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Subcritical Turbulence in 3D Yukawa Liquids

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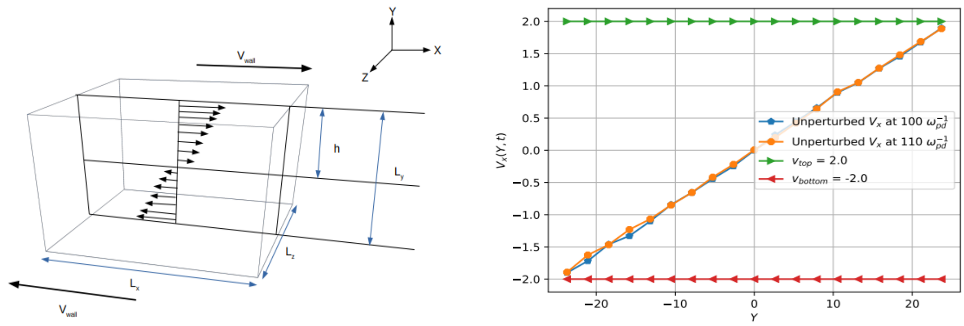


FIG. 1: Demonstration of plane Couette flow (a) Apparatus to create PCF. Lx, Lz is periodic and Ly is bounded. Vwall = 2.0. "h" is the half-channel height (b) From bottom to top along ˆy, the stream-wise fluid velocity Vx varies linearly. As the walls at top and bottom is moving opposite to each other, a linear velocity profile is the most stable state of the system.

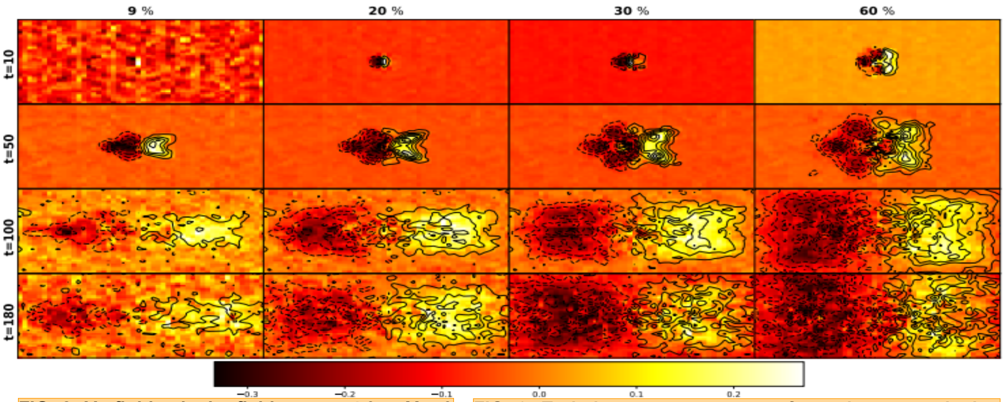
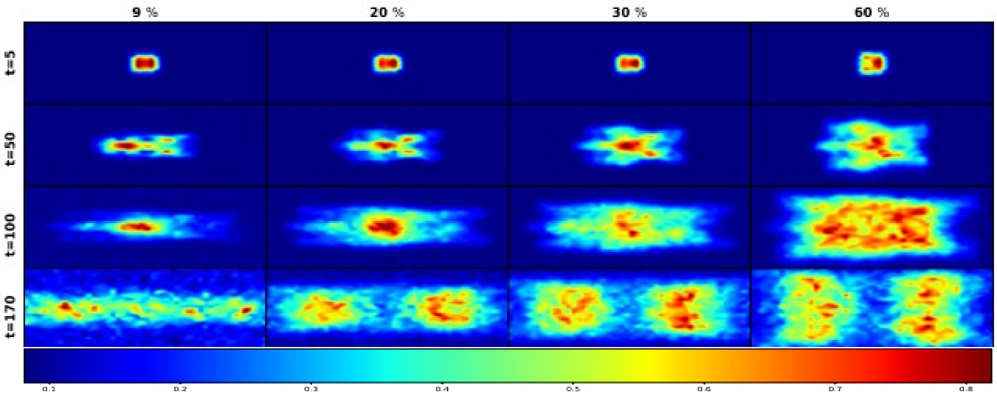


FIG. 2: Vx fluid velocity fields at κ = 4.0 at Y = 0 plane. The horizontal direction is X and the vertical direction is Z. (Above)

FIG. 3: Turbulent energy contours for various perturbation strengths are shown in XZ plane. The turbulent energy maximizes with the increasing perturbation strength (Below)



In nature, we observe non-equilibrium systems in abundance. All living biological systems, Turbulent heat convection in earth's outer core and solar outer core, cosmic dust in between stars, Earth's outer atmosphere, oceans etc. are all examples of non-equilibrium systems. In such systems, pattern formation occurs, e.g., granular structures in solar surface, patterns in sand dunes, patterns on the surface of fish, leave pattern (as a result of fractal law), pattern formation in turbulent flows, etc. Out of all the above pattern forming examples, we shall discuss about the pattern formation in turbulent Plane Couette flow (PCF).

Fig.1 demonstrates PCF formation[1], which occurs in nature and also get produced in laboratory experiments. PCF is one of the simplest examples of wall-bounded shear flow, which is linearly stable at all the values of Reynolds number. Kelvin-Helmholtz instability (KH) [2], Rayleigh-Taylor instability (RT)[3], occurs in linearly unstable flows. These instabilities occur when the flow Reynolds number increases. However, flows like Plane Couette flow, Plane Poiseuille Flow in pipe (PPF) , counter-rotating Taylor Couette Flow (TCF) are linearly stable. How do such linearly stable flow become turbulent? There is only one way to make such flow turbulent is to apply a finite amplitude non-linear perturbations. Upon applying non-linear perturbations, the flow becomes turbulent and as a result of turbulence, turbulent spot in observed in PCF [1,4], PPF [4] and TCF [5].

The transition to turbulence which occur due to KH, RT instabilities are known as supercritical transition to turbulence, which occurs slowly and steadily upon increasing the Reynolds number of the flow. However, in subcritical transition to turbulence, there is an abrupt transition to turbulence upon increasing the non-linear perturbation strength. Subcritical turbulence occurs with the co-existence of laminar and turbulent flows. The laminar turbulent boundary is often oblique and spot formation occurs when the flow is turbulent.

In the past, numerical and experimental work have been performed to study subcritical transition to turbulence in PCF. However, in particle level and in Yukawa liquids, there is no study available to the best of our knowledge [1]. Therefore, to study subcritical turbulence and pattern formation at particle level, we have considered PCF in a 3D Yukawa liquid. We have used MD simulation as a tool to perform simulations at the particle level. The code that we use to perform the MD simulations is MPMD-3D [1], which is an in-house developed MD code. This code is available in both CPU (MPI) and GPU (openACC + MPI) versions. To perform the simulation, we have used 1000 CPU cores for the CPU version and 4 GPU cards for the GPU version in the ANTYA cluster. With ~ 0.614 million particles, the walltime for both the versions are 13, 19 hours respectively.

The Fig.1a shows the apparatus we use to simulate the system and Fig.1b shows the PCF profile. We use Lundbladh like [1] non-linear 3D perturbations to make the flow turbulent. The dust particles considered in the simulations are interacting via Yukawa potential. Fig.2 shows the turbulent spot formation as a result of subcritical transition to turbulence. In Fig.2, we can observe that for 9% perturbation strength, the turbulent spot dies very early or there is no turbulent structure at all. When we increase the perturbation strength, then we can observe the turbulent patches in Vx velocity contour plots. The turbulent patches 2 spreads with time because of the presence of large-scale flow in the system[1]. Fig.2 shows the process of subcritical transition to turbulence, where the flow is linearly stable but unstable to finite-amplitude non-linear perturbations .

For the first time, possibility of subcritical turbulence in a plane Couette flow in 3D Yukawa liquids is demonstrated using Molecular Dynamics

We can understand the subcritical nature of turbulence with the help of Fig.3. In Fig.3, turbulent energy contours are shown [1]. For 9% perturbation strength, the turbulent energy dissipates very fast and the flow becomes laminar up to time t = 170ω_{pd}^{-1}.

However, for increasing perturbation strength, the turbulent energy contours are distinctively observed and for the 60% perturbation strength the turbulent energy occupies the maximum area of XZ plane as compared to the rest of the cases. The nature of sub criticality is also reflected here.

More discussions regarding the sub critically of PCF can be fetched from the article in Ref.[1]. Turbulent spots as discussed here is observed in boundary layer flows[4], turbo-machinery in Jet engines[4], channel flows (PCF, PPF)[4] and pipe flows (PPF) [4], etc. Therefore, to have more understanding about the geophysical, astrophysical flows, to increase the efficiency of Jet engines, we need to perform a deep study about the turbulent spot formation

References:

1. *S Kalita, R Ganesh, Physics of Fluids 33, 095118 (2021)*
2. *A Joy, et al, Phys. Rev. Lett. 104, 215003 - Published 27 May 2010*
3. *H Charan, et al, Journal of Plasma Physics , Volume 80 , Issue 6 , December 2014*
4. *X Wu, Annu. Rev. Fluid Mech, 2023*
5. *A Prigent, (FMIA, volume 77)*

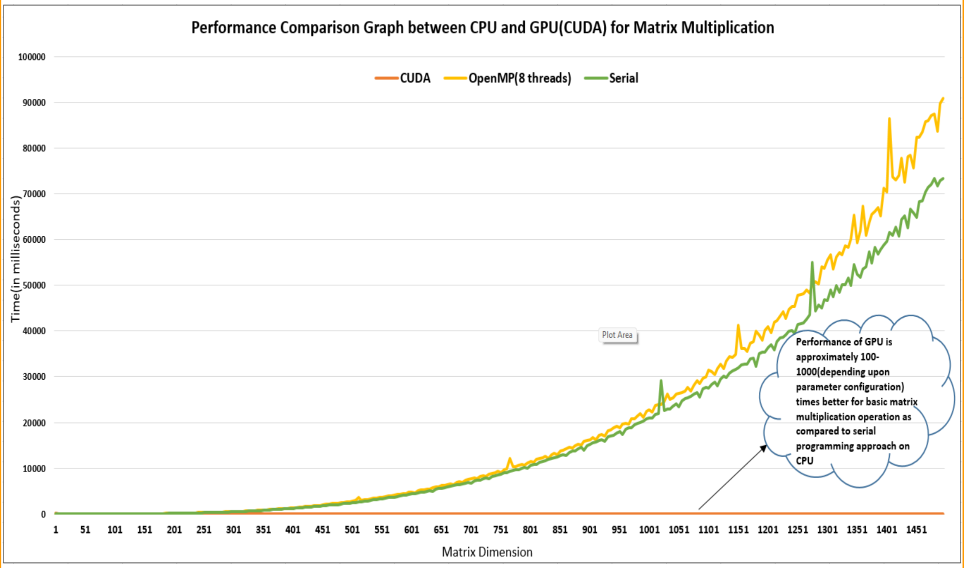
Optimizing GPU Workload with CUDA: A case study in Parallel Computing

Image source: Tejaswi Agarwal, Introducing NVIDIA's Compute Unified Device Architecture (CUDA), 2013. **Accessed via** https://www.opensourceforu.com/2013/12/introducing-nvidias-compute-unified-device-architecture-cuda/

CUDA, developed by NVIDIA, plays a pivotal role in leveraging parallelism, particularly in high-performance computing tasks. It capitalizes on the parallel processing capabilities embedded in Graphics Processing Units (GPUs). Unlike traditional single-threaded processing executed by a Central Processing Unit (CPU), CUDA enables the simultaneous execution of numerous parallel threads on a GPU. This parallelization is particularly advantageous for computationally intensive applications such as scientific simulations, data analytics, and machine learning. By distributing the workload across a multitude of GPU cores, CUDA significantly accelerates the execution of tasks, offering a scalable solution to the ever-growing demands of modern computing.

In practical applications, CUDA has proven indispensable in fields such as fluid dynamics simulations, where it significantly expedites the computation of complex fluid behaviors. This acceleration is particularly crucial in industries like aerospace, facilitating the rapid analysis of airflow patterns around aircraft for more efficient design. Additionally, in genomics, CUDA plays a pivotal role in expediting the analysis of vast datasets, notably in DNA sequencing algorithms. This accelerates the identification of genetic variations, advancing research in mapping the human genome and contributing to personalized medicine. Essentially, CUDA operates as a high-performance engine for parallel processing tasks, offering scalable solutions to the evolving demands of modern computing. NVIDIA's pioneering role in advancing parallel processing and high-performance computing is underscored by CUDA's tangible impact in these real-world applications, driving advancements in scientific research and technological innovation

In the conducted comparison study, we explored the performance disparity between traditional parallel programs executed on a Central Processing Unit (CPU) and parallel programming utilizing Graphics Processing Units (GPU) with **CUDA**. The focus of the study was a fundamental mathematical operation, matrix multiplication, executed across a range of matrix sizes from 1 to 1500 (Jobs related to larger matrix dimensions i.e. 4096 are running, will update it as soon as it is available). The associated code for this study can be found [here](). The matrix multiplication operation, being computationally intensive, serves as an ideal benchmark for evaluating the parallel processing capabilities of both architectures.



The results, visually represented in the plotted graph, underscore the considerable acceleration achieved by the GPU-based CUDA approach compared to traditional CPU parallelism. As the matrix size increased, the performance advantage of GPU-based parallel programming became more pronounced. This study demonstrates the superior parallel processing capabilities of GPUs using CUDA, making it a compelling choice for accelerating mathematical operations and handling large datasets efficiently.

GPU Accelerated Libraries will be covered in future articles.

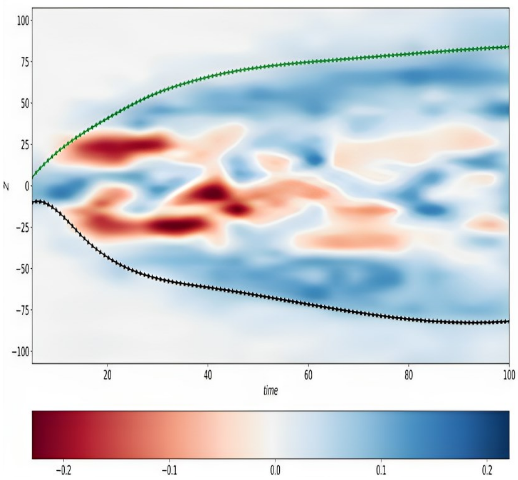
ANTYA UPDATES AND NEWS

1. New Packages/Applications Installed

=> LIGGGHTS 3.8
module load LIGGGHTS/LIGGGHTS-3.8

=> OpenFOAM 5.X
module load OpenFOAM-5.X

HPC PICTURE OF THE MONTH



Pic Credit: **Suruj Kalita**

Title: Spatio-temporal diagram in turbulent plane Couette flow

Description: The above figure shows the spatio-temporal diagram of a turbulent spot that forms in turbulent Plane Couette flow (PCF) [1]. In other words, the above figure shows the turbulence spreading. As there is a presence of large-scale flow in turbulent PCF, the turbulence spreads spatially. A co-existence of laminar and turbulent regions is also observed in this diagram. The regions outside the dotted lines are laminar and inside the dotted lines are turbulent, as we can observe turbulent fluctuation inside the dotted lines. Laminar and turbulent regions co-exists in subcriticaly turbulent PCF and the spatio-temporal diagram is consitant with this argument.

[1] S Kalita, R Ganesh, Physics of Fluids 33, 095118 (2021).

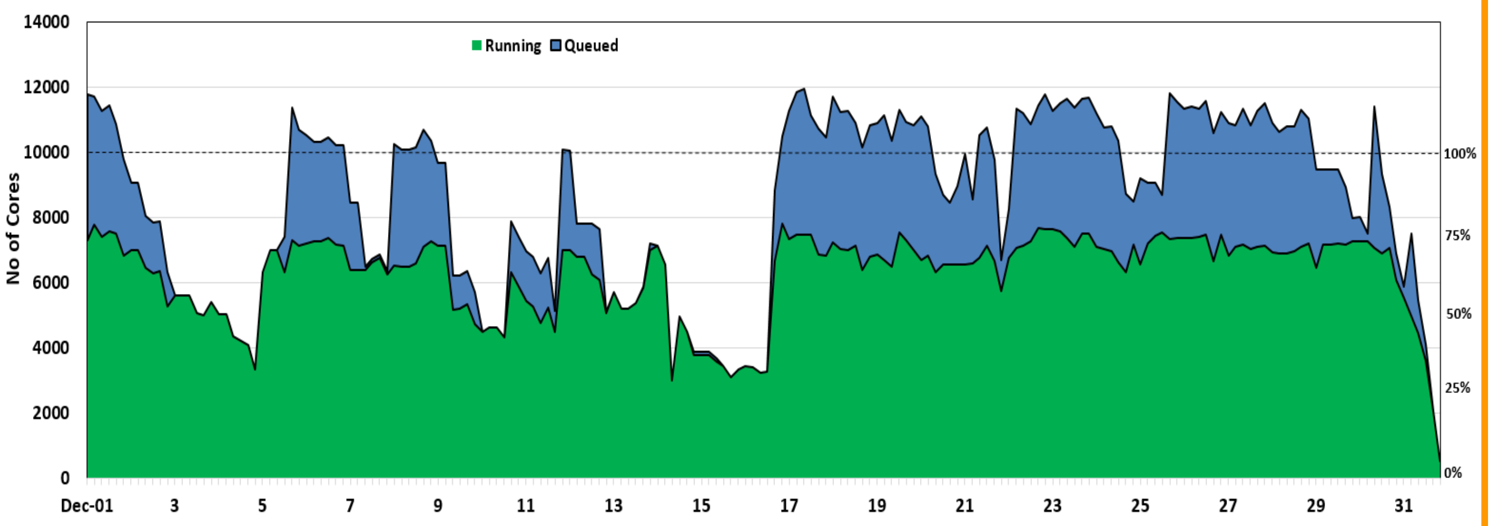
TIP OF THE MONTH

To put hold on running job for executing some higher priority job, a command called 'qhold' is used which puts job in held state in execution queue and resource assigned to jobs are released. To remove hold on job, there is command called 'qrls'.

```
[user@login1 ~]$ qhold 298760.ANTYA
# to release job from held state
[user@login1 ~]$ qrls 298760.ANTYA
```

ANTYA Utilization: DECEMBER 2023

ANTYA Daily Observed Workload



Other Recent Work on HPC (Available in IPR Library)

Disruption prediction on ADITYA/ADITYA-U using future sequence based time series neural network	**Rameshkumar Babubhai Joshi**
Generation of S-polarized Terahertz Radiation From Laser-Plasma Interactions	**Anjana K. P.**
Plasma boundary simulations of limiter ramp-up phase of ITER	**Arzoo Malwal**

ANTYA HPC USERS' STATISTICS— DECEMBER 2023

- **Total Successful Jobs~ 1834**
- **Top Users** (Cumulative Resources)
  - **CPU Cores** — **Amit Singh**
  - **GPU Cards** — **Shishir Biswas**
  - **Walltime** — **Vinod Saini**
  - **Jobs** — **Arzoo Malwal**

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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