ISSUE 12 NOVEMBER 2021

GAṆANAM (गणनम्)

HIGH PERFORMANCE *COMPUTING* NEWSLETTER

INSTITUTE FOR PLASMA RESEARCH, INDIA

INSIDE THIS ISSUE (3 Pages)

Turbulent Spots in a 3D Complex Plasma

Suruj Kalita (PhD Student, Plasma Devices Theory and Simulation Division, IPR)
Email: suruj.kalita@ipr.res.in

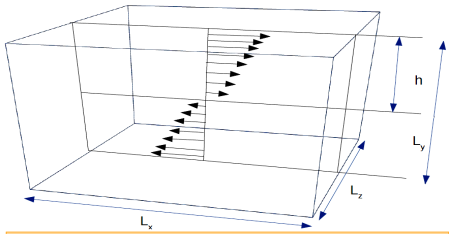


Figure 1 (a): (PCF) x and z directions are periodic while y is bounded, with L_x, L_z and L_y as respective lengths. V_{wall}=2.0, "h" is the half-channel height (L_y/2). The momentum from the walls is transferred to the particles, due to the presence of viscosity in the system. After achieving a steady state, the fluid flow (from macroscopic viewpoint) inside the system, takes the form of a PCF, as shown by the arrows in the diagram.

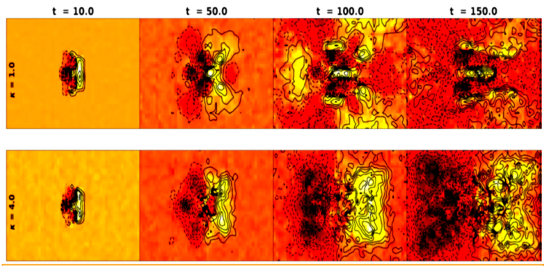


Figure 2: V_x fluid velocity fields at K = 1.0, 4.0 at Y = 0 plane. The horizontal direction is X and the vertical direction is Z.

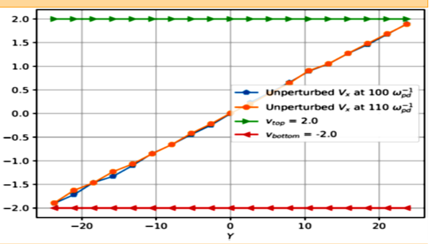


Figure 1 (b): From bottom to top along y, the stream-wise fluid velocity V_x, obtained from MD data, varies linearly. As the walls at top and bottom are moving opposite to each other, a linear velocity profile emerges, which is found to be linearly stable for all values of Re.

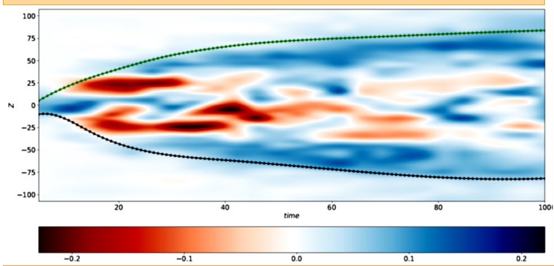


Figure 3: It shows the co-existence of laminar-turbulent regions in Z-t plane. The blue and red regions are non-zero and white regions are zero V_x fluid velocity regions. The non-zero regions are turbulent while the zero regions are laminar. As there is no base flow along ˆz direction, the velocity fluctuations shown in this figure are mainly due to the turbulence induced in the system.

Turbulence is an unsolved problem. Turbulence is commonly found in everyday phenomena such as blood flows in arteries, wind flow past a jet engine, fluid flow in boat wakes, atmosphere and ocean currents, and more. In the hydrodynamic context, we have two different classes of turbulence: "supercritical" and "subcritical". An equilibrium flow becoming unstable and leading to turbulence, slowly and progressively, due to an infinitesimal perturbation, provided the Reynolds number (Re) of the system is above a critical value Re_c, is termed as "supercritical transition" to turbulence. Some well-known examples of this class are turbulence generated due to Kelvin-Helmholtz instability, which occurs when there is a velocity difference across an interface between two fluids; ion temperature gradient driven instability leading to plasma turbulence; turbulence generated due to inertially driven Von Kármán flow; etc. On the other hand, "subcritical transition" to turbulence occurs very abruptly, in sharp contrast to a supercritical transition, which occurs gradually. Moreover "subcritical transition" displays the co-existence of laminar and turbulent regions. Some of the hydrodynamic flows, which show "subcritical transition" to turbulence are: Plane Couette flow (PCF) [1], Taylor-Couette flow (TCF) in between counter-rotating cylinders, rapidly rotating Rayleigh-Bénard convection cells, doubly periodic Kolmogorov flow, etc. Amongst the above, PCF is the most studied, as it is the easiest to create by simply moving the top and bottom walls in a laboratory as shown in Fig.1(a). The base flow of PCF (Fig.1b) is known to be linearly stable at all Reynolds numbers. Therefore, a finite-amplitude non-linear perturbation is required to make the flow unstable. We have chosen Yukawa liquids as a prototype to study the PCF, for a 3D Complex plasma. A Yukawa liquid mainly consists of negatively charged dust grains, often realizable in a complex plasma system. In this work, we have addressed the following questions: does the interaction range in a Yukawa liquid play a vital role in the turbulent dynamics of PCF ?, Can the turbulent dynamics be studied with a laminar initial state prepared at an empirically high initial Reynolds number?, is it possible to perform a quench study without changing Ly and wall speed Vwall, etc.?

> ***"A unique and novel feature of our study is that we can address the effect of changing Reynolds number on the turbulent spot dynamics, without altering the flow scale or its amplitude using our in-house developed MPMD-3D code which scales reasonably well on CPU and GPU."***

To investigate such problems at the particle level, we have chosen "Molecular-Dynamics (MD)" as our computational technique. The code that we use is MPMD-3D, which is an in-house developed 3D MD code. For this work, an existing 2D MD code developed in-house has been generalized to 3D. 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 computational walltime for both the versions are 13, 19 hours respectively.

When a finite amplitude non-linear perturbation [2] is applied to the plane Couette equilibrium (linear velocity profile from bottom to top along the bounded direction (see in Fig.1b)), the system becomes unstable and makes a transition to turbulence as a result of the applied perturbation. In Fig.2, we see velocity patches are growing within the laminar regions in XZ plane at Y = 0. Such velocity patches are termed as the turbulent spots. Formation of such turbulent spot is a signature of the occurrence of a subcritical transition in the system. Moreover, the co-existence of laminar and turbulent regimes, observed in Fig.3, [3] also indicates that the transition in the system is subcritical. We have started with a laminar initial state with a high Reynolds number chosen empirically and then performed a quench study. We can see in Fig.2 that the spot structure spreads spatially with time, while its intensity is found to reduce. This is because of the generation of turbulent large scales in our system. The nature of turbulent spot in a PCF depends particularly on the range of interaction in Yukawa liquids. When the range of interaction is increased by reducing the value of K to 1.0, we see a change in the spot structure. Such structures have been observed in the hydrodynamic studies of turbulent PCF. Therefore, we can conclude that the higher the range of interaction, the more the results will qualitatively tend to the hydrodynamic limit. One of the probable reasons behind this is that in hydrodynamics, the range of interaction between the fluid elements are infinite. So, the more we increase the range interaction, the more we tend towards the scale-free hydrodynamic limit. The above published work can be accessed in [1].

References:

1. *S. Kalita and R. Ganesh, Physics of Fluids 33, 095118 (2021), https://doi.org/10.1063/5.0060089.*
2. *A. Lundbladh and A. V. Johansson, Journal of Fluid Mechanics 229, 499 (1991).*
3. *M. Couliou and R. Monchaux, Journal of Fluid Mechanics 819, 1 (2017).*

Python Package Management Using Conda — Part-5
Making Conda Environments Visible in Jupyter Notebook

Working in multiple Conda environments allows us to have project-specific packages without having any conflict for different versions as the environments are isolated. Since at a time, only one of the Conda environments will be activated, the Jupyter Notebook launched will show only the kernel of the activated environment. This means that for accessing the packages from different environments, one has to run Jupyter Notebook from each environment separately. With the no. of steps involved in making Jupyter Notebook run on the local machine browser from ANTYA (refer to issue 3 on how to run Jupyter Notebook in local Browser, *https://www.ipr.res.in/ANTYA/Gananam_HPCNewsletter_IPR_Issue3_Feb2021.pdf*), it is certainly not the best approach. In this part-5 of the Conda series, we will cover how you can make all your Conda environments kernels visible in a single Jupyter Notebook.

How to Implement in ANTYA?

Suppose you have created 6 different Conda environments in your home. At a time, you are using, let us say "conda-hpc-python-course" environment. We will see how you can ensure all the other environments in the Jupyter Notebook launched from your say "conda-hpc-python-course" environment.

 # Activate one of the Conda environment.

```
[user@login1 ~]$ conda activate conda-hpc-python-course
(conda-hpc-python-course) [user@login1 ~]$
```

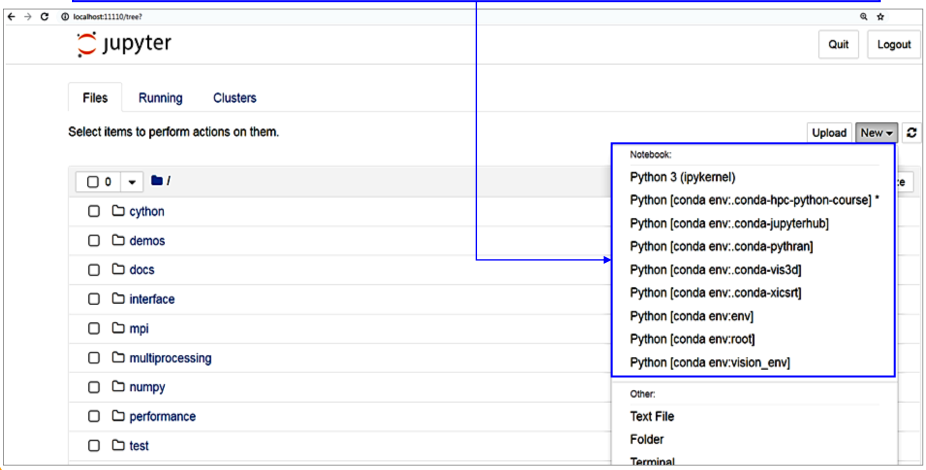
 # Install the nb_conda_kernels package in the environment.

```
(conda-hpc-python-course)[user1@login1 ~]$ conda install nb_conda_kernels
```

 # After installing the package, launch the Jupyter Notebook from ANTYA and access it on your local machine.

```
(conda-hpc-python-course)[user@login1 ~]$ jupyter notebook --no-browser
```

After Enabling Kernels, All the Conda Environments are Visible.



ANTYA UPDATES AND NEWS

1. New Packages/Applications Installed

⇒ **Updated NVIDIA HPC SDK modules with CUDA**

A separate article on how to use is on the next page.

⇒ **FFTW2 module**

The module file of fftw2/openmpi/gcc/64/double/2.1.5 module is corrected and now available for use.

2. NVIDIA GPU Drivers Upgraded

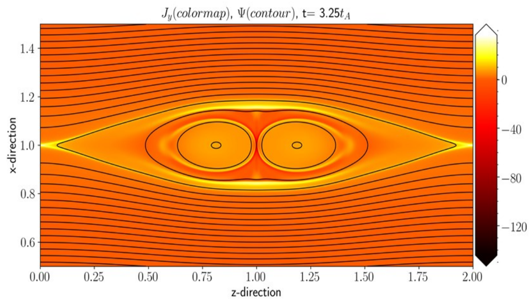
Version 460.32.03 on 50% GPU nodes which can now support CUDA11.2 toolkit.

3. GPU Bootcamp Material

The container image(nways_C_F.simg) used for the demonstration is available at /home/application/singularity_images/singularity_3.4.1

For running the image use module **singularity/3.4.1/3.4.1**

X-type Magnetic Reconnection in Hall MHD
(HPC Picture of the Month)



Pic Credit: **Jagannath Mahapatra**

X-type magnetic reconnection at the reconnecting current sheet (x=1, z=1 location) due to finite Hall effect during the coalescence of two magnetic islands (Jy: out of plane current density, and Ψ: out of plain vector potential). Simulation is performed by solving the incompressible Hall-MHD equations using BOUT++ framework on a 2048*4096 grid over 1024 CPU cores (simulation time~42 hrs). The image was generated in Python (Matplotlib) with data obtained from simulation run.

TO UNLOAD ALL LOADED MODULES IN YOUR PATH

```
$ module purge
```

NVIDIA HPC Software Development Kit (SDK) For GPU

HPC SDK Suite includes CUDA compilers, PGI compilers (OpenACC), optimized GPU libraries, profilers, debuggers along with MPI and OpenMP all in one single package. The old PGI compiler names still work too in the HPC SDK as well and are called nvfortran, nvc, and nvc++.

> ***"The PGI compilers have been rebranded into HPC SDK toolkit and no separate modules of PGI are further required for OpenACC. Similarly, separate CUDA toolkit modules are also not needed when using the HPC SDK module on ANTYA for GPU programming."***

You do not have to change the compilers names of PGI (pgfortran, pgf90, pgf95, pgcc, pgc++) as they have redirected to HPC SDK compilers by default. The name of the *HPC SDK* module installed on ANTYA is ***nvhpc***. We currently have version 21.7 which supports CUDA versions 10.2, 11.0 and 11.4, available as independent modules. For example, if you need OpenACC compilers with CUDA 10.2 compatibility, load the module *nvhpc/cuda10.2/21.7*.

```
[user@login1 ~]$ module avail nvhpc
nvhpc-byo-compiler/21.7  nvhpc-nompi/21.7  nvhpc/21.7  nvhpc/
cuda10.2/21.7  nvhpc/cuda11.0/21.7  nvhpc/cuda11.4/21.7
```

ANTYA HPC USERS' STATISTICS— OCTOBER

- **Total Successful Jobs — 5251**
- **Top Users (Cumulative Resources):**

⇒ **CPU Cores — Swarnima Singh**

⇒ **GPU Cards — Suruj Kalita**

⇒ **Walltime — Mywish Anand**

⇒ **Jobs — Mywish Anand**

Other Recent Work on HPC (Available in IPR Library)

RF design of power level 2.5 MW compatible transmission line components	AKHIL JHA
Hydrodynamic Matrix and Density Autocorrelation Function for Strongly Coupled Charged Fluids in Generalized Hydrodynamic Framework	ANKIT DHAKA
Laser-cluster interaction in a static magnetic field without dipole approximation	KALYANI SWAIN
ICRF Antenna Research For Tokamaks: Path From A Simplistic To Complex Approach	KISHORE KANTI MISHRA
An Artificial Intelligence based Solution for SST 1 Tokamak building monitoring	AGRAJ ABHISHEK
Effect of the Geometrical Configuration of Flexible Cryostat on the Hydraulic Characteristic of Cryogenic Ghe towards High-Temperature Superconducting Applications	MAHESH M GHATE
Electromagnetic wave transparency induced in a strongly magnetized plasma	DEVSHREE MANDAL
Observation of E x B electron drift instability in Hall-Thruster simulation	SNEHA GUPTA
Implementation of three-dimensional simulations for scrape-off layer transport in inboard limited Aditya-Upgrade plasma configuration	ARZOO MALWAL
Excitation of lower hybrid and magneto-sonic perturbations by laser in X-mode configuration of magnetized plasma	AYUSHI VASHISTHA
Kelvin-Helmholtz Instability in Two Dimensional Semi-bounded Active Yukawa Liquids	SOUMEN DE KARMAKAR
Quasi-longitudinal propagation of nonlinear electromagnetic excitations in magnetized plasma	GAYATRI B BARSAGADE
Multi-GPU Acceleration of Three Dimensional Pseudo-Spectral Magnetohydrodynamic Code for Large Scale Plasma Simulation: G-MHD3D	SHISHIR BISWAS
A Novel Method for the Measurement of the N|| Spectrum and RF Characterisation of the PAM Launcher for ADITYA -U Tokamak	PROMOD KUMAR SHARMA
Mechanical Design of Prototype Center Stack (PCS) for Spherical Tokamak Based Technologies Development	ADITYA KUMAR VERMA
Overview of the Recent Investigations on the Surrogate-Particle-Irradiation in Tungsten Plasma-Facing-Materials	MAYA P.N.
Eliminating flux contributed by external currents and eddy current from magnetic probe measurement in SST-1 discharges	SAMEER KUMAR
Modelling of Tritium-Titanium target degradation for the DT neutron production	MAYANK RAJPUT
Ab-Initio selection of transition metal species for incorporation in ZSM-5 zeolite framework to improve dihydrogen binding for nuclear fusion applications	GAYATHRI V DEVI
Liquid metal MHD flow analysis in presence of a physical obstruction in a rectangular flow path	ANITA PATEL
Web Editor for Configuration Management of Laboratory Plasma Experiments	RITESH SUGANDHI

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.***

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***