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ontrolled thermonuclear fusion from magnetically confined plasmas could be a viable source of clean and unlimited energy, resolving most of the world's energy-related issues. In this quest, tokamaks and stellarators are the leading contenders to achieve thermonuclear fusion from toroidal burning plasmas. The stellarators are gaining interest due to the absence of toroidal current, which leads to the avoidance of disruptions and lower MHD activities [1]. However, these benefits come at the cost of increased neoclassical transport. Several techniques have been reported for stellarator optimization by reducing the neoclassical transport to an advanced stellarator. Even after the reduction of neoclassical transport, microturbulent transport in stellarators remains a major cause of heat and particle flux loss. Furthermore, the universal aspects of drift-wave turbulence are microturbulence and self-generated zonal flows [2]. Hence, the microturbulent transport and its interaction with the self-generated zonal flow must be adequately understood. We used the gyrokinetic toroidal code (GTC) [3] to perform electrostatic self-consistent global gyrokinetic simulations of the ion temperature gradient (ITG) and trapped elec-

tron mode (TEM) driven microturbulence in the large helical device (LHD) stellarator. GTC is a global nonlinear gyrokinetic particle-in-cell code used to study the physics

"GTC simulations of microturbulence in the LHD stellarator show that, in contrast to the TEM turbulence, the ITG turbulent transport is regulated by the zonal flow."

associated with Alfvén waves, energetic particles, microturbulence, and radio frequency waves in the fusion plasma.

In this work, one-tenth of the LHD torus is simulated due to the field symmetry of the stellarator, as shown by the 'eye' in Figure 1. GTC simulations have been carried out to study the ITG turbulence and the zonal flow dynamics with the adiabatic electron model and the fluid-kinetic hybrid model, well benchmarked in GTC [4]. ITG turbulence simulations have been carried out with adiabatic electrons as well as with kinetic electrons. Figure 2

<u>(NSIDE THIS ISSUE</u>) GANANAM (गणनम्)

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

Global Gyrokinetic Simulations of Electrostatic Microturbulent Transport Using Kinetic Electrons in LHD Stellarator

Tajinder Singh (PhD Student, Department of Physics, IISc Bangalore) BRNS Project (Sanctioned No. 39/14/05/2018-BRNS) Email: stajinder@iisc.ac.in



Figure 1: The 3D real space contour plot Figure 2: The contour plots of the electrostatic potential on the of magnetic field amplitude on the flux poloidal plane in the linear phase of (a) ITG turbulence and (b) TEM surface with Ψ =0.36 Ψ_{w} . turbulence.



Figure 3: The comparison of the time history of the Figure 4: Time history of the ion diffusivity averaged ion heat conductivity averaged over $\Psi \in [0.19, 0.38] \Psi_w$ over $\Psi \in [0.19, 0.38] \Psi_w$ (red) and non-zonal electrostatic in the gyro-Bohm units for adiabatic and kinetic elec- perturbed potential (blue) with zonal flow (solid) and trons, with and without zonal flow.

shows the contour plots of the electrostatic potential corresponding to the ITG and TEM turbulence on the poloidal plane. For both cases, the linear eigenmode structure lies on the outer midplane side, where the curvature is bad. As shown in Figure 3, the kinetic electrons increase the linear growth rate of the ITG turbulence by ~1.5 times and the turbulent transport by ~2.5 times compared to the case with adiabatic electrons. The zonal flow plays a vital role in regulating ITG turbulent transport. However, in contrast to ITG turbulence, the zonal flow is found not to play an

essential role in TEM turbulence saturation (see Figure 4). However, the inverse cascade of the higher poloidal and toroidal

modes to the lower one acts as a dominant saturation mechanism for TEM turbulence.

The simulations discussed here have extensively used the computational resources of the ANTYA cluster at IPR to simulate the microturbulent transport in LHD. A typical GTC microturbulence simulation has used ~1000 cores for almost two days of real-time with ~250 GB of hard disk space. GTC simulations make use of the hybrid programming architecture (OpenMP + MPI) along with libraries such as NetCDF (for data writing) and PETSc (to solve the matrix

without zonal flow (dashed) and zonal electric field (black). The diffusivity is normalized by the gyro-Bohm diffusivity and the electrostatic potential is normalized by Te/e, the radial electric field resulting from the turbulence is normalized with $\sqrt{T_e/e}$

equations) installed on the ANTYA cluster.

The presented simulation study discusses the dynamics of electrostatic microturbulence and its interaction with the self-generated zonal flow. The zonal flow plays a crucial role in regulating ITG turbulent transport, whereas it has an almost negligible effect on TEM turbulence. This study also shows that global effects are essential in linking turbulent transport in LHD. The knowledge gained from these microturbulence simulations could be helpful on the path to an optimized advanced stellarator to harness the power of nuclear fusion. The detailed results of the present work are available in the published work [5]. This work is supported by the Board of Research in Nuclear Sciences (Sanctioned No. 39/14/05/2018-BRNS) project between the Indian Institute of Science, Bangalore, and the Institute for Plasma Research, Gandhinagar.

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Containerization in HPC Through Singularity on ANTYA

This article focuses only on the containerization of applications in HPC using singularity and does not cover different containerization approaches and how it is better than virtualization. It is well known that running user codes in an HPC environment requires a lot of effort because of compiler/library dependencies. To provide users with mobility of computing (porting) across the systems to run their scientific codes, containerization can help. Singularity is an open-source container software that allows packing an application with its dependencies into a single image file. Singularity has been designed for HPC where the user does not has the root privilege and can still use the container images.

What is Containerization?

It is the process to create containers (image files) that store everything to run scientific applications across HPC clusters. Containerization helps in hiding the complexity of scientific applications and makes their deployment easier.

When to use Containers?

There are cases where the dependencies of an application are either too complex to install or not compatible with the host operating system (OS). In such cases, creating singularity containers can help by building a container with a compatible OS and then running the container image file on HPC.

"Running commercial applications binaries that have specific OS requirements not met by host system." "Containers can be used for both CPU and GPU applications and also support MPI run across the compute nodes."

"For many applications, the container

images are available and can be directly downloaded from the internet (Singularity

hub: https://singularity-hub.org, NVIDIA

GPU Cloud: https://ngc.nvidia.com)"

"For inhouse developed applications, the

HPC Team may help the users create one to

improve portability across HPC clusters."

HOW to Implement in ANTYA?

ANTYA has singularity modules (singularity/3.4.1 and singularity/3.5.3) available for HPC Users to run the container image files built with singularity software only. The container images cannot be built on ANTYA by the users. The user can get the container images of the required applications using any of the following methods:

"The container images built by HPC Team are available at the shared directory on ANTYA (built with singularity/3.4.1\): /home/application/singularity_images/ singularity_3.4.1/"

"For creating application containers which are not available, the users may request the HPC Team or create one themselves."

Singularity Modules

[user@login1 ~]\$ module avail singularity singularity/3.4.1/3.4.1 singularity/3.5.3/3.5.3

Available container images on ANTYA

[user@login1 ~]\$ ls /home/application/singularity_images/ singularity_3.4.1/ cfd1.simg climate1.simg mayavi.simg nvhpc_21.2_devel.sif nways_C_F.simg nways_python_numba.simg ovito1.simg paraview57.simg scilab.simg

Singularity Workflow?

Build the singularity container image on your local Linux system (PC/ Laptop).

Once the image is built or available from internet, transfer it to ANTYA. Run the singularity container image using the batch script.

ANTYA UPDATES AND NEWS

1. New Packages/Applications Installed

- ⇒ Julia package available as module
- module load julia/julia-1.8.2
- ⇒ NAG library version upgraded

module load NAG/nag-intellibrary_28

⇒ User home directories backed up

HPC PICTURE OF THE MONTH

Generation of Magnetic Flux Ribbon for a Fast Dynamo Model



Pic Credit: Shishir Biswas

The figure shows ribbon like magnetic field iso-surface structure for a fast dynamo problem, in a three dimensional magnetohydrodynamic plasma. It is generated using an Inhouse developed multi-node multi-card weakly compressible magnetohydrodynamic GPU based solver GMHD3D.

[Ref: manuscript under review]

This figure is generated in Vislt with data generated from **GMHD3D** on *ANTYA*. The simulation took 63.526 hours on 4xP100 GPU cards from two GPU nodes for 256x256x256 grid resolution problem.

TIP OF THE MONTH

Pinning the processes and threads of MPI codes to cores/sockets: This is particularly helpful for memory bound applications and can result in improved performance. ANTYA compute nodes have 2 sockets with 20 cores each.

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ANTYA Utilization: OCTOBER 2022



ANTYA HPC USERS' STATISTICS-OCTOBER 2022

- Total Successful Jobs 2539
- ◆**Top Users** (Cumulative Resources):
- CPU Cores Suruj Kalita
- GPU Cards Suruj Kalita
 - Walltime Anshika Chugh

Someswar Dutta

Jobs

Other Recent Work on HPC (Available in IPR Library)

Systematic analysis of whistler wave from fluid to kinetic limit with phase space dynamics	Anjan Kumar Paul
Role of noise on directed motion of active particles on Ratchet	Anshika Chugh
Non-reciprocal reorientation mechanism exhibits flocking	Soumen De Karmakar
Excitation of electrostatics oscillations and their modification by nonlinear whistlers	Gayatri Bhayyaji Barsagade
Nonlinear propagation of quasi-longitudinal whistler wave in plasma	Gayatri Bhayyaji Barsagade
Experience in Developing LN2 Cooled Sorption Cryopump, Application and Technology Transfer	Samiran Mukherjee
Role of Neutral Gas Flows in Double Layer Formation and Thrust Generation in an Expanding Magnetic Field Plasma	Vinod Saini
Effect of flow shear on the onset of dynamo	Shishir Biswas
Active Complex Plasma: A new paradigm of research	Soumen De Karmakar
Compressible Effects On Force-free 2d Magnetic Flux Tubes	Jagannath Mahapatra
Hydrodynamic Stability of Convective Cells in 2D Complex Plasmas	Pawandeep Kaur
Collective excitations of strongly coupled systems under the Quasi-localized charge approximation (QLCA) framework	Prince Kumar
Universal Drift Modes In A Magnetized Plasma - A Study Using Gyrokinetic Particle-In-Cell Methods	Sagar Choudhary
Simulation of Toroidal B-field for tight aspect ratio torus: SMARTEX-C	Alli Amardas
Transient Lorentz Force Calculations on In-vessel Coils in SST-1 Operation	Alli Amardas
Finite Element Simulation of Plasma Production in a cusp field linear device	Alli Amardas
Development of an Alignment System for ITER-CXRS-Pedestal Diagnostics	Abha Maheshwari
Layer formation in stratified 3D Yukawa liquids	Suruj Jyoti Kalita
Emission of Terahertz Radiation by Oblique Incidence of Laser on Inhomogeneous Plasma	Anjana K. P.
Experiments on crystal dynamics in strongly coupled complex plasmas	Pintu Bandyopadhyay
3D Plasma transport equilibrium study in the inboard limited Aditya-Upgrade Scrape-off layer	Arzoo Malwal
Development of -5kV, 1A High Voltage DC Power Supply for Magnetron to develop ECR Plasma	Kiritkumar Maganbhai Parmar
Characterizations of Spontaneous Fluctuations in Strongly Coupled Dusty Plasmas	Ankit Dhaka
Comparison of time series forecasting of future sequence of signals using deep learning models at Aditya/Aditya-U data	Rameshkumar Babubhai Joshi
Directed motion in a 2D system of Yukawa particles on 1D Ratchet	Anshika Chugh
Parameter Choices and Constraints for Indian DEMO	Shishir P. Deshpande
Kelvin-Helmholtz instability in a compressible dust fluid flow	Krishan Kumar
Role of Section Modulus in Conceptualizing and Designing the Support Structure for Linear Induction Motor	Ritesh Kumar Srivastava
Design & analysis of hydrogen gas pre-cooler for fuel pellet injections system of tokamak	Pratikkumar A. Nayak
Thermal Performance Of Gate Valve Assembly With Cooling Provision For Safe Handling Of BioMedicalWaste Packets In Plasma Pyrolysis System	Atikkumar N. Mistry
A Collimated Electron Beam From The Laser-Driven Deuterium Cluster In Ambient Magnetic Field	Kalyani Swain
Ion Beam Induced Wettability Gradient Surface for Automated Droplet Motion	Vishakha Baghel
Experimental Demonstration of Structural Phase Transition in 2-D Complex Plasma Crystals	Swarnima Singh
Square Lattice Domains in 2D Plasma Crystal	Swarnima Singh
3D Computational Fluid Dynamics Simulation of Heat Transfer for PINI Ion Source Back Plate	Tejendrakumar Patel

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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 GAŅANAM, please write to us. Contact us HPC Team Computer Division, IPR Email: *hpcteam@ipr.res.in*

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