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## GANANAM (गणनम्)

HIGH PERFORMANCE COMPUTING NEWSLETTER  
INSTITUTE FOR PLASMA RESEARCH, INDIA



## Characterizing the Microscopic Density Fluctuations of Yukawa Fluids in Terms of Various Transport Coefficients

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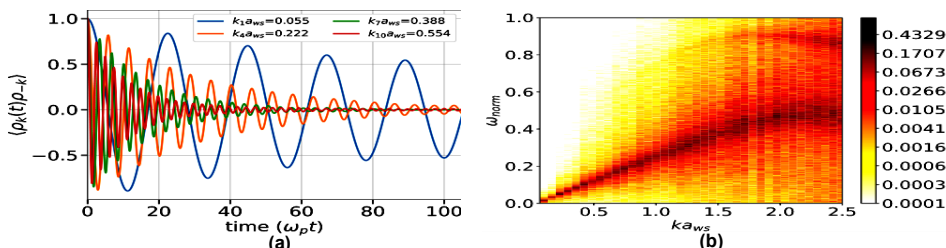


Figure 1: (a) A Density Autocorrelation Function (DAF) plot generated using MD simulation (Solid lines) and non-linear least square fitted curve in black broken lines for  $T = 80$  and  $K = 1.0$ . (b) FFT of longitudinal current fluctuation showing the acoustic mode dispersion.

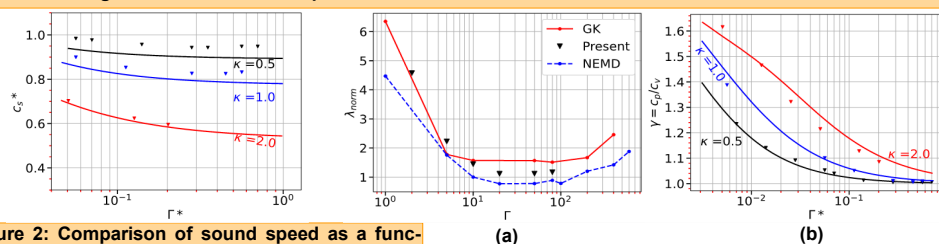


Figure 2: Comparison of sound speed as a function of Coulomb coupling parameter from present work (triangles) with ref [5] (solid lines). Following the same normalization used in [5], the sound speed is normalized as  $c_s^* = c_s / (\omega_{pd} a_{ws})$  and effective Coulomb coupling parameter as  $T^* = T/T_m$  where,  $T_m = [1 - 0.388\kappa^2 + 0.138\kappa^3 - 0.0138\kappa^4]$ .

Figure 3: (a) Comparison of estimated thermal conductivity normalised as  $\lambda_{norm} = \lambda / (nk_B \omega_p a_{ws}^2)$  with NEMD Method, GK Method and present work. (b) Comparison of variation of adiabatic constant  $\gamma$  with Coulomb Coupling Parameter from present work with reference [5].

Yukawa fluids [1] are systems of charged particles interacting with a screened Coulomb potential. These systems attract a lot of interest in research because of their importance in many fields such as astrophysical systems [2], gas discharges, microelectronics, thermonuclear fusion systems [3] and condensed matter physics. A popular way to form a Yukawa system in laboratory is suspension of micro to nano meter sized particles in a plasma system. These systems, known as Dusty Plasma or Complex plasma [1], are characterized by Coulomb Coupling parameter,  $\Gamma$  and screening parameter,  $k$ . There are many thermodynamic parameters of Yukawa fluids of which includes sound speed, adiabatic constant, thermal diffusivity and longitudinal viscosity that are examined in this study across range of coupling and screening regimes.

In this study we have used an analytical relationship of **Density Autocorrelation Function (DAF)** with various thermodynamic parameters obtained using the hydrodynamic matrix which, for a fluid, is derived from fluid momentum equation supplemented with energy and continuity equations in  $\omega$ - $k$  space. It relates the variations of microscopic density, current and temperature with their respective initial values in terms of various transport coefficients such as thermal diffusivity, viscosity and acoustic speeds [4]. Thus, an autocorrelation function can be obtained analytically from the hydrodynamic matrix in terms of these transport coefficients providing a framework to use in molecular dynamics (MD) simulations. In this framework, the particle trajectories obtained from MD simulations are used to generate DAF and best fitted through transport coefficients using nonlinear least square routines. The transport coefficients obtained from this method across the coupling regimes are compared with existing models and results.

**"A unified approach to obtain sound speed, thermal diffusivity and adiabatic constant from microscopic density fluctuations that can be applied to experiments as well as simulations was exercised. The parameters estimated were within <15% deviations with published results from different models."**

sively Parallel Simulator (LAMMPS) code on ANTYA. The typical simulation wall time for  $5 \times 10^5 \omega_p t$  time steps on 400 CPU cores was 14 hours. The velocities and positions of particles at all time steps, called trajectories, were stored and spatio-temporal Fourier transforms was performed to calculate DAF as shown in Figure 1(a). Also, longitudinal current correlation function was calculated to verify the parameters of simulation and obtain acoustic dispersion as shown in Figure 1(b). In order to compare the thermal conductivity, two separate calculations were performed using two well-established techniques namely Green-Kubo Method and a non-equilibrium MD method proposed by Müller-Plathe (MP) [6]. MP technique involves the idea of imposing a known heat flux and measure the temperature gradient of the system as a response followed by estimating thermal conductivity using Fourier's law. Figure 2 shows the comparison of sound speed with the established method. In Figure 3(a), a compilation of results obtained is plotted and the present method agrees well with NEMD method which is considered relatively accurate. Simultaneously the adiabatic constant also compared, in figure 3(b), with published result to verify the applicability of the study. **The disagreement of results in certain cases shown in figure 2 & figure 3 is because of the absence of viscoelastic terms in analytical treatment. A study with a Generalised Hydrodynamic model is currently underway to address this issue.**

**In order to Fourier transform large data files (~500 GB), a cluster scalable python script containing FFTs was developed in distributed computing framework with the help of DASK library.** This helped in speeding post processing of data by breaking the large data in blocks and parallelize the computation for FFTs. Now, the spatial Fourier transforms of the system at each time step can be processed by a single CPU core enabling linear scaling in computation. A **DASK\_jobqueue API** was used to provide interfacing with PBS job scheduler for scaling across multiple nodes and request computational resources from ANTYA. **A 40-fold reduction on a single node in computation time was achieved with the help of distributed computing.**

### References:

- André Melzer. *Physics of Dusty Plasmas*, volume 962 of *Lecture Notes in Physics*. Springer International Publishing, Cham, 2019.
- Pavel Bliokh, et al., *Dusty and Self-Gravitational Plasmas in Space*, volume 50 of *Astrophysics and Space Science Library*. Springer Netherlands, 1997.
- Vadim N Tsytovich and J Winter. On the role of dust in fusion devices. *Physics- Uspekhi*, 41(8):815–822, Aug 1998.
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- I. L. Semenov, et al., On the estimation of sound speed in two-dimensional Yukawa fluids. *Physics of Plasmas*, 22(11), 2015.
- Patrick K. Schelling et al., Comparison of atomic-level simulation methods for computing thermal conductivity. *Physical Review B - Condensed Matter and Materials Physics*, 65(14):1–12, 2002.

## Python Package Management Using Conda — Part-6 Working with GPU Dependencies in Conda Environment

Working with AI/ML/DL work that requires GPU cards to carry out the intensive work in the HPC cluster can be a very daunting task given the number of GPU dependencies (Cuda toolkit, various libraries optimized for GPUs) that need to be installed. With frequent updates in the library packages, managing the GPU dependencies with support from HPC Admin would not be an effective approach to follow. Also, the chances of having one package conflicting with others are more for GPU-dependent packages. Similar to the CPU packages, Conda allows us to manage GPU dependencies independently in userspace without the need for admin privileges. In this last part of the Conda series, we will cover what are the most common GPU packages, and how these packages can be installed with GPU compatibility.

### Which GPU libraries are available via Conda Channels?

Nvidia maintains its channel for Nvidia CUDA Toolkit versions which are also available in the default Conda channel. GPU enabled versions of CUDA Deep Neural Network library (cuDNN), NVIDIA Collective Communications Library (NCCL), PyTorch (through pytorch channel), Tensorflow, Horovod for distributed learning, etc. are available via Conda Channels.

### Why use GPUs for AI/ML/DL within Conda Environment in ANTYA?

GPUs are not mandatory but extremely efficient for such workloads because of the massive number of cores available in them that can perform multiple and simultaneous computations. With ANTYA having a total of 44 P100 GPU cards, the work can be massively sped up and scaled.

### How to implement GPU compatible Conda packages in ANTYA?

We will create an environment wherein the required packages are the GPU version of TensorFlow with other dependent packages.

# Create the project name with Conda.  
[user@login1 ~]\$ conda create --name tensorflow-gpu

# Now activate the created environment.  
[user@login1 ~]\$ conda activate tensorflow-gpu  
(tensorflow-gpu)[user@login1 ~]\$ conda list

# Since there are no packages installed, this will not list any packages. Now install the tensorflow gpu package.  
(tensorflow-gpu)[user@login1 ~]\$ conda install tensorflow-gpu

# This will take few minutes to install the tensorflow-gpu along with other dependent packages given below which are required for a GPU run.  
(tensorflow-gpu)[user@login1 ~]\$ conda list | grep -

E 'toolkit|cudnn|tensorflow-gpu|nccl'

cudatoolkit	11.5.0	h36ae40a_9	conda-forge
cudnn	8.2.1.32	h86fa8c9_0	conda-forge
nccl	2.11.4.1	hdc17891_0	conda-forge
tensorflow-gpu	2.6.0	cuda112py39h0bbbad9_2	conda-forge

## ANTYA UPDATES AND NEWS

### 1. New Packages/Applications Installed

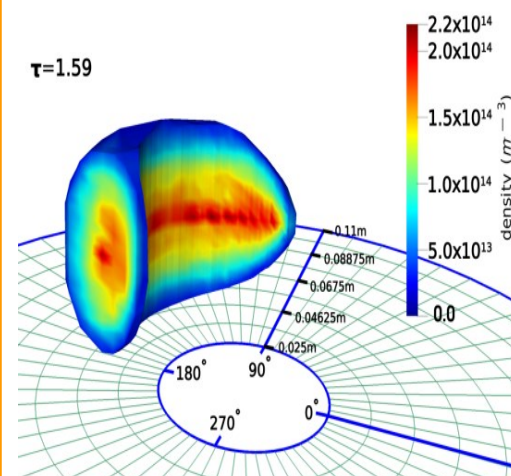
Nanoscale Molecular Dynamics  
Software available as modules  
[NAMD/2.13-CPU & NAMD/2019-GPU](#)

### 2. NVIDIA GPU Drivers Upgraded

Version 460.32.03 on all the GPU nodes which can now support upto CUDA11.2 toolkit.

## HPC PICTURE OF THE MONTH

### 3D Electron Density Profile of the Electron Cloud in Electrostatic Magnetized Incomplete Toroid (EMIT)



Pic Credit: [Swapnali Khamaru](#)

This figure shows 3D electron density profile of the electron cloud in Electrostatic Magnetized Incomplete Toroid (EMIT). Green grid is the toroidal midplane, blue borders are the toroidal and poloidal boundaries. -400 V potential is applied at the toroidal end points (0° to 90° span). The density profile is plotted on only 90° toroidal domain for illustrative purpose. [Ref: Meghraj Sengupta, Swapnali Khamaru, Rajarman Ganesh, J. Appl. Phys. 130, 133305 (2021); <https://doi.org/10.1063/5.0055828>]

This figure is generated using in-house developed particle-in-cell code PEC3PIC with simulation run on ANTYA, which took around 2 minutes to complete on 40 CPU cores for 2560640 particles.

## TIP OF THE MONTH

### To Load The Software Modules Automatically in User Environment

Put the module load command for the required modules in your .bashrc file

## Submit Conda Environment Jobs with Job Scheduler in ANTYA

A sample script has been given below with comments to show how the Conda environment job can be launched as a batch job.

```
#!/bin/bash

----- # PBS Scheduler Parameters Section -----
#PBS -N tf_test           # Name of the job which the user can give
#PBS -q serialq           # Name of the queue from the list of available queues in the cluster

#PBS -l select=1:ncpus=1:ngpus=2  # Compute resources requested for the job
                                # select = no. of chunks/nodes, ncpus = no. of cores per chunk/node,
                                # ngpus = no. of gpu cards per node

#PBS -l walltime=24:00:00  # Execution time of the job (HRS:MINS:SECS). This should not exceed the
                                # walltime limit of the selected queue.
#PBS -j oe                # Join the output and error files into a single file with name <jobname>.<jobid>
##PBS -V                  # Export user environment paths is commented.
#PBS -m bea               # Email is sent when the job starts, terminates and aborts
#PBS -M abc@ipr.res.in    # Specify the email address for getting the notifications

cd $PBS_O_WORKDIR         # PBS environment variable for current working directory

----- # Environment Modules/Paths -----
module load miniconda/3    # Load the miniconda module for getting the conda command
source /home/application/miniconda/miniconda/etc/profile.d/conda.sh  # Necessary to initialize user shell
conda activate tensorflow-gpu  # Activate the user-created conda environment

----- # Running the Job Executable -----
echo "Job starts from here"
python example.py          # The executable Python and required packages
                            # will be from the user created Conda environment
```

## Other Recent Work on HPC (Available in IPR Library)

Conceptual Design of Large Cryopumping Test Facility (LCTF)	SAMIRAN MUKHERJEE
Localized absorption of laser energy in X-mode configuration of inhomogeneous magnetized plasma	AYUSHI VASHISTHA
Cool down and testing of Nb3Sn based solenoid	ARVIND KUMAR TOMAR
On the Growth and Texturing of Ultrathin Zinc Oxide Films in Sol-gel Spin Coating	MAYA P.N.
Plasma Position measurements for SST1 discharges using function parameterization (FP) Method	SAMEER KUMAR
Large scale magnetic field generation in a 3D MHD plasma via Induction Dynamo Action: A numerical study	SHISHIR BISWAS
Ratchet Dynamics of Active Yukawa Particles	ANSHIKA CHUGH
Towards a 3D Quiescent Nonneutral Plasma State in Small Aspect Ratio Torus - A Particle-In-Cell Simulation Study	SWAPNALI KHAMARU
Strong magnetic field effects in the strongly coupled rotating dusty plasma	PRINCE KUMAR
Rotational Kelvin-Helmholtz instability and anomalous transport in a 2D strongly coupled Yukawa liquid	SURUJ JYOTI KALITA

## Acknowledgement

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

## ANTYA HPC USERS' STATISTICS— NOVEMBER

♦ Total Successful Jobs — **5936**

♦ Top Users (Cumulative Resources):

- ⇒ CPU Cores — **Suruj Kalita**
- ⇒ GPU Cards — **Shishir Biswas**
- ⇒ Walltime — **Anjan Paul**
- ⇒ Jobs — **Mywish Anand**

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

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