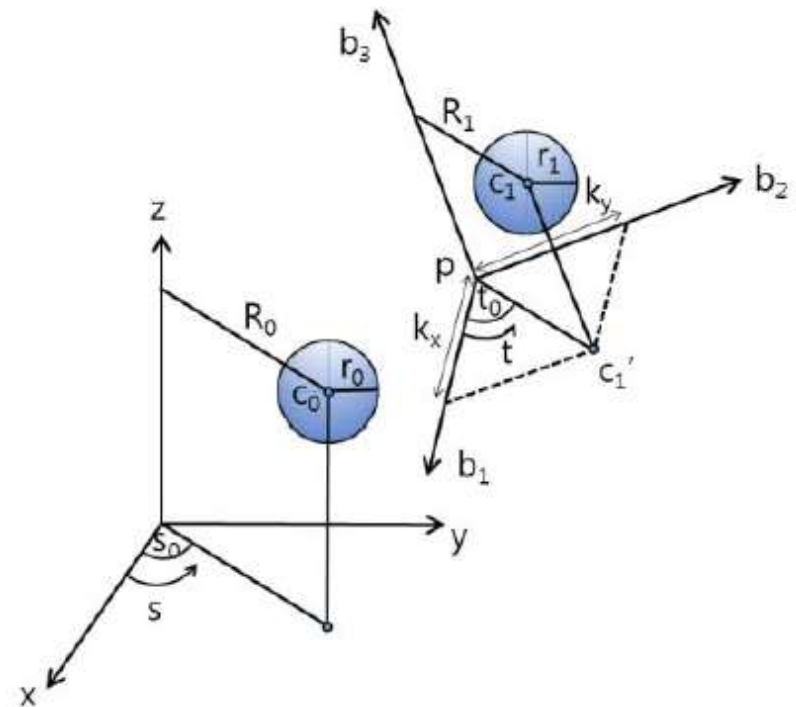


<Rotating side chain animation>



Collision region for two spheres(1)

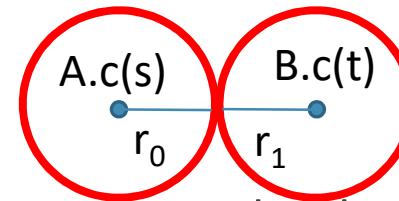
- Center location of rotating spheres A and B
 - $A.c(s) = (R_0 \cos (s + s_0), R_0 \sin (s + s_0), z_0)$
 - $B.c(t) = \mathbf{p} + R_1 \cos (t + t_0) \mathbf{b}_1 + R_1 \sin (t + t_0) \mathbf{b}_2 + ||c_1 - c_1' || \mathbf{b}_3$



Collision region for two spheres(2)

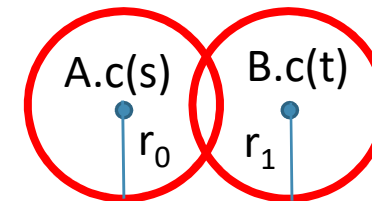
Case 1: Two spheres at (s^*, t^*) tangentially contact each other

$$||A.c(s^*) - B.c(t^*)||^2 = (r_0 + r_1)^2$$



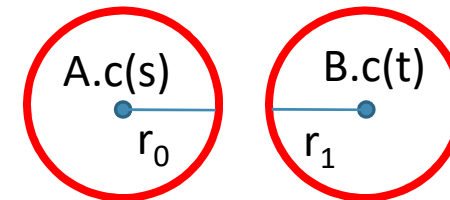
Case 2: Two spheres at (s^*, t^*) have an intersection each other

$$||A.c(s^*) - B.c(t^*)||^2 < (r_0 + r_1)^2$$

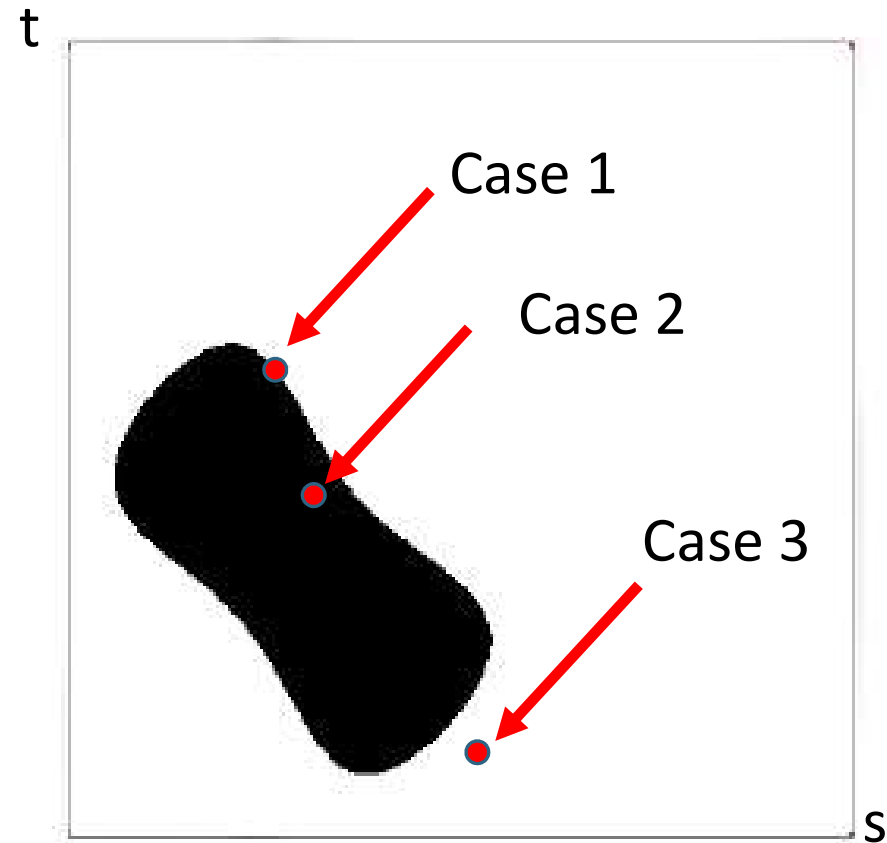
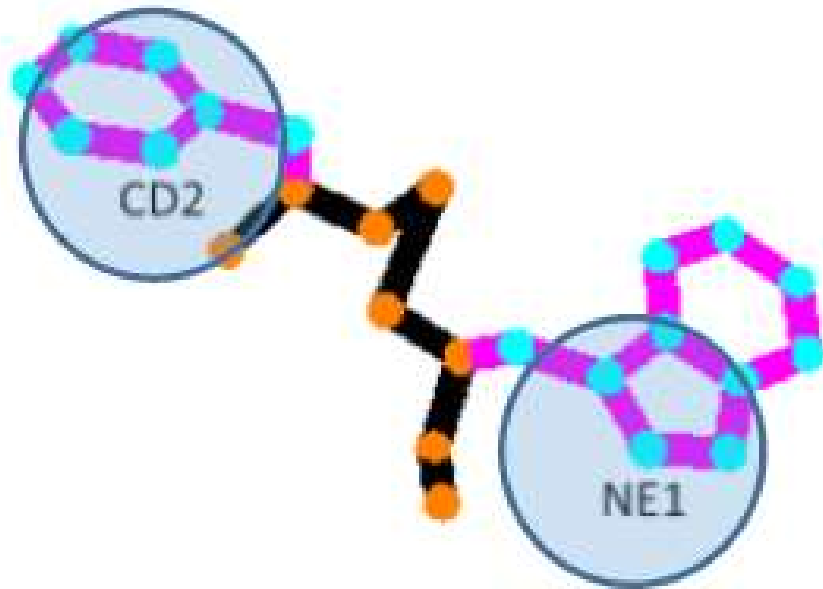


Case 3: Two spheres at (s^*, t^*) are apart

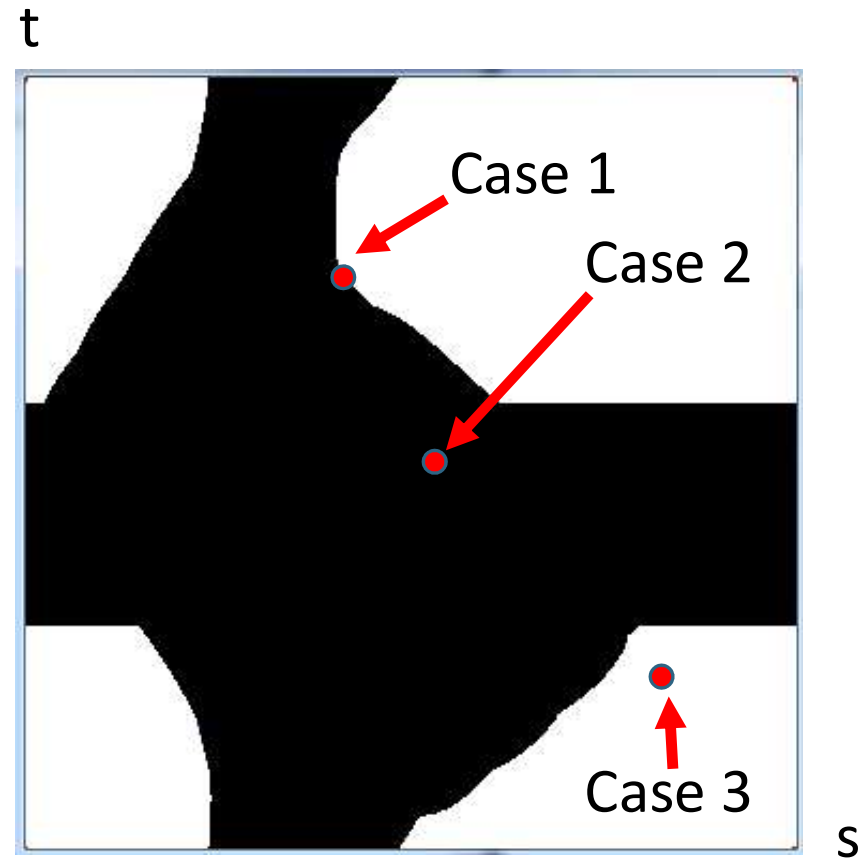
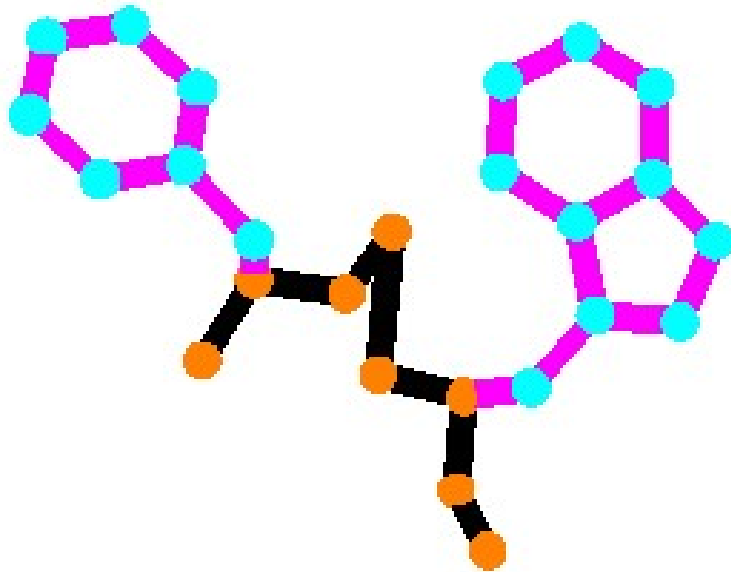
$$||A.c(s^*) - B.c(t^*)||^2 > (r_0 + r_1)^2$$



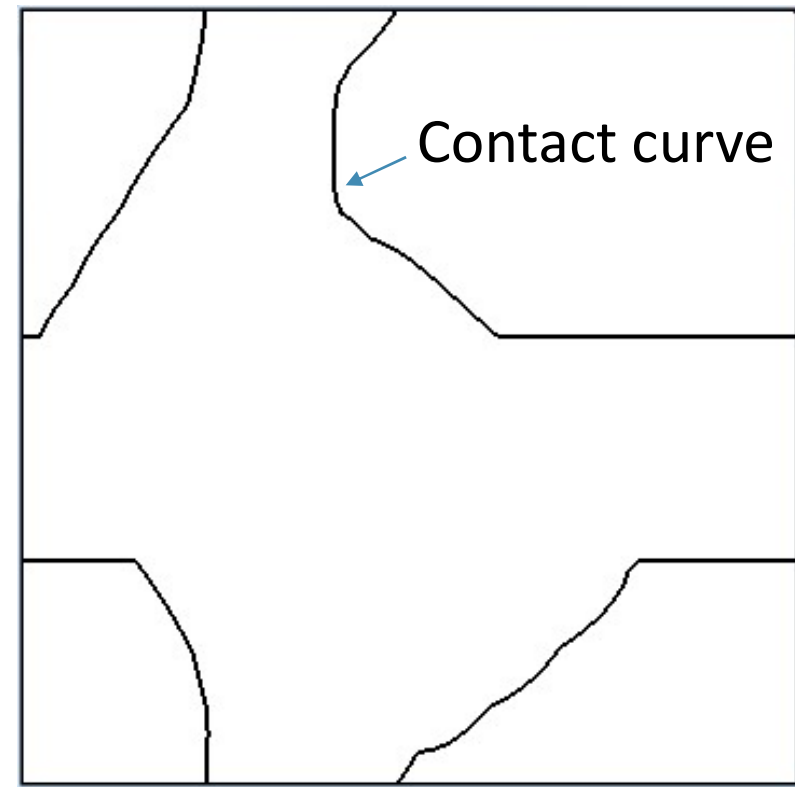
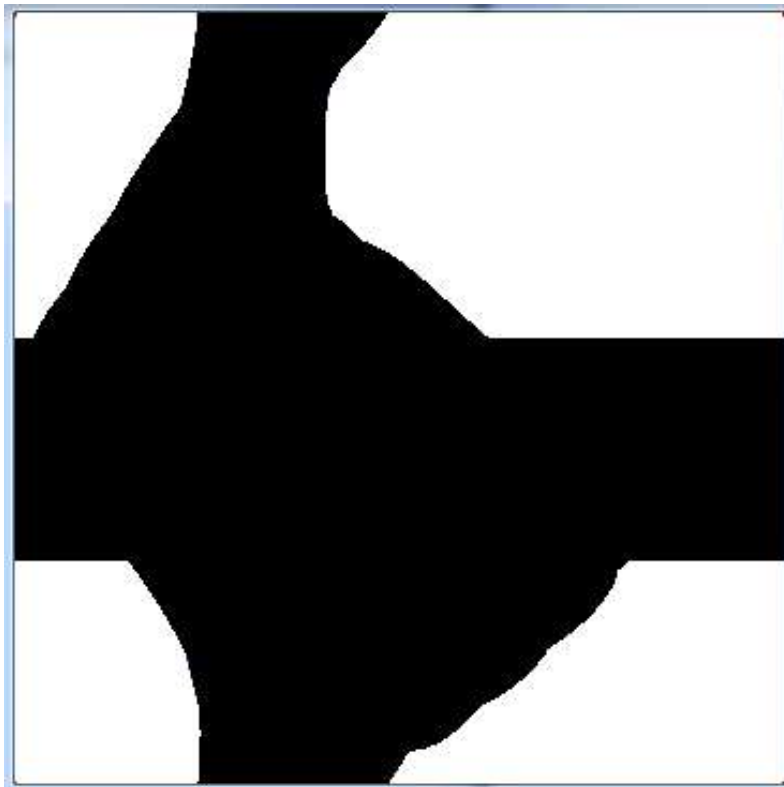
Collision region for two spheres(3)



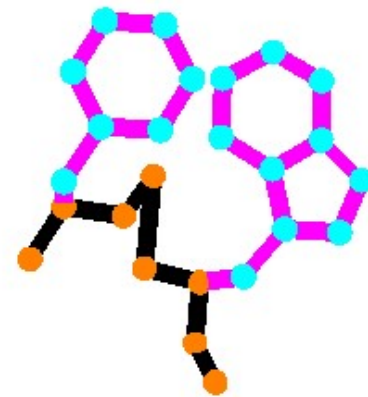
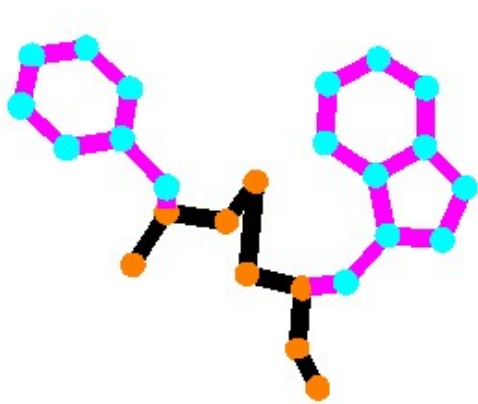
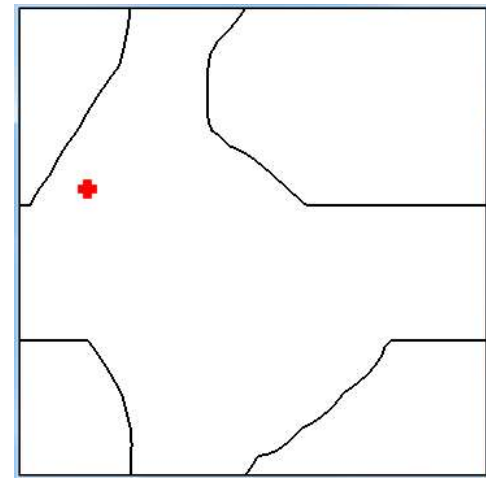
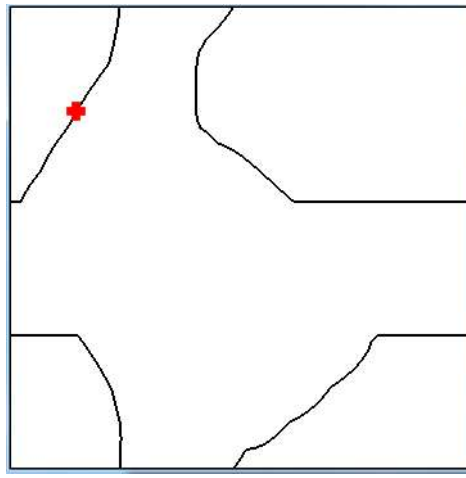
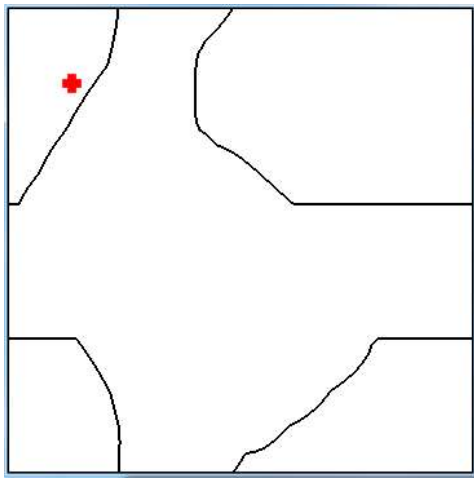
Contact curve for two amino acids (1)



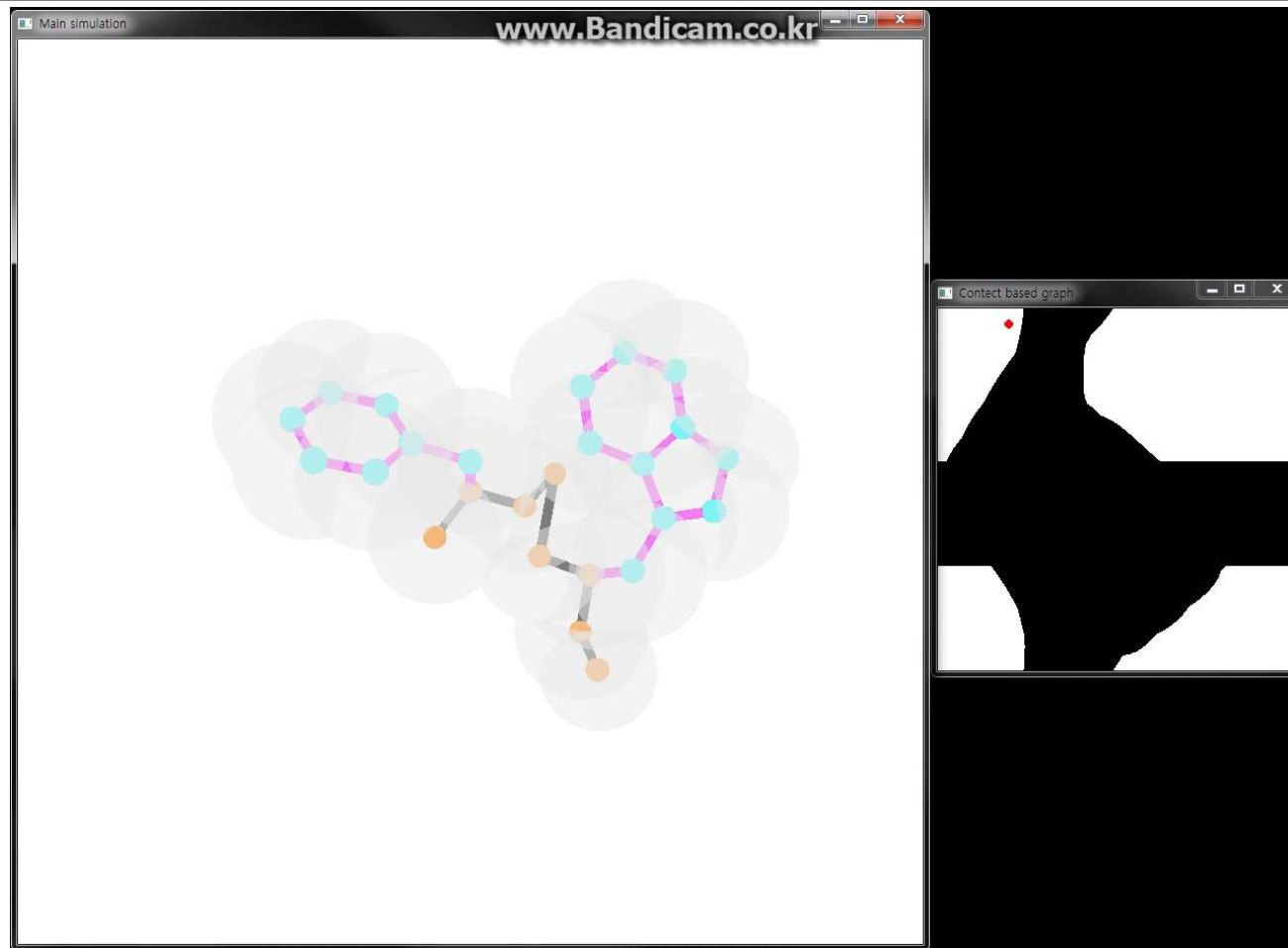
Contact curve for two amino acids (2)



Simulation along contact curve (1)



Simulation along contact curve (2)



Conclusion

- Analysis of contact configuration of two amino acids
- Computation of the contact curve
- Simulation based on the contact curve

Thank you

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