# COLLECTIVE BEHAVIOUR IN NON EQUILIBRIUM ACTIVE MATTER

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# COLLECTIVE BEHAVIOUR IN NON EQUILIBRIUM ACTIVE MATTER

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*Dedicated to my mother and father*

# Certificate

This is to certify that the thesis entitled **"COLLECTIVE BEHAVIOUR IN NON EQUILIBRIUM ACTIVE MATTER"**, submitted by **MOHD YASIR KHAN** to the Indian Institute of Technology Delhi, for the award of the degree of **Doctor of Philosophy** in Physics, is a record of the original, bona fide research work carried out by him under our supervision and guidance. The thesis has reached the standards fulfilling the requirements of the regulations related to the award of the degree.

The results contained in this thesis have not been submitted in part or in full to any other University or Institute for the award of any degree or diploma to the best of our knowledge.

**Prof. Sujin B. Babu**
Department of Physics,
Indian Institute of Technology Delhi.

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# *Abstract*


This PhD project is motivated to design artificial microswimmers for targeted drug delivery applications and to understand the collective behaviour in active matter at the fundamental levels. The pursuit of designing nanoscopic/microscopic machines is inspired by Feynman's address "There is Plenty of Room at the Bottom, 1959" and by Purcell's famous piece "Life at low Reynolds number, 1977". This thesis has carried out this quest by exploiting the complex geometrical structures such as boundaries and obstacles(mimicking red blood cells) to direct the motion of microswimmers towards a specific ailing tissue by theoretically and computationally modelling the organisms. When present in numbers, the dynamics of these organisms lead to emergent phenomenons, and in this thesis, we probed this collective behaviour in microswimmers, self-propelled particles and Vicsek agents.

We have modelled an artificial swimmer(Taylor line) by a bead spring arrangement with a sine wave passing through it using a bending wave potential. The fluid is modelled using the particle-based simulation method of multiparticle collision dynamics. We took a binary mixture of swimmers with the same propulsion speed, but they differ from each other in the shape of the Taylor line. We observe that an optimal amplitude exists, leading to large cluster formation as well as enhancements of swimming efficiency.

For circling(chiral) self-propelled rods, we modelled by connecting beads, interacting with each other with LJ potential and simulated using the overdamped Langevin equation. With equal fractions as clockwise, anticlockwise circling particles, the dynamical response follows subdiffusive behaviour at lower particle fractions and gradually increases to diffusive behaviour at higher particle fractions. Spheres show a similar response to conclude that the shape plays no role.

We also modelled the dynamics of self propelled particles following the Standard Vicsek model mimicking the dynamics of birds. Such agents dwell in an inhomogeneous environment with different behaviours in different regions. We modelled a complex noise regime using the Vicsek model and observed that the time taken or the escape profile from the noiseless to the noisy regime broadens as the noise gradient increases. This concludes that the Vicsek agents avoid the noisy region. We proposed a sorting mechanism for Vicsek agents by quantitatively analysing the escape time.

# सारांश

यह शोध  ग्रंथ दवाओं के ऊतकों में लक्षित अनुप्रयोग के लिए कृत्रिम सूक्ष्म-तैराकों के आविष्कार एवं निर्माण के साथ-साथ सक्रिय पदार्थ में सामूहिक व्यवहार के मूल नियमों के अध्ययन के उद्देश्य से प्रेरित है। अति लघु मशीनों का निर्माण तथा व्यवहार का अध्ययन  महान वैज्ञानिक फेनमैन के संबोधन "देयर इज़ प्लेंटी ऑफ़ रूम ऐट द बॉटम, १९५९" तथा पर्सेल की प्रसिद्ध रचना "लाइफ एट लो रेनॉल्ड्स नंबर, १९७७" से प्रेरित माना जाता है। सूक्ष्मयंत्रों को विशिष्ठ ऊतकों की दिशा में लक्षित करने के उद्देश्य हेतु जटिल ज्यामितीय संरचनाओं तथा उनपर सीमाओं और बाधाओं के प्रभाव को उजागर एवं उपयोग करते हुए, सुक्ष्म जैविकीय के सैद्धांतिक एवं गणनीय प्रतिरूपण के आधार पर, विज्ञान की इस महान यात्रा को आगे बढ़ाने का प्रयास किया गया है। अत्यधिक संख्या में लेने पर, ये सुक्ष्म-जैविकीय-निकाय उद्भित प्रभाव प्रदर्शित करते हुए पाए जाते हैं जिन्हें हम सामूहिक व्यवहार कहते हैं । प्रस्तुत शोधरचना, इन्ही सामूहिक व्यवहारों, जो की सूक्ष्मयंत्रों, स्वचालित कणों, विकसेक-प्रतिनिधियों के निकायों द्वारा परिलक्षित होती है, पर एक  अध्ययन है।

इस शोध-रचना में, कृत्रिम सूक्ष्म-तैराकों का प्रतिरूपण बीड-स्प्रिंग व्यवस्था में बेन्डिंग तरंग विभव के   प्रयोग का उपयोग करते हुए, आवर्ती तरंग के प्रेशण द्वारा किया गया है। द्रव का प्रतिरूपण कण आधारित संगणक अनुरूपण विधि मल्टी-पार्टिकल-कोलिसन-डायनामिक्स द्वारा किया गया है।  हमने सुक्ष्म-तैराकों के द्वैत-मिश्रण को लिया, जिनका प्रणोदन समान परन्तु टेलर रेखा आकृति भिन्न थी। हमने पाया कि एक सर्वोत्तम आयाम  मौजूद है जो बड़े गुच्छों के निर्माण तथा कुशल प्रणोदन में वृद्धि करता है।

आवर्ती स्वचालित लघु-छड़ों के विरुपन के लिए, हमने बीड़ों को एल जे विभव के माध्यम से जोड़ा तथा उनका संगणक अनुरूपण अति-अवमन्दित लेंगेविन समीकरण द्वारा किया। निम्न कण घनत्व के स्तिथि में, वामावर्त तथा दक्षिणावर्त दोनों छड़ों के सामान मात्रा में लेने पर, गति को उप-प्रसारी पाया गया। जबकि दोनों छड़ों का घनत्व अधिक लेने पर गति परासरी पायी गयी। गोलीय कड़ों द्वारा समान व्हार प्रदर्शित किया गया, जो कि गति पर आकृति के प्रभाव को नकारता है।

हमने स्वचालित कड़ों के गतिकीय का विरुपन मानक विकसेक-रचना द्वारा भी किया जोकि पक्षियों के गति का ही अनुरूपण करता है। विषम माध्यम में ये विकसेक प्रतिनिधि, विभिन्न स्थानों में विविध व्यवहार प्रदर्शित करते हुए पाए गए।  हमने जटिल कोलाहल स्थानों का निरूपण भी विकसेक- प्रतिमान द्वारा किया और पाया की कोलाहल परिपूर्ण परिवेश से कोलाहल मुक्त परिवेश की ओर गमन दोनों स्थानों के सीमा पर कोलाहल दर परिवर्तन पर निर्भर करता है। निष्कर्ष रूप से विकसेक-प्रतिनिधि कोलाहल-युक्त स्थानों से प्रतिकर्षित होते हुए पाए गए। इस प्रकार यह शोध, विकसेक प्रतिनिधिओं के लिए, लघुकीय-तंत्र की प्रस्तावना, परिगमन समय के मात्रात्मक विश्लेषण द्वारा करता है।

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# Abbreviations

| | |
|---|---|
| **AM** | **A**ngular **M**omentum |
| **LM** | **L**inear **M**omentum |
| **MPCD/MPC** | **M**ulti **P**article **C**ollision **D**ynamics |
| **SPP** | **S**elf **P**ropelled **P**articles |
| **MD** | **M**olecular **D**ynamics |
| **DPD** | **D**issipative **P**article **D**ynamics |
| **SRD** | **S**tochastic **R**otation **D**ynamics |
| **COM** | **C**enter **O**f **M**ass |
| **BC** | **B**oundary **C**ondition |
| **pBC** | **p**eriodic **B**oundary **C**ondition |
| **bbBC** | **b**ounce **b**ack **B**oundary **C**ondition |
| **MSD** | **M**ean **S**quare **D**isplacement |
| **2D** | **2D**imention |