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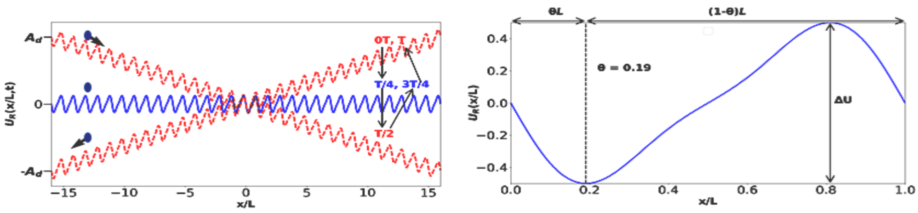
INSIDE THIS ISSUE
(3 Pages)

Is Directed Motion Possible in a Noisy System With Zero Average Force?

Anshika Chugh (PhD Student, Plasma Devices Theory and Simulation Division, IPR)
Email: anshika.chugh@ipr.res.in



(a) Diagram of time dependent Ratchet (rocking Ratchet), $U(x,t) = U_R(x) - A_d \cos(\omega t)x$. The form for Ratchet profile $U_R(x)$ is shown in (b).

(b) Ratchet profile over one spatial period is shown in blue. $U_R(x) = -(\sin(2\pi x/L) + 0.25 \sin(4\pi x/L))$. In normalised units $\Delta U = 1$.

Figure 1: Diagram of Rocking Ratchet U(x,t) and form of Ratchet profile $U_R(x)$.

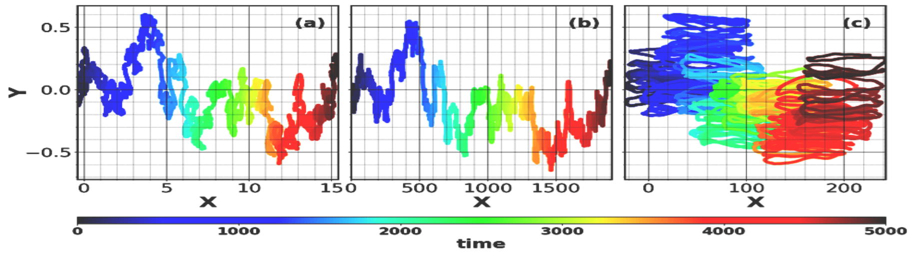


Figure 2: Time evolution of average position of system of interacting particles for three different values of amplitudes of driving strengths A_d at driving frequency $\omega = 0.2$, (a) For $A_d = 0.50$ average distance travelled in x-direction is 15L in 5000 τ_0, (b) For $A_d = 1.60$ average distance travelled in x-direction is 1900L in 5000 τ_0 , (c) For $A_d = 4.50$ average distance travelled in x-direction is 330L in 5000 τ_0.

In non-equilibrium systems, transport is a widely studied phenomenon. In a macroscopic world, a ball rolls down an inclined plane due to potential difference, heat flow occurs from hotter end of a rod to colder end of the rod due to thermal gradient, osmosis is known to occur due to concentration gradient, electric current flows due to potential difference. In these examples, forces in the form of gradients are involved to generate directed flow or motion in the system. Hence, force-free or gradient-free systems are known not to lead to directed motion at macroscopic scales. At microscales, thermal fluctuations become dominant, therefore it requires incessant input of energy to maintain gradients at such scales. The order of input energy to perform work is continually washed out by thermal fluctuations. Hence transport mechanism becomes complex. But, surprisingly, protein motors in our body can transport cargo or energy packets across microtubules in the face of inescapable thermal noise. What happens to transport at microscales? Can the same idea of transport via gradients be implemented at a microscale? Will transport be efficient? In this article, we talk about the transport mechanisms at scales as small as a living cell. Inspired by the fascinating mechanism by which protein motors move in the face of thermal noise, many physicists are working to understand these molecular motors . Among the various models proposed to explain the working of molecular motors, the Brownian motor is one such model [1]. A Brownian motor combines Brownian motion with an external asymmetric profile called ratchet to help achieve directed motion. But asymmetry alone cannot lead to directed motion until unless time-reversal symmetry is broken. In literature, asymmetric periodic forces in combination with Brownian motion are considered as an archetype for bio-engines that work on chemical synthesis and conformational changes [2].

> ***"In noisy systems, fluctuations can be rectified to obtain directed motion with zero average force using ratchet mechanism"***

We have performed 2D Langevin simulations on Yukawa particles to demonstrate the emergence of directed motion in a system dominated by fluctuations [3]. We have used an in-house developed parallelized version of MPMD (Multi-Potential Molecular Dynamics) code. The code was modified to include ratchet profile, time-periodic drive, and related diagnostics to perform measurements on the system. Figure 1 shows the ratchet profile used in this study. The simulation is carried out with 1024 particles in a 32 x 27.71 box with periodic boundary conditions along with both directions on ANTYA HPC Cluster. We used the Leapfrog integration scheme with step size 0.001 for the time integrating the equation of motion for each particle.

Yukawa system act as an interesting 'test bed' for investigating ratchet dynamics owing to its ease in tuning the interaction radius via screening length and its experimental viability through dusty plasma experiments. We use a time-periodic drive to take the system out of equilibrium which in combination with thermal fluctuations help break time-reversal symmetry. The beauty of this study is that directed motion can be achieved even if all the external forces involved has zero spatial-temporal average. Fig. 2 shows the time evolution of the average position of the system defined through average over a number of interacting particles for three different values of the amplitude of driving Ad at driving frequency ω = 0 .2. One advantage of performing molecular dynamics simulation is that information about particles' positions and velocities can be known from the first principles and dynamics of the system can be extracted at both local and global scales. However, this information comes at the price of storing a large amount of data. In Figure 2, local information of the particles' average position can be seen in the form of oscillations which are large for the large amplitude of the periodic drive, while on a global time scale i.e. throughout total simulation time, forward motion is observed. The simulation data has been obtained using 32 cores with a run time of 13 hours. The above plot has been generated using 500000 data points amounting to 17 Mb of data.

We conclude that it is possible to achieve directed motion in the absence of any net force in the system with the help of a ratchet mechanism. This detailed published results are available in [3].

References:

1. *R.D. Astumian, P. Hänggi, Brownian motors, Phys. Today 55 (11) (2002) 33–39.*
2. *P. Hänggi, Fabio Marchesoni, and Franco Nori, Brownian motors, Ann. Phys. (Leipzig) 14, No. 1 – 3, 51 – 70 (2005).*
3. *Anshika Chugh and Rajaraman Ganesh, Emergence of directed motion in a 2D system of Yukawa particles on 1D Ratchet, Physica A 593 (2022) 126913.*

Running MATLAB Programs on ANTYA

Part-3: Access/Run MATLAB via Your Local Web Browser

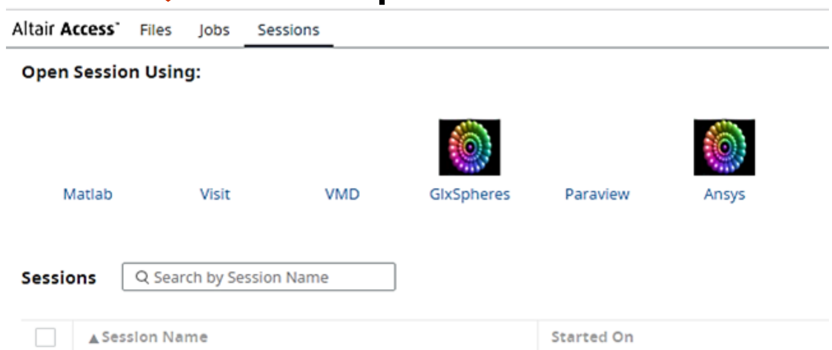
For users not so much familiar with the Linux terminal command line and feel there are just too many things to learn before doing anything with MATLAB on ANTYA HPC cluster, then this part-3 of the MATLAB article shows the simplest way to use MATLAB through a web interface. MATLAB users need to have an HPC account in ANTYA and the same details are required on the login page of the web interface (Altair Access). This part-3 of the MATLAB series will demonstrate through snapshots how MATLAB can be accessed on ANTYA through a web interface. First open the URL in your local browser, provide your login credentials. To open a MATLAB session, click on "Sessions" Tab and then click on "Matlab". This will submit a job on the visualization node of ANTYA.

Web Interface URL: https://10.20.39.6:4443/pbsworks/login

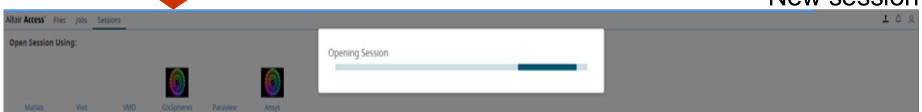
Enter your ANTYA **Username** and **password**

In Sessions Tab, click on "**Matlab**" which will submit a job and open a new session.

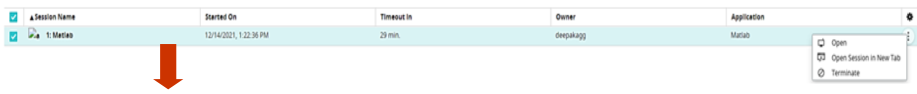
Note: There are no active sessions here

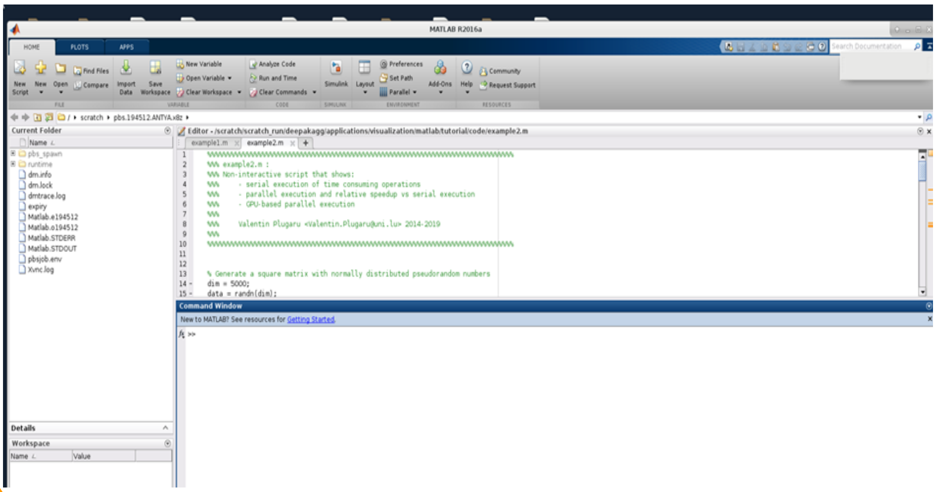


New session



Click on triple dots under Session Name "…" and click on "**Open Session in New Tab**"





ANTYA UPDATES AND NEWS

1. New Packages/Applications Installed

⇒ **Upgraded NAG Compiler and NAG Library**

The latest available versions are available with **modules:**
NAG/nag-compiler_71
NAG/nag-intel32-library_27

⇒ **DMTCP (Distributed Multi-Threaded Checkpointing) Tool**

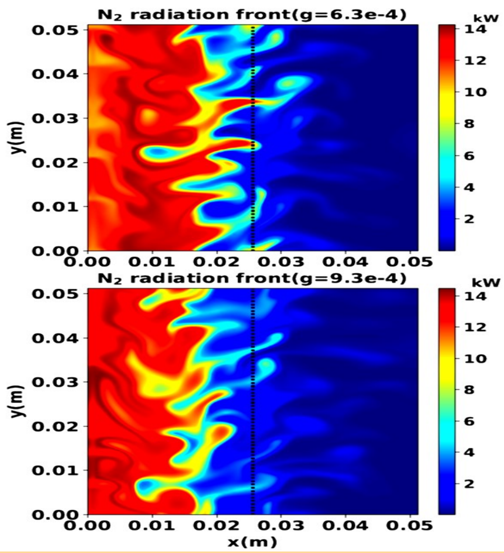
This is a checkpoint/restart tool for applications. The tool is available as module with name **dmtcp**.

⇒ **OpenFOAM new module**

OpenFoam 'plus' version, exclusively made for developers available as module with name **OpenFOAM-plus**

HPC PICTURE OF THE MONTH

Effect of Turbulence on Impurity Transport in Boundary Region of a Tokamak



Pic Credit: **Shrish Raj**

The figure shows an induced inward shift of the radiation cooling front with an increase in magnetic curvature induced effective gravity obtained with non-linear 2D BOUT++ simulation of plasma-impurity interaction in the tokamak boundary for nitrogen gas seeding conditions. The vertical dotted line indicates the edge-to-SOL transition.

Data is obtained from BOUT++ code simulations on ANTYA and plotted with Python scripts.

TIP OF THE MONTH

Did you know that PGI Compilers suite was rebranded and packaged as part of the NVIDIA HPC SDK (See issue12, page#3)?

pgcc => nvc
pgc++ => nvc++
pgfortran and pgf90 => nvfortran

Converting Dos Files To Linux Compatible Files on ANTYA:

Running Script Files Created on Windows Machine in a Linux Shell on ANTYA

This article covers the issue faced while running a bash script on ANTYA that has either been written or modified in a text editor on an MS Windows machine and how such an issue can be resolved.

Demonstration of the Issue and Resolution on ANTYA

Suppose you have created/modified a simple bash script for printing the hostname of the machine in an MS Windows system. The script, hostname.sh looks like the following (it has a blank line#2 introduced in the Windows editor):

```
#!/bin/bash

echo $HOSTNAME
```

> ***"In ANTYA, if you get obscure errors like***
> ***$'\r': command not found***
> ***when running a script, most likely it is related to Windows file formatting"***

 # Transfer this script to ANTYA and then run it which will give an unknown error about command not found.

```
[user@login1 ~]$ bash hostname.sh
hostname.sh: line 2: $'\r': command not found
login1
```

 # There is Linux tool called dos2unix which is available by default on ANTYA to convert the files edited in Windows machine to Linux compatible format. Run this tool on the hostname.sh file.

```
[user@login1 ~]$ dos2unix hostname.sh
dos2unix: converting file hostname.sh to Unix format ...
```

 # Now run the same script again which should give the correct output without any error.

```
[user@login1 ~]$ bash hostname.sh
login1
```

What dos2unix did?: There are different conventions about text files formats in Windows and Linux environments. Editing in Windows, when you "ENTER" to introduce a newline, it comprises two symbols **"\r\n"** to mark the end of a line whereas Linux systems use just a **"\n"** to mark the end of a line. **dos2unix** removes extra "\r" from Windows edited scripts and make them compatible to run on Linux.

Other Recent Work on HPC (Available in IPR Library)

Study of magnetized multi-component plasma sheath containing charged dust particle in presence of oblique magnetic field: A fluid approach	AKSHAYA KUMAR SHAW
Square lattice formation in a mono-dispersive complex plasma	SWARNIMA SINGH
Long time fate of 2D incompressible High Reynolds number Navier-Stokes turbulence: a relook!	SHISHIR BISWAS
The Quasi-localized charge approximation (QLCA) approach for the nonlinear structures in strongly coupled Yukawa systems	PRINCE KUMAR
RCS reduction of Microstrip antenna using Ku-band Perfect Polarization Convertor Metasurface	PRIYANKA TIWARI
Tritium-Titanium target degradation due to deuterium irradiation for DT neutron production	MAYANK RAJPUT
A criterion to aid direct tracking of plasma blobs in a tokamak	NIRMAL K. BISAI
Artificial Intelligence tool for Cancer Detection	AGRAJ ABHISHEK
Water Droplet Motion Dynamics on Linear Wettability Graded Surface for Microgravity Applications	VISHAKHA BAGHEL
Study of Electrode Biasing in the Edge and SOL regions of a Tokamak	VIJAY SHANKAR

ANTYA HPC USERS' STATISTICS— FEBRUARY

- **Total Successful Jobs — 3848**
- **Top Users (Cumulative Resources):**
  - CPU Cores — Vikram Dharodi
  - GPU Cards — Swapnali Khamaru
  - Walltime — Shishir Biswas
  - Jobs — Shrish Raj

Acknowledgement

The HPC Team, Computer Division IPR, would like to thank all Contributors for the current issue of *GAṆANAM*.

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

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

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