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HIGH PERFORMANCE *COMPUTING* NEWSLETTER

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Wettability Gradient Driven Automatic Movement of Liquid Droplet on a Surface

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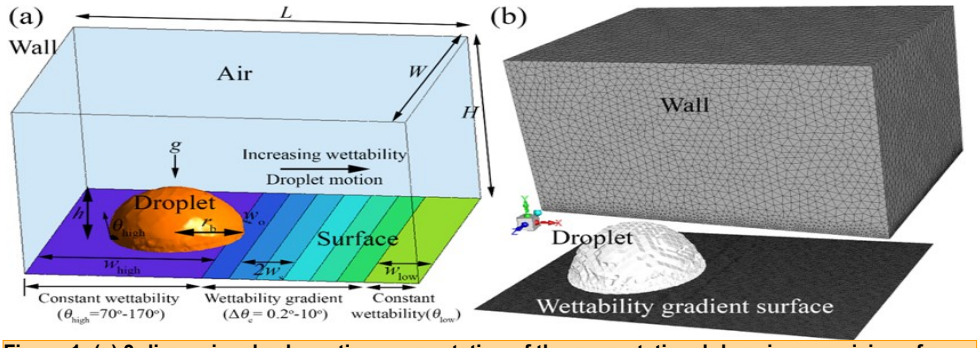


Figure 1: (a) 3-dimensional schematic representation of the computational domain comprising of a water droplet on a horizontal wettability graded surface in presence of atmospheric air. (b) Exploded view of the meshed computational domain, comprising triangular elements on the surface and tetrahedrons in the volume.

The controlled directional motion of a liquid droplet is an important phenomenon and has a lot of applicability in microfluidics/ biofluidic, self-cleaning, anti-icing, water harvesting, etc. In the recent era, wettability gradient surfaces (WGS) are employed for controlling the automatic/ self-sustained motion of liquid droplets from one point to another on these specially designed surfaces. Droplet moves on WGS from the low wettability side towards a highly wetted region of these surfaces. In 1978, Greenspan [1] was the first to propose the concept of wettability gradient. Later, Brochard [2] presented an analytical study for droplet motion on graded surfaces. Since then, several experimental and numerical studies have been performed to investigate the drop dynamics of WGS. WGS enables droplet motion purely due to the presence of a wettability gradient across the surface, hence it also promotes automatic droplet motion where gravity-driven droplet motion is completely non-functional.

The present study will estimate the drop dynamics of single water droplet shape evolution on WGS under gravity and microgravity environments. The numerical simulations play a crucial role in understanding the intricacies of spatial-temporal shape evolution of small and large volume droplets in various gravity and microgravity engineering processes incorporating droplet motion, splitting, spreading, merging, coalescence, bouncing, etc. on WGS. Herein, transient, laminar, 3-dimensional Continuity and Navier-Stokes equations are solved for the computational domain consisting of a liquid water droplet on a wettability gradient surface in presence of atmospheric air as shown in figure 1. Finite Volume Method based Computational Fluid Dynamics software *ANSYS FLUENT® (ANSYS-v221 licensed version installed on ANTYA)* is used for numerically simulating the directional motion of water droplets on linear wettability gradient surface and the Volume of Fluid method is adopted for interface tracking at the Three-Phase Contact Line of the droplet. The simulations were performed for the computational domain with a 5 ×10^5 grid size. The simulations were performed on ANTYA HPC with 32 cores for a single run. The simulation run time of 40 ms took 3 hours of real-time on ANTYA. ANTYA helped in completing all the simulations very fast and efficiently, which would otherwise have taken 2 days of real-time on a 16 GB desktop to complete 40 ms of simulation run time.

"The obtained results of the simulation study predict the drop dynamics and shape evolution on WGS using the Volume of Fluid method which can be useful in designing and optimizing WGS for many different applications"

The presented simulation study demonstrates shape evolution of droplets moving on WGS is attributed to caterpillar alike inching motion in both gravity and microgravity conditions as shown in figure 2. The droplet is almost stagnant on the surface with an initial superhydrophobic angle (θ_{high} > 150°) with a low gradient ($\Delta\theta_e$ = 0.2° and 1°). However, despite higher spreading droplet accelerates on hydrophobic surfaces (θ_{high} = 100°) with a higher gradient ($\Delta\theta_e$ = 10°).

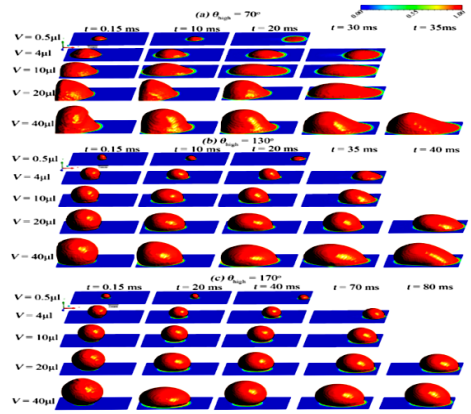


Figure 2: Spatial-temporal water volume fraction contours of a water droplet in the presence of gravity on wettability graded surface ($\Delta\theta_e$) = 10°.

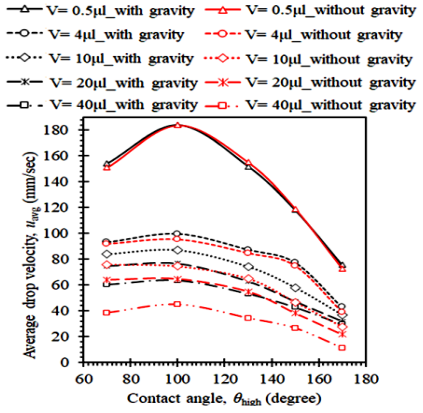


Figure 3: Average droplet velocity (u_{avg}) as a function of low wettability region initial contact angle (θ_{high}) at various values of droplet volume.

The effect of gravity is negligible for smaller droplets. However, substantially affects large droplets due to the increased value of the Bond number as shown in figure 3. The obtained results are helpful for designing and optimizing wettability-graded surfaces that endure droplet splitting and coalescence in various microgravity engineering systems. In addition, the WGS is also advantageous for heat transfer augmentation. The detailed results of the present research are available in the published work [3].

References:

1. *H. P. Greenspan, "On the motion of a small viscous droplet that wets a surface," Journal of Fluid Mechanics, 125 (**1978**).*
2. *F. Brochard, "Motions of Droplets on Solid Surfaces Induced by Chemical or Thermal Gradients," Langmuir, 432 (**1989**).*
3. *V. Baghel and M. Ranjan, "Numerical Estimation of Droplet Motion on Linear Wettability Gradient Surface in Microgravity Environment, " Materials Today Communications, 103916 (**2022**).*

Storage Space Allocation and Sharing of Data in ANTYA

ANTYA has GPFS (General Parallel File System) high-performance cluster file system and is sized at around ***2 Petabytes (PB)***. This storage space is divided into two partitions of ***300 TB "HOME"*** and **1700 TB *"SCRATCH"***. Both these partitions are available to all the users with a default quota. This article covers some of the ***FAQs*** related to storage space on ANTYA.

What is the Default User Storage?

The default quota for each user in the home directory is ***200 GB*** and in the scratch directory, it is ***10 TB***. The scratch directory space is equally divided into two scratch partitions, ***scratch_run***, and ***scratch_data***.

How can User Check Quota and Available Free Space?

 # The command to check your current storage and quota limits. The blocks column represent the storage space being used by the user out of the total allocated space provided in limit column.

```
[user@login1 ~]$ mmlsquota --block-size auto home scratch
                         Block Limits
Filesystem Fileset     type         blocks      quota      limit   in_doubt    grace
home       root        USR          110.4G       195G       200G          0     none
scratch    root        USR        no limits
scratch    scratch_run USR          762.8G     4.951T         5T          0     none
scratch    scratch_data USR          340.4G     4.951T         5T          0     none
```

How does a User Request for a Quota Increase?

The scratch quota can be increased upto ***25 TB*** if the default quota has been used, by simply sending an email to HPC Team at *hpcteam@ipr.res.in*. For increasing quota beyond *25 TB*, a storage extension form available at *https://cc.ipr.res.in/ccfiles/HPC_storage_request_form.pdf* has to be filled and submitted. The home quota can be increased only in cases of justified requests.

Is there any Backup of User Data?

User data in the home directory is backed up in a *monthly cycle* usually at the start of the month. However, any data that the Users consider irreplaceable like source codes should also be saved to their local storage to avoid loss of data in case of any catastrophic event in the storage system. There is no backup provided for the user scratch directory.

Is there any Purging of User Data in the Scratch Directory?

There is no purging of user data in the scratch directory.

Is User Data Accessible by Other Users?

By default, one user's data is not accessible by any other users on ANTYA. However, a user may give permission to allow other users for accessing the data.

How can User Give Permission to Other Users for Accessing the Data?

HPC users collaborating on a project can share their working directories with selective users on ANTYA using ***"setfacl"***. The *setfacl* utility sets Access Control Lists (ACLs) of files and directories. For detailed procedures and how to use *setfacl,* please refer to *page#2 of issue2* of GANANAM. , Consider carefully whether it's really necessary before sharing write permissions on data, often just read permissions are enough.

How can User Transfer Data?

Windows: For Windows machine users, open source third-party tools like WinSCP, FileZilla, MobaXterm, etc. can be used for transferring data to/from ANTYA.

Linux/Mac: These users can use command line tools like scp, rsync for transferring data to/from ANTYA.

 # To copy files from local computer to ANTYA

```
[user@local~]$ scp local_file username@antya.ipr.res.in:/home/username/
```

 # To copy files from ANTYA to local computer

```
[user@local~]$ scp username@antya.ipr.res.in:/home/username/cluster_file .
```

Note: *There are 1024 bytes in a KB, 1024 KBs in an MB, 1024 MBs in a GB, 1024 GBs in a TB, and 1024 TB in a PB.*

ANTYA UPDATES AND NEWS

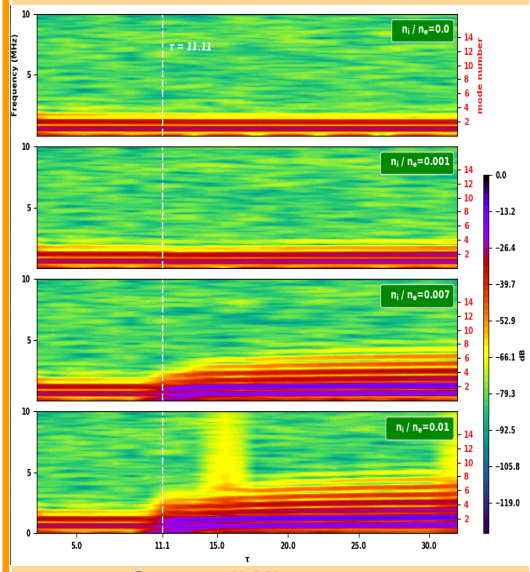
1. New Packages/Applications Installed

⇒ **The no. of Applications stays the same for this issue.**

⇒ **ANTYA Users /home data monthly backed up cycle completed.**

HPC PICTURE OF THE MONTH

Spectrogram of the Wall Probe Current: Ion-driven Destabilization of a Toroidal Electron Plasma



Pic Credit: **Swapnali Khamaru**

The figure shows the Spectrogram analysis of the wall probe data obtained from toroidal electron cloud dynamics in an axisymmetric toroidal device, in the presence of small ion density in the device. For higher ion density values (n_i/n_e>0.005), the spectrogram shows the presence of higher mode numbers in the system. The white dotted line represents the time at which ions were introduced into the system.

The data has been obtained from the in-house developed 3D3V OpenMP parallelized particle-in-cell code, **PEC3PIC**. Each simulation ran on 10 cores and a total walltime of 800 hours was used for obtaining the data.

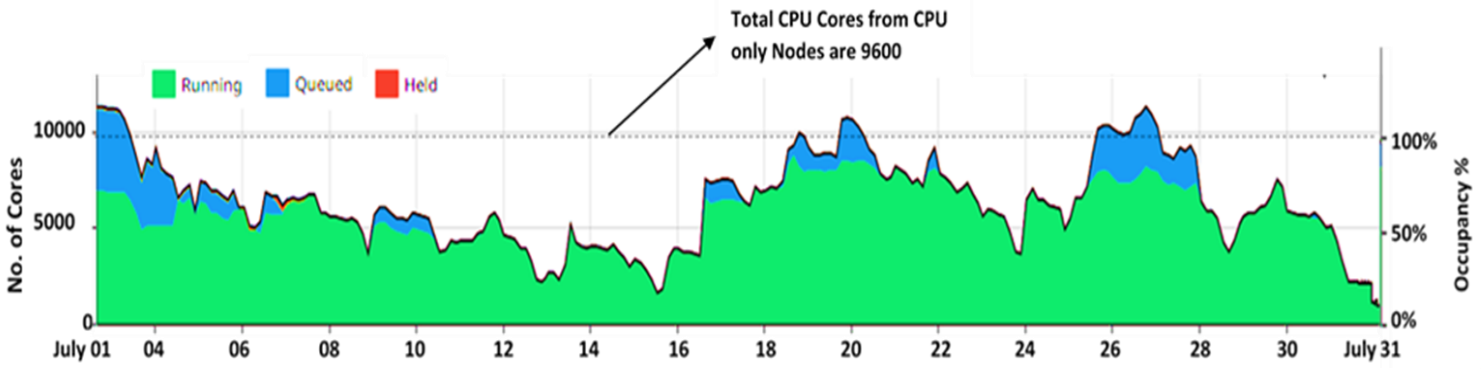
TIP OF THE MONTH

Using passwords with special characters in the export proxy commands:

```
@ can be replaced with %40
$ can be replaced with %24
# can be replaced with %23
: can be replaced with %3A
```

ANTYA Utilization: JULY 2022

ANTYA Daily Observed Workload



Other Recent Work on HPC (Available in IPR Library)

Effect of DBD Plasma treatment on surface modification of aramid fibers: XPS Study	SADAF JETHVA
First MHD experiment at IPR in LLMHD loop	ANITA PATEL
Numerical study of DBD plasma based Inline textile treatment system	JYOTI AGARWAL
Electromagnetic & Structural Analysis of in-vessel Coils of SST-1	ALLI AMARDAS
Short pulse laser-cluster interaction in ambient magnetic fields	MRITYUNJAY KUNDU
Large Scale Molecular Dynamics Study on Phase Dynamics of mixture of active and passive finite mass Yukawa particles	ANSHIKA CHUGH
Implementation of 3D Monte-Carlo simulations in the inboard limited Aditya-U scrape-off layer Plasma	ARZOO MALWAL
Kinetic plasma modelling, GPU parallelization and application to physics problem	ANJAN PAUL
Simulation of nonlinear whistler wave in plasma	GAYATRI BARSAGADE
Development and Validation of Room Temperature Bore Cryostat for HTS Solenoid Magnet Testing	MAHESH GHATE
Scaling of magnetic reconnection parameters with and without in-plane shear flow in the magnetic island coalescence problem	JAGANNATH MAHAPATRA
Hydrodynamic matrix for Yukawa Fluids in the Generalized Hydrodynamics Framework	ANKIT DHAKA
Role of ion beam parameters in formation of faceted ridges on soda-lime glass for wettability tuning	SUKRITI HANS
Ion-driven destabilization of a toroidal electron cloud - A 3D3VPIC Simulation	SWAPNALI KHAMARU
Bifurcation behaviour of RMP control of ELMs in tokamaks: nonlinear simulation results	CHANDRA DEBASIS
Induction dynamo using Yoshida-Morrison flow: Generation of large scale magnetic energy	SHISHIR BISWAS
Quasi-localized charge approximation (QLCA) approach for the nonlinear structures in strongly coupled Yukawa systems	PRINCE KUMAR
Fate of Convection Cells in 2D Yukawa Liquids via Molecular Dynamics Simulations	PAWANDEEP KAUR
Dynamics of shear flows in magnetic island coalescence problem using Hall-MHD model	JAGANNATH MAHAPATRA
Role of in-plane and out-of-plane shear flow on island coalescence problem	JAGANNATH MAHAPATRA
Propagation large amplitude oblique whistler wave in plasma	GAYATRI BARSAGADE
Understanding subcritical turbulence in 3D Yukawa liquids using large scale Molecular Dynamics simulations	SURUJ KALITA

ANTYA HPC USERS' STATISTICS–

JULY 2022

- Total Successful Jobs — **3703**
- **Top Users** (Cumulative Resources):

• CPU Cores	Amit Singh
• GPU Cards	Suruj Kalita
• Walltime	Gayathri
• Jobs	Soumen Dekarmakar

Acknowledgement

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

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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