ISSUE 2 JANUARY 2021

HAPPY NEW YEAR 2021

GAṆANAM (गणनम्)

HIGH PERFORMANCE *COMPUTING* NEWSLETTER

INSTITUTE FOR PLASMA RESEARCH, INDIA

INSIDE THIS ISSUE
(2 Pages)

- Research Highlight: **Understanding a Collection of Self-propelling Particles or An Active System Using Computer Simulations!**
- HPC Article: **Securely Granting Your Working Directory Access...**
- ANTYA Updates and News
- Upcoming HPC Event: AI Bootcamp for Physics @IPR
- Other Recent Work on HPC

Understanding a Collection of Self-propelling Particles or An Active System Using Computer Simulations!

Soumen De Karmakar
Email: soumen.dekarmakar@ipr.res.in

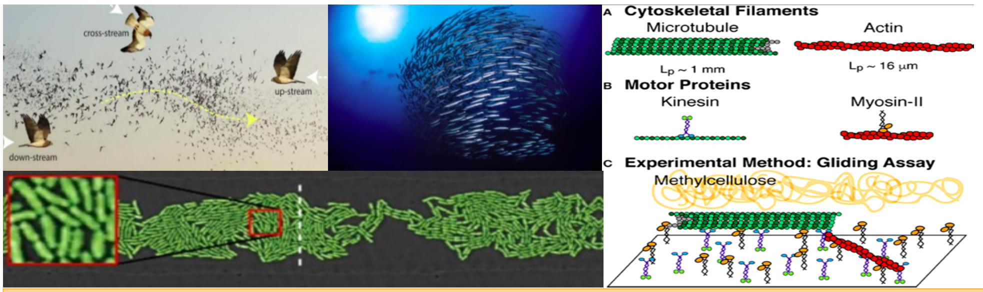


Figure 1: (Top left) A flock of birds (Top right) Collective motion of school of fish (Bottom left) Experimental image of a bacterial colony (Bottom right) Cartoon diagram of microtubules bound with motor proteins[1].

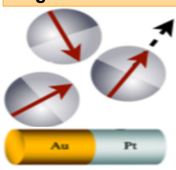


Figure 2: Janus or two faced self-propelled particle possesses different properties due to different materials present on the two opposite faces. Hence, each half of the particle respond in a different way in an external driving field or in a background solvent. As a result rotational symmetry breaks and the particle propel in a preferred direction until rotational diffusion changes the direction of propulsion. Persistent Brownian motion in a dilute limit. (Top): Cartoon of isotropic Janus particles. (Bottom): Cartoon of anisotropic or rod like Janus particle with gold and platinum coating in two halves.

All of us are familiar with a thermodynamic system, e.g. ideal gas. State variables, such as temperature, pressure, density, completely characterize a thermodynamic system and the laws of thermodynamics, relating the thermodynamic variables, can predict, to a limited extent, the future of a thermodynamic system. Likewise, laws of mechanics can explain the motion of Earth around the Sun or the motion of a car on a road. Similar laws of other branches of physics, such as quantum mechanics or hydrodynamics, can describe respective systems, to a certain extent. Many of us are fascinated by a dancing flock of birds on a nice evening just after the sunset or a beautiful collective motion of a fish school in the ocean (see Figure-1). Are there any laws that govern the motion of these systems of biological origin? Can we predict the future of such systems? Can we define thermodynamic-like variables that obey thermodynamic-like equations of state? Tremendous effort has been put in the past two decades to understand some of these questions.

Active or self-propelled systems [2,3] are the ones where each entity in the system can be thought of as a self-propelled particle i.e. they propel themselves using an internal source of energy or using energy from an external source but energy injection and dissipation happens at the individual particle level. Apart from the above mentioned two, there are numerous examples of active systems shown in Figure-1 over a vast range of scales, like microtubule propelled by motor proteins inside a cell, a group of single cell bacteria and even herds of animals, and human crowds belong to this class of non-equilibrium system. Moreover, there has been a great effort in recent past to produce artificial self-propelled particles from nanoscales to microscales to macroscales (see Figure-2) [4,5,6]. Apart from understanding some of the fundamental questions of non-equilibrium statistical physics, studying active systems could find potential applications in disease detection to targeted drug delivery [5], security, and environmental applications [6], to name a few.

Researchers have been trying to understand active systems performing experimental, numerical, and theoretical studies. Experimental studies over the vast range of scales have been shown to possess various dynamic states [7], phase transition between these states, crystallization and jamming [8], turbulent behavior [9], giant number fluctuations, motility induced phase separation [10], thermodynamic-like properties, etc. But there are clear differences between these non-equilibrium properties and their passive counterparts (in few cases when they exist). Various simple models [2,11,9] have been proposed for active systems. To understand some of the properties of active systems, our group has been working on simple numerical models of microscale active systems. Microscale active particles are also known as micromotors or microswimmers [6]. They are, generally, immersed in a background solvent, e.g. water. Typical velocities of the microswimmers are tens of micrometers per second. Hence, Reynolds number of a system of microswimmers turns out to be very low ($Re \sim 10^{-4}$ — 10^{-5}). Consequently, inertial forces or the effective accelerations can be neglected in comparison to other forces, and the microswimmers acquire a constant propulsion speed; an over-damped system. Now, there are several mechanisms through which the propulsion speed of the microswimmers can be increased by a few orders of magnitude [12,13]. If we immerse those highly motile microscopic self-propelled particles in a low viscous solvent, then the Reynolds number can become few orders of magnitude higher than that of over-damped systems. Such highly motile self-propelled particles in a low viscous solvent are also known as microflyers[12]. We can not neglect the inertial contributions of microflyers. Recently, we have performed [14] numerical simulations of an agent-based model of microflyers. Our simulation techniques are similar to the Brownian dynamics simulation with some minor changes due to the active nature of the particles. For this purpose, we have upgraded the molecular dynamics code (MPMD[15]) to a multi-GPU code, which can run on modern hybrid CPU-GPU cluster (like ANTYA at IPR). Surprisingly enough, our study demonstrates that despite its non-equilibrium nature, the system of microflyers is found to observe equilibrium like Gaussian velocity distributions. We have extracted the equilibrium-like temperature of an inherent non-equilibrium system. With the accessibility of bigger and powerful computing facilities, many unknown areas that can be studied now which are difficult to study experimentally or analytically.

> ***"In near future, we hope to perform new studies that will eventually lead to general theories or laws in this domain of interdisciplinary science"***

References:

1. *Leila Farhadi, et al., Active self-organization of actin-microtubule composite self-propelled rods, Frontiers in Physics, 6:75, 2018.*
2. *Tam´as Vicsek, et al., Novel type of phase transition in a system of self-driven particles. Phys. Rev. Lett., 75:1226–1229, Aug 1995.*
3. *Sriram Ramaswamy, The mechanics and statistics of active matter. Annual Review of Condensed Matter Physics, 1(1):323–345, 2010.*
4. *Ivo Buttinoni, et al., Dynamical clustering and phase separation in suspensions of self-propelled colloidal particles. Phys. Rev. Lett., 110:238301, 2013.*
5. *Joseph Wang and Wei Gao. Nano/microscale motors: Biomedical opportunities and challenges. ACS Nano, 6 (7):5745–5751, 2012.*
6. *Clemens Bechinger, et al., Active particles in complex and crowded environments, Rev. Mod. Phys., 88:045006,2016.*
7. *Tam´as Vicsek and Anna Zafeiris. Collective motion. Physics Reports, 517(3):71 – 140, 2012. Collective motion.*
8. *Guillaume Briand, et al., Spontaneously flowing crystal of selfpropelled particles, Phys. Rev. Lett.,120:208001, 2018.*
9. Henricus H. Wensink, et al., Meso-scale turbulence in living fluids, PNAS, 109(36):14308–14313, 2012.
10. Jeremie Palacci, et al., Living crystals of light-activated colloidal surfers. Science, 339(6122):936–940, 2013.
11. M. Cristina Marchetti, et al., Minimal model of active colloids highlights the role of mechanical interactions in controlling the emergent behavior of active matter, Current Opinion in Colloid & Interface, Science, 21:34–43, 2016.
12. Hartmut L¨owen, Inertial effects of self-propelled particles: From active brownian to active langevin motion, The Journal of Chemical Physics, 152(4):040901, 2020.
13. Kilian Dietrich, et al., Microscale marangoni surfers. Phys. Rev. Lett., 125:098001, Aug 2020.
14. Soumen De Karmakar and Rajaraman Ganesh, Phase transition and emergence of active temperature in an active Brownian system in underdamped background. Phys. Rev. E, 01:032121, Mar 2020.
15. *Harish Charan, Yukawa liquids under external forcing: A molecular dynamics study, HBNI, PhD Thesis, IPR, 2017.*

Securely Granting Your Working Directory Access to Specific Users for Collaborative Work in ANTYA

The **"HOME"** and **"SCRATCH"** directories on ANTYA are by default not shared among the users. HPC users collaborating on a project can share their working directories with selective users on ANTYA using **"setfacl"**. The setfacl utility sets Access Control Lists (ACLs) of files and directories. For further read link

Syntax

Suppose user1 (Ma'am) has the following directory structure in her scratch area:

```
[user1@login2 user1]$ ls -ltr
drwx------   3 user1 user1  4096 Dec 26   2019 359lrnln.kqt
drwx------   2 user1 user1 16384 Feb 13   2020 test
```

To allow the access (read & execute) only to test directory for student1 only, she can do it in the following two steps:

```
$ setfacl -m u:student1:rx /scratch/scratch_run/user1/
$ setfacl -m u:student1:rx /scratch/scratch_run/user1/test1/
```

To revoke the permissions:

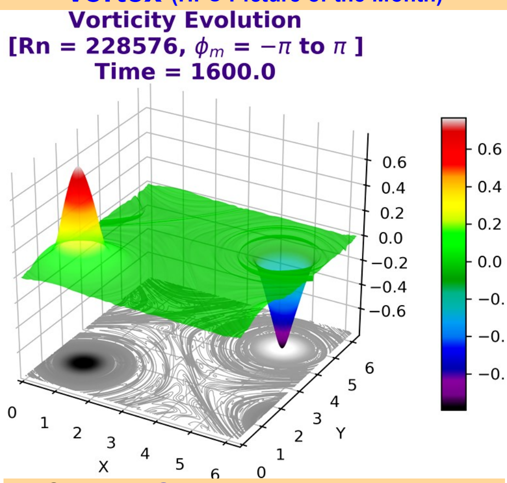
```
$ setfacl -x u:student1 /scratch/scratch_run/user1/test1/
```

ANTYA UPDATES AND NEWS

1. **New Software Installed**
   - ⇒ **CUDA 11.1.0 and 11.1.1 modules**
   - ⇒ **Tensorflow-2.3 now available in python379 module**
   - ⇒ **Python version 3.8.5 now available in python385 module**
   - ⇒ **PyEVTK/EVTK module useful for converting ASCII data file to .vtk binary format**
2. **GPU CUDA Drivers Updated**

AI Bootcamp for Physics @IPR
Registrations are Open
Registration link
Last date to register 7th Jan 2021

Kelvin-Helmholtz Unstable Strip Vortex (HPC Picture of the Month)



Pic Credit: **Mr Shishir Biswas**
Generated using in house developed incompressible hydrodynamic GPU solver **GIHD2D** with Python on ANTYA visualization node. The simulation took ~100 hours in a single P100 GPU card with a grid size of 2048x2048.

Other Recent Work on HPC

Effect of In-Plane Shear Flow on Magnetic Island Coalescence Instability	JAGANNATH MAHAPATRA

Acknowledgement

The HPC Team, Computer Division IPR, would like to thank all Contributors who helped to make this newsletter available in time. Thanks to Dr Promit Moitra for helping to write the HPC article through cartoon illustrations.

FORCEFULLY DELETE A STUCK JOB

```
$ qdel -W force JobID
```

On Demand Online Tutorial Session on HPC Environment for New Users Available

Please send your request to ***hpcteam@ipr.res.in.***

Join the HPC Users Community

hpcusers@ipr.res.in

If you wish to contribute an article in GAṆANAM, please write to us.

Contact us

HPC Team
Computer Division, IPR
Email: ***hpcteam@ipr.res.in***