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Application of Selection Rejection Methodology to Molecular Dynamics

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Abstract: In this paper I have applied the Selection-Rejection Methodology to Molecular Dynamics to select collision pairs of particles.

Keywords: -relative velocity, position vector and collision probability.

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I. INTRODUCTION

The Selection-Rejection Methodology was developed based on the idea of Acceptance-Rejection Method by the renowned mathematician, Von Neumann, from the University of Berlin. Von Neumann[1] came forward with his method during 1950's but later on Karl Sigman[2] from Columbia University gave the similar methodology in 2007.Again in 1989,Bernard D.Flury[3] from Indiana University came forward with the theory "Acceptance-Rejection Sampling Made Easy".D.P.Kroese[4] from University of Queensland put forward his theory of Acceptance-Rejection in 2011.Selection-Rejection Methodology can be applied to almost all statistical distributions and hence it has got immense physical significance.

II. CONCEPT OF COLLISION PAIRS OF PARTICLES

In Molecular Dynamics the state of a system is given by the positions and velocities of the particles consisting the system. Let N be the number of particles in a system.

Let $\vec{r}_i; i = 1, 2, ...N;$ be the position vector of the i^{th} particle.

$\vec{v}_i; i = 1, 2, ...N;$ be the velocity vector of the i^{th} particle.

Let τ = time step ie τ is the time taken by the particles to move from one position to another position without interactiong with each other.

Let $\vec{r}_i^{\,new}$ be the new position of the i^{th} particle after the elapse of time τ .

Then $\vec{r}_i^{\,new} = \vec{r}_i + \vec{v}_i \tau$

Once the particles start moving some particles are selected for collision after a certain period of time. The rules for this random selection process are obtained from kinetic theory. After the velocities of all colliding particles have been reset, the process is repeated for the next time step.

In each cell, a set of representative collisions is processed at each time step. All pairs of particles in a cell are considered to be candidate collision partners, regardless of their positions within the cell.In the hard sphere model,the collision probability for the pair of particles at the i^{th} and j^{th} position is proportional to their relative speed.

Let $\vec{v}_i =$ velocity of the i^{th} particle and $\vec{v}_j =$ velocity of the j^{th} particle.

Then the relative speed for the i^{th} and j^{th} particle is given by $\left|\vec{v}_i - \vec{v}_j\right| = V_{relative}(say)$.
(1)

The maximum relative speed of the collided particles in the hard sphere model is given by

$$\sum_{m=1}^{N_c}\sum_{n=1}^{m-1}\left|\vec{v}_m - \vec{v}_n\right| = V_{\max}(say) \qquad (2)$$

Where $N_c =$ no of collided particles in the hard sphere model.

Now the probability of collision between the i^{th} and j^{th} particle is given by

$$P_{coll}(i,j) = \frac{\left|\vec{v}_i - \vec{v}_j\right|}{\sum_{m=1}^{N_c}\sum_{n=1}^{m-1}\left|\vec{v}_m - \vec{v}_n\right|} \qquad (3)$$

III. SLECTION-REJECTION METHODOLOGY FOR COLLISOION PAIRS.

Step (1):- Let i^{th} and j^{th} particles are chosen at random as candidate particles.

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Step (2):-Let $V_{relative}$ be the relative speed of the i^{th} and j^{th} particle.

Step (3):- Let $0 < R < 1$ be a random number.

Step (4):- Let $V_{\max}$ be the maximum relative speed of the i^{th} and j^{th} particle.

Step (5):- Set $P_{coll}(i,j) = \frac{V_{relative}}{V_{\max}}$

Step (6):- If $R \le P_{coll}(i,j)$,then select i^{th} and j^{th} particle; otherwise reject the i^{th} and j^{th} particle and repeat the process from step (1).

IV. CONCLUSION.

In this paper I have calculated the probability of collision between two particles in terms of their minimum and maximum relative velocities.

REFERENCES

[1] JOHN VON NEUMANN, "Various techniques used in connection with random digits, in *Monte Carlo Method,* Appl. Math. Series, vol, 12, U. S. Nat. Bureau of Standards, 1951,pp. 36-38 (Summary written by George E. Forsythe);reprinted in John von Neumann, *Collected Works*. Vol. 5, Pergamon Press; Macmillan, New York, 1963, pp. 768-770. MR 28#1104.

[2] Acceptance-Rejection Method by Karl Sigman, 2007, Columbia University.

[3])BERNARD D. FLURY, "ACCEPTANCE-REJECTION SAMPLING MADE EASY",SIAM Review, Vol. No. 3. Pp 474-476, September 1990.

[4] D.P.Kroese, "Acceptance-Rejection Method", 2011, University of Queensland.

[5] Loernzo Pareschi,"Part III: Monte Carlo methods",2003,University of Ferrara,Italy.

[6] WILLIAM FELLER, "An Introduction to Probability Theory and its Applications", Vol I, Wiley, New York, 1950, Lemma 2, P-131(P-166 of 2nd ed).MR 12,424.

[7] Richard Saucier, "Computer Generation of Statistical Distributions", March 2000, *ARMY RESEARCH LABORATORY.*

[8] J.H. Ahrens and U. Dieter, Computer Methods for Sampling from Exponential and Normal Distributions, Comm. A.C.M 15 (1972), 873-882.

[9] Fill, J. A. (1998) An interruptible algorithm for perfect sampling via Markov chains. *Annals of Applied Probability,* 8(1) 131-162. MR1620346.

[10] Fill, J. A. Machide, M., Murdoch, D.J. and Rosenthal, J. S. (1999). Extension of Fill's perfect rejection sampling algorithm to general chains. Random *Structures and Algorithms* **17** 219-316. MR1801136.

[11] Gilks, W. R. and Wild, P. (1992). Adaptive rejection sampling for Gibbs sampling. *Appl. Statist.* **41** 337-348.

[12] Propp, J.G. and Wilson, D. B. (1996). Exact sampling with coupled Markov chains and applications to statistical mechanics. *Random Structures and* Algorithms. **9**(1 & 2), 223-252. MR1611693.