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GAṆANAM (गणनम्)

HIGH PERFORMANCE *COMPUTING* NEWSLETTER
INSTITUTE FOR PLASMA RESEARCH, INDIA

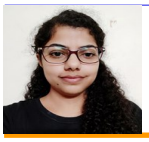
INSIDE THIS ISSUE

(2 Pages)

Message from the Director,

Dr. Shashank Chaturvedi

*"To friends of the IPR's High Performance Computing community, I'm happy to inform you all that we now have a new dedicated newsletter christened **"गणनम्"**, meaning **Computing**, for the scientific simulation activities performed on the Institute's HPC resources. It will serve as a platform for sharing the research and make the IPR HPC community stronger. Enjoy the newsletter with highlights of the exciting research."*



Can a Tail Wag a Dog : Particle Phase Controls the Macrostate in Rayleigh-Bénard System!

Pawandeep Kaur
Email: ***pawandeep.kaur@ipr.res.in***

Rayleigh-Bénard system, where a thin layer of fluid confined between two conducting plates with bottom plate maintained at relatively higher temperature is placed in an external gravity, is a well-known paradigm to study thermal convection in many experimental as well as numerical systems. When the temperature difference between the top and bottom plates is increased beyond a critical value, the system attains a quasi steady-state with the emergence of convection rolls, widely known as Rayleigh Bénard convection cells (RBCCs). Using 2D molecular dynamics (MD) simulations, we have investigated the effect of particle-level velocity perturbations on the RBCCs formed in the system taking Complex plasma as a prototype, which is composed of negatively charged micron sized dust-grains, electrons, ions and neutrals [1]. The grain medium embedded in a Complex plasma is considered to be in liquid phase, which is decided by the values of two dimensionless parameters, (i) coupling parameter, and (ii) screening parameter.

Simulation details: Using an in-house developed MPMD-v2.0 [2], on HPC ANTYA, we simulate N=7200 dust-grains in *x*–*y* plane (Γ = 50; κ = 4) under the effect of an external gravity *g* = 0.00019 and external relative temperature difference, $\Delta T/T_0 = 1$ between the top and bottom plates. The grain dynamics is modeled using Yukawa potential. Once the system attains a quasi steady-state forming RBCC, we superpose a perturbation on the x-component of particle velocities:

$$v_{x,i}^{new} = v_{x,i} + \alpha |v_{x,i}| \cos(\pi y_i / L_y + \phi)$$

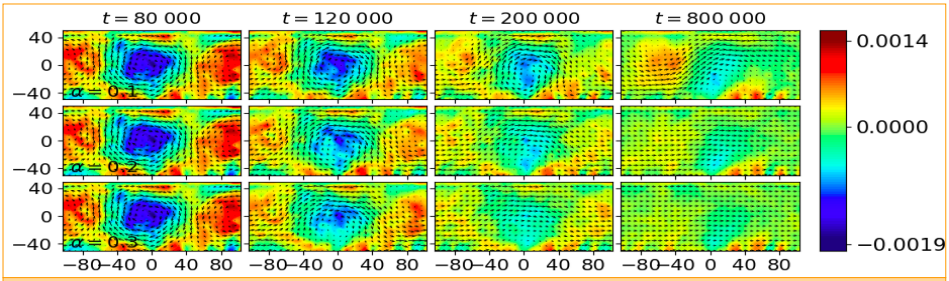


Figure 1: Time-evolution of fluid velocity and vorticity plots for various α values under an even-phase, Φ = nπ, n = 0 of particle-level velocity perturbation. Colorbar labels represent local vorticity values and black arrows represent the relative local fluid velocities. The fluid quantities plotted here are constructed by dividing the simulation domain into (30x15) grid and averaging over time, t indicated on each column.

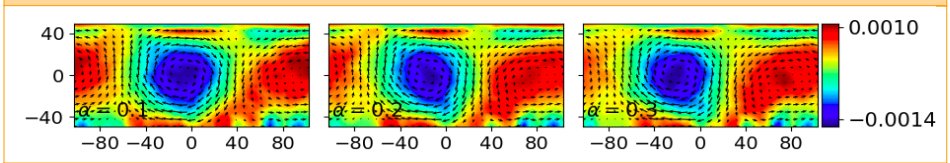


Figure 2: Fluid velocity and vorticity plots for an odd-phase, Φ = (n +1/2)π, n = 1 of particle-level velocity perturbation at t = 800,000ω^{-1}_{pd} for various α values.

where $v_{x,i}^{new}$ and $v_{x,i}$ respectively represents the velocity of particle i before and after applying perturbation, L_y is system size along y, y_i is the y-component of the instantaneous position vector of i^{th} particle, α represents the amplitude of perturbation with respect to the magnitude of particle's velocity and Φ represents the phase of perturbation. *For all perturbation amplitudes considered in this work, the perturbed energy introduced by the perturbations lie within the energy fluctuations present in the quasi-steady state.* For each set of (α,Φ), we run the simulation till t = 800,000ω^{-1}_{pd}, with time-step, dt = 0.01, where ω_{pd} is the dusty plasma frequency. A total of 30 simulation runs were performed on ANTYA, each finishing within 3 days on 10 CPU cores delivering much higher performance with simultaneous runs than one could get out of a typical desktop computer or workstation.

> ***"Particles when perturbed with certain phase can change the fate of the entire fluid"***

Our results indicate that the phase and amplitude of particle-level velocity perturbations introduced in the steady-state determines the fate of RBCCs at later times. Under even phase values of particle-level velocity perturbations Φ = nπ, RBCCs become unstable to a 1D shear flow, which at later times gives way to shearless unidirectional fluid flow (see Figure. 1). On the other hand, the odd phase values Φ = (n + 1/2)π, of particle-level velocity perturbations do not affect the RBCCs formed in the system (see Figure. 2).

References:

1. ***Pawandeep Kaur***, *Rajaraman Ganesh, Phase of particle-level velocity perturbations determine the fate of Rayleigh-Bénard convection cells in 2D Yukawa liquids, (Under Review, Oct 2020)*

2. ***H. Charan***, *Ph.D. thesis, Homi Bhabha National Institute (2017).*

Running Interactive Jobs in ANTYA

What

Interactive job sessions allow a user to connect to a compute node from a login node and work on compute node directly. Both interactive and the usual batch jobs are managed by PBS in ANTYA.

When

For running an application or software with a graphical interactive element, like Matlab, or VisIt, or something like Python for performing analysis without having to write a batch submission script.

"For running applications like MATLAB, IDL, Visit, Paraview, Python or compiling software"

Syntax

```
$ qsub -I -X -q serialq -l select=1:ncpus=4,walltime=15:00:00
```

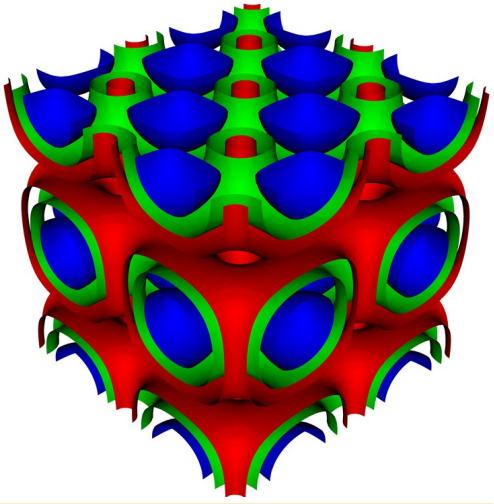
*The parameters like **serialq , no. of cores, no. of GPU cards and walltime** can be selected as per the requirement. On the compute node, user can execute any application or command similar to login node. The interactive GUI application can also be run directly after loading the required modules on compute node.*

ANTYA UPDATES AND NEWS

1. New Software Installed
   - ⇒ CUDA 10.2 module
   - ⇒ Singularity-3.5.3 module for precompiled images
   - ⇒ OpenFOAM-8.0 module
2. Profiling of a GPU code can be submitted as a batch job on gn07 node.
3. No Scheduled Downtime in the Coming Month

UDAY and UDBHAV clusters will not be available for use after 31st December 2020

HPC PICTURE OF THE MONTH
Recurring Taylor-Green (TG) Flow



Pic Credit: **Mr Shishir Biswas**
Generated using in house developed code **GMHD3D** on ANTYA with **VisIt 3.0**

Other Recent Work on HPC

Effective thermodynamic properties of inertial active micro-swimmers with alignment interaction	SOUMEN DE KARMAKAR
Driven dust vortex characteristics in plasma with external transverse and weak magnetic field	LAISHRAM M. SINGH
Non-isothermal CFD simulation of solid hydrogen flow through single-screw extruder	VISHAL GUPTA
Real Time Close Circuit Television: Artificial Intelligence Monitoring Solution	AGRAJ ABHISHEK
3D Magnetic Field Analyses of Linear Induction Motor (LIM) for Electromagnetic Launching Applications	ANANYA KUNDU

Acknowledgement

The HPC Team, Computer Division IPR, would like to thank all Contributors who helped to make this newsletter available in time. We would also like to acknowledge the support provided by IPR Library and Dr Arkaprava Bokshi during template finalization.

TO CHECK YOUR QUOTA IN ANTYA

```
$ mmlsquota --block-size auto home scratch
```

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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